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COST 507

Definition of thermochemical and thermophysical properties to provide a database for the development of new light alloys

Thermochemical database for light metal alloys

Volume 2

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Edited by
I. Ansara, A. T. Dinsdale, M. H. Rand

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COST 507
COORDINATION GROUP C

Final Report Round 2
July 1998

Partners in Coordination Group C, whose results are presented in the pages of this report, are:

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Istituto di Chimica Generale, Università di Genova, Genova, Italy

Senter for Industriforskning, Blindern, Oslo, Norway

Division of Physical Metallurgy, Royal Institute of Technology, Stockholm, Sweden

Laboratory of Materials Processing and Powder Metallurgy, Helsinki University of Technology, Espoo, Finland

Centre for Materials Measurement and Technology, National Physical Laboratory, Teddington, U.K.

Institut für Physikalische Chemie, Universität Wien, Austria

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INTRODUCTION

The COST-Action 507 has the official title:

Measurement and Evaluation of Thermochemical and Thermophysical Properties to Provide a Database for the Development of New Light Alloys

There are 14 signatory countries to the Action, which had an official commencement date on January 1, 1990.

The countries concerned are:

Austria
Belgium
France
Finland
Germany
Greece
Italy
Netherlands
Norway
Portugal
Spain
Sweden
Switzerland
United Kingdom

In addition, the Baikov Institute of Metallurgy, Moscow (Russia) is taking part in the Action.

The work of COST 507 is shared amongst partners in 4 Coordination Groups whose areas of interest are:

Coordination Group A	:	Experimental measurement of thermochemical properties
Coordination Group B	:	Critical compilation and assessment of constitutional data prior to thermodynamic calculation
Coordination Group D	:	Experimental measurement and compilation of thermophysical data

Coordination Group C, whose work is presented in this report, is concerned with the general theme:

Critical thermodynamic evaluation of relevant binary, ternary and higher-order alloy systems to produce a set of optimized coefficients for the light metal alloy database.

The evaluations of Group C incorporate experimental data from Group A and Group D partners, and use the critically compiled constitution data from Group B as basis for the evaluation work.

Using this computer database, which is now in an impressive state of development, it will be possible to calculate the phase equilibria to be expected in complex light alloy systems as a function of a wide range of compositions and temperatures. For example calculation can be made of liquidus and solidus temperatures, crystallization paths for equilibrium and non-equilibrium conditions, nature and amounts of precipitated phases, enthalpy effects associated with phase transformations, etc.

The rapid accessibility of such information will considerably assist the design, manufacture and utilization of a wide range of different alloy types.

The alloy systems towards which the experimental and evaluation work is being directed, together with some major applications, are listed below:

Al-Mg-Mn-Fe-Si : cans

Al-Mg-Si-Cu (-Fe) : extrusions, automobiles

Al-Zn-Cu-Mg (-Zr,Cr,rare earth metals) : aerospace, transport

Al-Li-Cu-Mg-Zr (-H) : airframes

Ti-Al-Mo-Zr (Cu,B,C,N,O,Si) : gas turbines

Ti-Al (-V,Cr,Mn,Ni,Fe,Nb), (B,C,N,O,Si) : gas turbines

EVALUATION PROCEDURE

Bearing in mind the alloy categories defined by industrial partners at the beginning of the Action, a matrix was drawn up to define the binary systems forming the building blocks for the evaluation of higher-order systems. These binaries were then allocated to the different partners in Group C for evaluation.

All partners made use of the selected data for the elements published by A.T. Dinsdale [1] on behalf of SGTE.

There was also agreement amongst partners with respect to the modelling of particular phases so that consistency could be maintained on proceeding from binary to higher-order systems combining evaluations originating from different laboratories. All results were prepared in exactly the same format to facilitate exchange of data and to provide a standard format for computer storage of the data by the database manager, Dr.Ansara, in Grenoble.

Evaluations to produce optimized sets of coefficients were carried out using one or

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[1] A.T. Dinsdale, Calphad, 15, 4, 317-425 (1991).

both of the two programs *Bingss/Tergss* written by Lukas [2] and *Parrot* developped by Jansson [3] contained in the *Thermo-Calc* databank system [4].

These programs make use of experimental thermodynamic and phase diagram data, which are fed in as measured values with error limits. Using defined models for the different phases of the systems concerned, optimized coefficients are produced which permit a self-consistent description of the thermodynamic properties and the phase boundaries of the alloys.

For some alloy systems the available experimental information is very scarce or unreliable. In such cases, only a part of the system may have been dealt with. In other cases, recourse may have had to be made to estimation procedures to obtain input data for the optimization process. The accuracy of the calculations involving these data will consequently be reduced.

The following pages present in summarized form a complete description of the evaluation work carried out by the partners in Coordination Group C during the course of Round 1 and 2 of COST 507. The brief reports for each system contain a calculated phase diagram, information on the structures of the phases in the system. The thermodynamic coefficients used to produce the calculated information are also given.

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[2] H.L. Lukas, J. Weiss, and E.-Th. Henig, Calphad, 6, 229-251 (1982)

[3] B. Jansson, Ph. D. Thesis, (1984), Div. Phys. Met., Royal Inst. Tech., Stockholm, Sweden.

[4] B. Sundman, B. Jansson, and J.-O. Andersson, Calphad, 2, 9, 153-190 (1985).

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I. Ansara and N. Dupin

Introduction

Standard CALPHAD procedures were used to assess the binary and ternary systems defined in the COST507 project. In Round 1, binary systems have been assessed. Several ternary systems have been analysed during Round 2.

In many ternary systems, the three pure elements exhibit different stable crystal structure. Hence data for metastable binary solutions have been obtained and are presented in the tables.

In these systems, there are also many binary phases stable on one binary edge which extend into the ternary system but not all the way across to the other binary edges. (for example, the Laves-$C15$ in the Cu-Mg-Zn system or the AlM-$D0_{19}$ in the Al-Ti-X (X=Mo, Nb, Ti, W) systems). Thus to model the intrusion of these phases into the ternary systems, the Gibbs energies of the metastable counterparts of the intruding phase must be defined in the other binary system(s). This means that when the data of these binary systems are retrieved, there will be data for these metastable "counterparts".

As the number of ternary systems increases, the number of metastable solution phases or counterphases will increase sharply and this may lead to increasing computing time and possible problems due to metastable equilibria which may appear during the calculation.

The main characteristics of each system are given in individual chapters which include:

- a summary of the various stable and metastable phases defined in the system, the thermodynamic model used to decribe their thermodynamic properties, the name of the assessor and the reference of the publication in which the evaluation is described,
- the thermodynamic properties of the compound and solution phases,
- for the binary systems: the phase diagram,
- for the binary systems: a table giving the invariant reactions,
- a table presenting the crystal structure for each phase in a given system, the structural type, the Pearson Symbol and space group as well as the occupation of the sublattices and comments when necessary. This information is taken from Massalski *et al.* [90Mas] and Villars *et al.* [91Vil].

In Appendix I, the thermodynamic functions for the elements in stable or metastable states are listed as a function of temperature. For magnetic ordering the functions are given in Appendix II.

Thermodynamic Description

Elements

The Gibbs energy of the pure element i, ${}^{\circ}G_i^{\phi}(T)$, referred to the enthalpy for its stable state ϕ at 298.15 K, ${}^{\circ}H_i^{\phi}(298.15\mathrm{K})$, is denoted by GHSER$_i$. This quantity is described as a function of temperature by the following equation:

$$\begin{aligned}\mathrm{GHSER}_i &= {}^{\circ}G_i^{\phi}(T) - {}^{\circ}H_i^{\phi}(298.15\ \mathrm{K}) \\ &= a + b\,T + c\,T\cdot\ln T + d\,T^2 + e\,T^3 + f\,T^{-1} + g\,T^7 + h\,T^{-9} \quad (1)\end{aligned}$$

The first and second derivatives of this quantity with respect to temperature are related to the absolute entropy and heat capacity of the compound at the same temperature. Experimental values for heat capacities can thus be directly used in the optimisation and will be related to the coefficients c, d, e, f, g and h.

For elements which display a magnetic ordering (Cr, Fe, Ni and Mn),the term GHSER will be referred to a para-magnetic state. The magnetic contribution is treated explicity. An additional term is thus added to the molar Gibbs energy of the magnetic phase.

For elements as well as for solutions, this term is equal to:

$$G^{\mathrm{mag}} = RT\ln(\beta+1)f(\tau) \quad (2)$$

where τ is T/T^* , T^* being the critical temperature for magnetic ordering (Curie temperature T_c for ferromagnetic materials or the Néel temperature T_N for antiferromagnetic materials), and β the average magnetic moment per atom of the alloy expressed in Bohr magnetons.

The function $f(\tau)$ is given as:

$$\tau < 1 \ : \ f(\tau) = 1 - [79\tau^{-1}/140p + (474/497)(1/p - 1)(\tau^3/6 + \tau^9/135 + \tau^{15}/600)]/A$$

$$\tau > 1 \ : \ f(\tau) = -[\tau^{-5}/10 + \tau^{-15}/315 + \tau^{-25}/1500]/A$$

with $A = 518/1125 + (11692/15975)(1/p - 1)$.

These equations were derived by Hillert *et al.* [78Hil] from an expression of the magnetic heat capacity C_p^{mag} proposed by Inden [81Ind].

The value of p depends on the structure. For example, p is equal to 0.28 for fcc and hcp metals and 0.40 for bcc metals [81Ind].

For each element, equation 1 is taken from the SGTE database [91Din]. These equations and the magnetic parameters for pure elements are given in Appendices I and II.

The function GHSER$_i$ is also often used to express the thermodynamic functions of a structure φ^* different from the stable structure of the pure element. The expression $G_i^{o,\varphi^*}(T) - H_i^{o,\phi}(298.15\text{K})$ is equivalent to $G_i^{o,\varphi^*}(T) - G_i^{o,\phi}(T) + \text{GHSER}_i$. The term $G_i^{o,\varphi^*}(T) - G_i^{o,\phi}(T)$ is often called the lattice stability of element i.

Binary Compounds

The Gibbs energy of formation of the compound A_aB_b is expressed as:

$$G^o_{A_aB_b}(T) - a\ H_A^{o,\phi}(298.15\ \text{K}) - b\ H_B^{o,\phi}(298.15\ \text{K}) \ = \ f(T) \qquad (3)$$

The expression for $f(T)$ is identical to that given by equation 1.

Equation 3 can be transformed by applying equation 1 for each component

$$\begin{aligned} f(T) &= G^o_{A_aB_b}(T) - a\ G_A^{o,\phi}(T) - b\ G_B^{o,\phi}(T) + a\ \text{GHSER}_A + b\ \text{GHSER}_B \\ &= \Delta_f G^T_{A_aB_b} + a\ \text{GHSER}_A + b\ \text{GHSER}_B \qquad (4) \end{aligned}$$

The term $\Delta_f G_{A_aB_b}(T)$ is the Gibbs energy of formation of the compound referred to the stable elements at temperature T.

Gaseous species

An expression identical to equation 3 is used to describe the Gibbs energy of formation of the gaseous species with the additional $RT\ \ln P$ term, where P is the total pressure. The gas phase is assumed to form an ideal solution. The reference state for each vapor species is taken to be the pure component at 0.1 MPa pressure.

Condensed phases

1: Substitutional solutions:

For the substitutional solution ϕ, the Gibbs energy of mixing is expressed as follows:

$$G_m = G^{\phi,\text{id}} + G^{\phi,\text{xs}} \qquad (5)$$

with

$$G^{\phi,\text{id}} = R\ T\ \sum_i x_i \ln x_i \qquad (6)$$

The Redlich - Kister equation [48Red], a power series expansion, is used to express the excess Gibbs energy, $G_m^{\phi,xs}$, as follows:

$$G_m^{\phi,xs} = x_i x_j \sum_{\nu=0} L_{ij}^{\nu,\phi} (x_i - x_j)^\nu \tag{7}$$

x_i is the molar fraction of component i with $\sum_i x_i = 1$. The model parameter L_{ij}^ν can be temperature dependent as follows:

$$L_{i,j:i} = y_i' y_j' [a_0 + b_0 T + c_0 T \cdot \ln T (a_1 + b_1 T)(y_i' - y_j')] \tag{8}$$

For a ternary solution, the excess Gibbs energy is expressed as follows:

$$G^{\phi,xs} = \sum_i \sum_{j>i} x_i^\phi \, x_j^\phi \sum_\nu L^{\nu,\phi} - (x_i^\phi - x_j^\phi)^\nu \tag{9}$$

If experimental information relative to ternary solutions are available then an extra term can be added to 9. For a ternary system A–B–C, this term is equal to:

$$x_A x_B x_C (\alpha_1 x_A + \alpha_2 x_B + \alpha_3 x_C.) \tag{10}$$

For magnetic alloys, the composition dependence of T_c and β are expressed by:

$$T_c^*(x) = \sum_i x_i T_{c,i}^{\circ,*} + T_c^{*,xs} \tag{11}$$

$$\beta(x) = \sum_i x_i \beta_i^\circ + \beta^{xs} \tag{12}$$

where $T^{*,xs}$ and β^{xs} are both represented by an equation similar to 7.

2: Ordered Phases:

The use of the sublattice model, developed by Hillert and Staffansson [70Hil] based on Temkin's model for ionic solutions [45Tem] and extended by Sundman and Ågren [81Sun], allows a variety of solution phases to be treated, in particular ordered phases.

As non-stroichiometric phases are formed by several sublattices, they can be schematically described as follows:

$$(\mathrm{A}_{y_A'} \mathrm{B}_{y_B'} \ldots)_p (\mathrm{A}_{y_A''} \mathrm{B}_{y_B''} \ldots)_q \ldots$$

where the species A, B, ... can be atoms, vacancies or ions on the different sublattices ', ", ... The number of sites are p, q, ... If $p + q + \ldots = 1$, then the thermodynamic quantities are referred to one mole of sites.

For each sublattice s, the site fraction of the species i is equal to

$$y_i^s = \frac{n_i^s}{\sum_j n_j^s} = \frac{n_i^s}{n^s} \qquad \text{with} \qquad \sum_i y_i^s = 1 \qquad \text{and} \qquad \sum_s n^s = n \tag{13}$$

where n_i^s is the number of species i in sublattice s, n^s the number of sites in sublattice s, and n the total number of sites. n^s is related to n by $n^s = n \cdot p/(p + q + \ldots)$. The number of sublattices and the species occupying them, is generally obtained from crystallographical information.

This model also describes stoichiometric phases, in which case the sublattices are occupied by a single atom, and substitutional phases which only contain one sublattice.

The molar Gibbs energy expressed by the sublattice model is equal to

$$G_m = G^{\mathrm{ref}} + G^{\mathrm{id}} + G^{\mathrm{ex}} \tag{14}$$

For a two sublattice phase taken as an example, with two elements A and B in each of the sublattices, the term G^{ref}, which defines a surface of reference, is equal to

$$G^{\mathrm{ref}} = y'_{\mathrm{A}} y''_{\mathrm{A}} G^{\circ}_{\mathrm{A:A}} + y'_{\mathrm{A}} y''_{\mathrm{B}} G^{\circ}_{\mathrm{A:B}} + y'_{\mathrm{B}} y''_{\mathrm{A}} G^{\circ}_{\mathrm{B:A}} + y'_{\mathrm{B}} y''_{\mathrm{B}} G^{\circ}_{\mathrm{B:B}} \tag{15}$$

The terms $G^{\circ}_{\mathrm{A:A}}$ and $G^{\circ}_{\mathrm{B:B}}$ represent the Gibbs energy of formation of the constituent elements A and B. The colon separates the different sublattices.

The terms $G^{\circ}_{0}\mathrm{A:B}$ and $G^{\circ}_{\mathrm{B:A}}$ represent the Gibbs energy of formation of the stoichiometric compounds $\mathrm{A}_p\mathrm{B}_q$ and $\mathrm{B}_p\mathrm{A}_q$, which may be stable or metastable.

The term G^{id} is related to the molar configurational entropy and is equal to:

$$G^{\mathrm{id}} = R\,T[p(y'_{\mathrm{A}} ln y'_{\mathrm{A}} + y'_{\mathrm{B}} ln y'_{\mathrm{B}}) + q(y''_{\mathrm{A}} ln y''_{\mathrm{A}} + y''_{\mathrm{B}} ln y''_{\mathrm{B}})] \tag{16}$$

Finally, the excess Gibbs energy $G^{\mathrm{xs}}$is equal to

$$\begin{aligned} G^{\mathrm{xs}} = {} & y'_{\mathrm{A}} y'_{\mathrm{B}} [y''_{\mathrm{A}} L_{\mathrm{A,B:A}} + y''_{\mathrm{B}} L_{\mathrm{A,B:B}}] \\ & + y''_{\mathrm{A}} y''_{\mathrm{B}} [y'_{\mathrm{A}} L_{\mathrm{A:A,B}} + y'_{\mathrm{B}} L_{\mathrm{B:A,B}}] \\ & + y'_{\mathrm{A}} y'_{\mathrm{B}} y''_{\mathrm{A}} y''_{\mathrm{B}} L_{\mathrm{A,B:A,B}} \end{aligned} \tag{17}$$

The terms $L_{i,j:i}$ and $L_{i:i,j}$ represent the interaction parameters between the atoms on one sublattice for a given occupancy of the other, and can be described by a polynomial, as follows:

$$L_{i,j:i} = y'_i y'_j [a_0 + b_0 T + (a_1 + b_1 T)(y'_i - y'_j)] \tag{18}$$

The above equations can be expressed for ternary systems and they become more complicated when the number of species increases in each sublattice.

3. Order-disorder transformation:

For the COST project, only the order-disorder transformation relative to the bcc-$A2$ and bcc-$B2$ was considered. A unique function representing the Gibbs energy is used to describe the thermodynamic properties of both phases as follows:

$$G_m = G_m^{dis}(x_i) + \Delta G_m^{ord}(y_i^s) \tag{19}$$

where $\Delta G_m^{ord}(y_i^s)$ and $G_m^{dis}(x_i)$ are respectively the ordering energy, equal to zero in the disordered state, and $G_m^{dis}(x_i)$ the molar Gibbs energy of the disordered phase. $\Delta G_m^{ord}(y_i^s)$ is equal to:

$$\begin{aligned}
\Delta G_m^{ord}(y_i^s) \;=\; & \sum_i \sum_j y_i' y_j'' \, \Delta {}^{\circ}G_{i:j}^{ord} + RT\left(a \sum_i y_i' \ln y_i' + b \sum_i y_i'' \ln y_i''\right) \\
& + y_{\mathrm{A}}' y_{\mathrm{B}}' \sum_i y_i'' \; L_{\mathrm{A,B}:i}^{0,ord} + y_{\mathrm{A}}' y_{\mathrm{B}}' (y_{\mathrm{A}}' - y_{\mathrm{B}}') \sum_i y_i'' \; L_{\mathrm{A,B}:i}^{1,ord} \\
& + y_{\mathrm{A}}'' y_{\mathrm{B}}'' \sum_i y_i' \; L_{i:\mathrm{A,B}}^{0,ord} + y_{\mathrm{A}}'' y_{\mathrm{B}}'' (y_{\mathrm{A}}'' - y_{\mathrm{B}}'') \sum_i y_i' \; L_{i:\mathrm{A,B}}^{1,ord} \\
& + y_{\mathrm{A}}' y_{\mathrm{B}}' y_{\mathrm{A}}'' y_{\mathrm{B}}'' L_{\mathrm{A,B:A,B}}^{ord}
\end{aligned} \tag{20}$$

$G_m^{dis}(x_i)$ is given in the Redlich-Kister formalism by equation 7. x_i and y_i^s are the molar fraction of element i in the phase and its site fraction in sublattice s respectively.

To ensure stability of the disordered phase, the first derivative of G_m with respect to the site occupation must be zero for any given composition. This condition and the fact that the ordering energy is zero for disorder leads to constraints between the thermodynamic parameters describing ordering [88Ans]. Using these constraints and converting the Gibbs energy of the disordered state into the sublattice formalism, allows to express the whole Gibbs energy of both phases ($A2$ and $B2$) in the sublattice formalism as follows:

$$G^{\circ}(T) - H_{\mathrm{A}}^{\circ,\mathrm{ref}}(298.15\ \mathrm{K}) = \mathrm{G(A{:}A)} = \mathrm{GREF_A}$$

$$\begin{aligned}
G^{\circ}(T) - 0.5\ H_{\mathrm{A}}^{\circ,\mathrm{ref}}(298.15\ \mathrm{K}) - 0.5\ H_{\mathrm{B}}^{\circ,\mathrm{ref}}(298.15\ \mathrm{K}) = \mathrm{G(A{:}B)} = \\
0.5\ \mathrm{GREF_A} + 0.5\ \mathrm{GREF_A} + \Delta {}^{\circ}G_{\mathrm{A:B}}^{ord} + \tfrac{1}{4}\ {}^{0}L_{\mathrm{A,B}}^{dis}
\end{aligned}$$

$$\begin{aligned}
G^{\circ}(T) - 0.5\ H_{\mathrm{A}}^{\circ,\mathrm{ref}}(298.15\ \mathrm{K}) - 0.5\ H_{\mathrm{B}}^{\circ,\mathrm{ref}}(298.15\ \mathrm{K}) = \mathrm{G(B{:}A)} = \\
0.5\ \mathrm{GREF_A} + 0.5\ \mathrm{GREF_A} + \Delta {}^{\circ}G_{\mathrm{A:B}}^{ord} + \tfrac{1}{4}\ L_{\mathrm{A,B}}^{0,dis}
\end{aligned}$$

$$G^{\circ}(T) - H_{\mathrm{B}}^{\circ,\mathrm{ref}}(298.15\ \mathrm{K}) = \mathrm{G(B{:}B)} = \mathrm{GREF_B}$$

$$\begin{aligned}
L_{\mathrm{A,B:A}}^{0} &= L_{\mathrm{A:A,B}}^{0} = -\Delta {}^{\circ}G_{\mathrm{A:B}}^{ord} - L_{\mathrm{A,B:A}}^{1,ord} + \tfrac{1}{4}\ L_{\mathrm{A,B}}^{0,dis} + \tfrac{3}{8}\ L_{\mathrm{A,B}}^{1,dis} + \tfrac{3}{16}\ L_{\mathrm{A,B}}^{2,dis} \\
L_{\mathrm{A,B:A}}^{1} &= L_{\mathrm{A:A,B}}^{1} = L_{\mathrm{A,B:A}}^{1,ord} + \tfrac{1}{8}\ L_{\mathrm{A,B}}^{1,dis} + \tfrac{4}{16}\ L_{\mathrm{A,B}}^{2,dis} \\
L_{\mathrm{A,B:A}}^{2} &= L_{\mathrm{A:A,B}}^{2} = \tfrac{1}{16}\ L_{\mathrm{A,B}}^{2,dis} \\
L_{\mathrm{A,B:B}}^{0} &= L_{\mathrm{B:A,B}}^{0} = -\Delta {}^{\circ}G_{\mathrm{A:B}}^{ord} + L_{\mathrm{A,B:B}}^{1,ord} + \tfrac{1}{4}\ L_{\mathrm{A,B}}^{0,dis} - \tfrac{3}{8}\ L_{\mathrm{A,B}}^{1,dis} + \tfrac{3}{16}\ L_{\mathrm{A,B}}^{2,dis} \\
L_{\mathrm{A,B:B}}^{1} &= L_{\mathrm{B:A,B}}^{1} = L_{\mathrm{A,B:B}}^{1,ord} + \tfrac{1}{4}\ L_{\mathrm{A,B}}^{1,dis} - \tfrac{4}{8}\ L_{\mathrm{A,B}}^{2,dis} \\
L_{\mathrm{A,B:B}}^{2} &= L_{\mathrm{B:A,B}}^{2} = \tfrac{1}{16}\ L_{\mathrm{A,B}}^{2,dis}
\end{aligned}$$

$$L_{\mathrm{A,B:A,B}} = 4L_{\mathrm{A,B:A}}^{1,ord} - 4L_{\mathrm{A,B:B}}^{1,ord} - \frac{24}{16} L_{\mathrm{A,B}}^{2,dis} \tag{21}$$

where $\Delta {}^{\circ}G^{ord}_{\mathrm{A:B}}$, $L^{1,ord}_{\mathrm{A,B:A}}$, $L^{1,ord}_{\mathrm{A,B:B}}$ are the independent ordering parameters and $L^{0,dis}_{\mathrm{A,B}}$, $L^{1,dis}_{\mathrm{A,B}}$, and $L^{2,dis}_{\mathrm{A,B}}$[1] are parameters of the disordered state.

In the binary systems Al-Fe, Cu-Mg, Cu-Zn, Fe-Si and Mg-Zn, the equations 21 were used with $L^{1,ord}_{\mathrm{A,B:A}}$ and $L^{1,ord}_{\mathrm{A,B:B}}$ equal to zero.

In a ternary system A-B-C, the relations 21 stand for each binary system. Moreover, the following constraints have to be fulfilled:

$$\begin{aligned}
L^{0}_{\mathrm{C:A,B}} &= L^{0}_{\mathrm{A,B:C}} = L^{0,ord}_{\mathrm{A,B:C}} + \tfrac{1}{4}\, L^{0,dis}_{\mathrm{A,B}} - \tfrac{1}{8}\left(L^{1,dis}_{\mathrm{A,C}} + L^{1,dis}_{\mathrm{B,C}}\right) \\
&\quad + \tfrac{1/2}{16}\left(L^{2,dis}_{\mathrm{A,C}} + L^{2,dis}_{\mathrm{B,C}}\right) \\
L^{0}_{\mathrm{B:A,C}} &= L^{0}_{\mathrm{A,C:B}} = L^{0,ord}_{\mathrm{A,C:B}} + \tfrac{1}{4}\, L^{0,dis}_{\mathrm{A,C}} - \tfrac{1}{8}\left(L^{1,dis}_{\mathrm{A,B}} - L^{1,dis}_{\mathrm{B,C}}\right) \\
&\quad + \tfrac{1/2}{16}\left(L^{2,dis}_{\mathrm{A,B}} + L^{2,dis}_{\mathrm{B,C}}\right) \\
L^{0}_{\mathrm{A:B,C}} &= L^{0}_{\mathrm{B,C:A}} = L^{0,ord}_{\mathrm{A:B,C}} + \tfrac{1}{4}\, L^{0,dis}_{\mathrm{B,C}} + \tfrac{1}{8}\left(L^{1,dis}_{\mathrm{A,B}} + L^{1,dis}_{\mathrm{A,C}}\right) \\
&\quad + \tfrac{1/2}{16}\left(L^{2,dis}_{\mathrm{A,B}} + L^{2,dis}_{\mathrm{A,C}}\right) \\
L^{1}_{\mathrm{C:A,B}} &= L^{1}_{\mathrm{A,B:C}} = L^{1,ord}_{\mathrm{A,B:C}} + \tfrac{1}{8}\, L^{1,dis}_{\mathrm{A,B}} \\
&\quad - \tfrac{1/2}{16}\left(L^{2,dis}_{\mathrm{A,C}} - L^{2,dis}_{\mathrm{B,C}}\right) \\
L^{1}_{\mathrm{B:A,C}} &= L^{1}_{\mathrm{A,C:B}} = L^{1,ord}_{\mathrm{A,C:B}} + \tfrac{1}{8}\, L^{1,dis}_{\mathrm{A,C}} - \tfrac{1/2}{16}\left(L^{2,dis}_{\mathrm{A,B}} - L^{2,dis}_{\mathrm{B,C}}\right) \\
L^{1}_{\mathrm{A:B,C}} &= L^{1}_{\mathrm{B,C:A}} = L^{1,ord}_{\mathrm{B,C:A}} + \tfrac{1}{8}\, L^{1,dis}_{\mathrm{B,C}} - \tfrac{1/2}{16}\left(L^{2,dis}_{\mathrm{A,B}} - L^{2,dis}_{\mathrm{A,C}}\right) \\
L^{2}_{\mathrm{C:A,B}} &= L^{2}_{\mathrm{A,B:C}} = \tfrac{1}{16}\, L^{2,dis}_{\mathrm{A,B}} \\
L^{2}_{\mathrm{B:A,C}} &= L^{2}_{\mathrm{A,C:B}} = \tfrac{1}{16}\, L^{2,dis}_{\mathrm{A,C}} \\
L^{2}_{\mathrm{A:B,C}} &= L^{2}_{\mathrm{B,C:A}} = \tfrac{1}{16}\, L^{2,dis}_{\mathrm{B,C}} \\
L_{\mathrm{A,B:A,C}} &= L_{\mathrm{A,C:A,B}} = -\,\Delta {}^{\circ}G^{ord}_{\mathrm{A:B}} - \Delta {}^{\circ}G^{ord}_{\mathrm{A:C}} - \Delta {}^{\circ}G^{ord}_{\mathrm{B:C}} - L^{0,ord}_{\mathrm{A,B:C}} - L^{0,ord}_{\mathrm{A,C:B}} \\
&\quad - L^{0,ord}_{\mathrm{B,C:A}} + L^{1,ord}_{\mathrm{A,B:A}} - L^{1,ord}_{\mathrm{A,B:C}} + L^{1,ord}_{\mathrm{A,C:A}} - L^{1,ord}_{\mathrm{A,C:B}} \\
&\quad - \tfrac{1}{16}\left(5\, L^{2,dis}_{\mathrm{A,B}} + 5\, L^{2,dis}_{\mathrm{A,C}} + 2\, L^{2,dis}_{\mathrm{B,C}}\right)
\end{aligned}$$

---

[1] In the tables, the following substitutions were made: $\Delta {}^{\circ}G^{ord}_{\mathrm{A:B}} = G^{\bullet}_{\mathrm{A:B:\square}}$, $\tfrac{1}{4}\, L^{0,dis}_{\mathrm{A,B}} = L^{0}_{\mathrm{A,B}}$, $\tfrac{1}{8}\, L^{1,dis}_{\mathrm{A,B}} = L^{1}_{\mathrm{A,B}}$, $\tfrac{1}{16}\, L^{2,dis}_{\mathrm{A,B}} = L^{2}_{\mathrm{A,B}}$

$$\begin{aligned}
L_{\mathrm{A,B:B,C}} &= L_{\mathrm{B,C:A,B}} = -\Delta{}^{\circ}G^{ord}_{\mathrm{A:B}} - \Delta{}^{\circ}G^{ord}_{\mathrm{A:C}} - \Delta{}^{\circ}G^{ord}_{\mathrm{B:C}} - L^{0,ord}_{\mathrm{A,B:C}} - L^{0,ord}_{\mathrm{A,C:B}} \\
&\quad - L^{0,ord}_{\mathrm{B,C:A}} + L^{1,ord}_{\mathrm{A,B:B}} - L^{1,ord}_{\mathrm{A,B:C}} + L^{1,ord}_{\mathrm{B,C:A}} - L^{1,ord}_{\mathrm{B,C:B}} \\
&\quad - \tfrac{1}{16}\left(5\, L^{2,dis}_{\mathrm{A,B}} + 2\, L^{2,dis}_{\mathrm{A,C}} + 5\, L^{2,dis}_{\mathrm{B,C}}\right) \\
L_{\mathrm{B,C:A,C}} &= L_{\mathrm{A,C:B,C}} = -\Delta{}^{\circ}G^{ord}_{\mathrm{A:B}} - \Delta{}^{\circ}G^{ord}_{\mathrm{A:C}} - \Delta{}^{\circ}G^{ord}_{\mathrm{B:C}} - L^{0,ord}_{\mathrm{A,B:C}} - L^{0,ord}_{\mathrm{A,C:B}} \\
&\quad - L^{0,ord}_{\mathrm{B,C:A}} + L^{1,ord}_{\mathrm{A,C:B}} - L^{1,ord}_{\mathrm{A,C:C}} + L^{1,ord}_{\mathrm{B,C:A}} - L^{1,ord}_{\mathrm{B,C:C}} \\
&\quad - \tfrac{1}{16}\left(2\, L^{2,dis}_{\mathrm{A,B}} + 5\, L^{2,dis}_{\mathrm{A,C}} + 5\, L^{2,dis}_{\mathrm{B,C}}\right) \\
L_{\mathrm{A:A,B,C}} &= L_{\mathrm{A,B,C:A}} = \tfrac{1}{32}\left(3\, L^{2,\mathrm{dis}}_{A,B} + 3\, L^{2,\mathrm{dis}}_{A,C} \right) \\
L_{\mathrm{B:A,B,C}} &= L_{\mathrm{A,B,C:B}} = \tfrac{1}{32}\left(3\, L^{2,\mathrm{dis}}_{A,B} + 3\, L^{2,\mathrm{dis}}_{B,C} \right) \\
L_{\mathrm{C:A,B,C}} &= L_{\mathrm{A,B,C:C}} = \tfrac{1}{16}\left(3/2\, L^{2,\mathrm{dis}}_{A,C} + 3/2\, L^{2,\mathrm{dis}}_{B,C} \right) \\
L_{\mathrm{A,B:A,B,C}} &= L_{\mathrm{A,B,C:A,B}} = 0 \\
L_{\mathrm{A,C:A,B,C}} &= L_{\mathrm{A,B,C:A,C}} = 0 \\
L_{\mathrm{B,C:A,B,C}} &= L_{\mathrm{A,B,C:B,B}} = 0 \\
L_{\mathrm{A,B,C:A,B,C}} &= 0
\end{aligned} \tag{22}$$

where $L^{0,ord}_{\mathrm{A,B:C}}$, $L^{0,ord}_{\mathrm{A,C:B}}$, $L^{0,ord}_{\mathrm{B,C:A}}$, $L^{1,ord}_{\mathrm{A,B:C}}$, $L^{1,ord}_{\mathrm{A,C:B}}$, $L^{1,ord}_{\mathrm{B,C:A}}$ are the independent ternary parameters of ordering.

In the ternary system Cu-Mg-Zn, the regular interaction parameters $L^{0,ord}_{\mathrm{A,B:C}}$, $L^{0,ord}_{\mathrm{A,C:B}}$ and $L^{0,ord}_{\mathrm{B,C:A}}$, were taken respectively identical to $-\Delta{}^{\circ}G^{ord}_{\mathrm{A:B}}$, $-\Delta{}^{\circ}G^{ord}_{\mathrm{A:C}}$ and $-\Delta{}^{\circ}G^{ord}_{\mathrm{B:C}}$, and the sub-regular terms $L^{1,ord}_{\mathrm{A,B:C}}$, $L^{1,ord}_{\mathrm{A,C:B}}$ and $L^{1,ord}_{\mathrm{B,C:A}}$ equal to zero like in the corresponding binary systems.

Neverthless, the use of this sublattice formalism to describe the order – disorder transformation requires the conversion of the parameters of the disordered state into the sublattice model which is cumbersome. A new treatment of the order–disorder transformation was introduced later on by Sundman [91Sun] where G_m is expressed as follows :

$$G_m = G^{dis}_m(x_i) + \Delta G^{ord*}(y_i', y_i'') - \Delta G^{ord*}(x_i, x_i) \tag{23}$$

with

$$G^{dis}_m(x_i) = \sum_i x_i\, {}^{\circ}G^{dis}_i + RT \sum_i x_i \ln x_i + x_{\mathrm{A}} x_{\mathrm{B}} \sum_\nu L^{\nu,dis}_{\mathrm{A,B}} (x_{\mathrm{A}} - x_{\mathrm{B}})^\nu \tag{24}$$

$$
\begin{aligned}
\Delta G^{ord*}(y'_i, y''_i) &= \sum_i \sum_j y'_i y''_j \; \Delta{}^{\circ}G^{ord*}_{i:j} + RT\left(a \sum_i y'_i \ln y'_i + b \sum_i y''_i \ln y''_i\right) \\
&\quad + y'_A y'_B \sum_i y''_i \; L^{0,ord*}_{A,B:i} + y'_A y'_B (y'_A - y'_B) \sum_i y''_i \; L^{1,ord*}_{A,B:i} \\
&\quad + y''_A y''_B \sum_i y'_i \; L^{0,ord*}_{i:A,B} + y''_A y''_B (y''_A - y''_B) \sum_i y'_i \; L^{1,ord*}_{i:A,B} \\
&\quad + y'_A y'_B y''_A y''_B \; L^{ord*}_{A,B:A,B} \qquad (25) \\
\Delta G^{ord*}(x_i, x_i) &= \sum_i \sum_j x_i x_j \; \Delta{}^{\circ}G^{ord*}_{i:j} + RT\left(a \sum_i x_i \ln x_i + b \sum_i x_i \ln x_i\right) \\
&\quad + x_A x_B \sum_i x_i \; L^{0,ord*}_{A,B:i} + x_A x_B (x_A - x_B) \sum_i x_i \; L^{1,ord*}_{A,B:i} \\
&\quad + x_A x_B \sum_i x_i \; L^{0,ord*}_{i:A,B} + x_A x_B (x_A - x_B) \sum_i x_i \; L^{1,ord*}_{i:A,B} \\
&\quad + x_A x_B x_A x_B \; L^{ord*}_{A,B:A,B} \qquad (26)
\end{aligned}
$$

Hence, the disordered and ordered phases can be treated separately. The parameters of the disordered phase, $L^{\nu,dis}_{A,B}$, and those describing the ordering $\Delta{}^{\circ}G^{ord*}_{A:B}$, $L'^{\nu,ord*}_{A,B:i}$, $L^{\nu,ord*}_{i:A,B}$ and $L^{ord*}_{A,B:A,B}$ are introduced as usual thermodynamic parameters of the sublattice model and a special command then allows their combination to define the expression of the order-disorder sublattice following equation 23.

Constraints must still be introduced between the thermodynamic parameters of the function $\Delta G(y'_i, y''_i)$ to ensure stability of the disordered state. But the value zero for the ordering energy is now built in. This allows to simplify the expression of the constraints linking the ordering parameters.

The ternary systems Al-Ti-(Mo,Nb,Ta,W) were assessed with equation 23 assuming

$$
\begin{aligned}
\Delta{}^{\circ}G^{ord*}_{i:j} = \Delta{}^{\circ}G^{ord*}_{j:i} &= -L^{0,ord*}_{i,j:i} = -L^{0,ord*}_{i,j:j} = -L^{0,ord*}_{i,j:k} \\
&= -L^{0,ord*}_{i:i,j} = -L^{0,ord*}_{j:i,j} = -L^{0,ord*}_{k:i,j} = \alpha_{ij} \qquad (27)
\end{aligned}
$$

These relations are identical to 21 and 22 when disordered parameters are not considered and sub-regular ordering terms are zero. The use of equation 23 allows a simpler but mathematically equivalent description with only two ordering parameters:

$$
\Delta{}^{\circ}G^{ord*}_{i:j} = \Delta{}^{\circ}G^{ord*}_{j:i} = 2\alpha_{ij} \qquad (28)
$$

When such simplication is possible, the two descriptions (the original using equations 27 and the modified using equations 28) are presented in this report.

For sake of uniformity, the descriptions using the sublattice model with the constrainsts 21 and 22 were also converted for use of equation 23 in the simpler way possible .

Only the parameters derived from the simpler description are in the database. In this report, they are presented in a frame. An example is shown hereunder for a binary system.

Phase bcc–$B2$

$G^{\circ}(T) - H_{\mathrm{A}}^{\circ,\mathrm{ref}}(298.15\ \mathrm{K}) = \mathrm{G(A{:}A)} = 0.0$

$G^{\circ}(T) - 0.5\ H_{\mathrm{A}}^{\circ,\mathrm{ref}}(298.15\ \mathrm{K}) - 0.5\ H_{\mathrm{B}}^{\circ,\mathrm{ref}}(298.15\ \mathrm{K}) = \mathrm{G(A{:}B)} = 2.0\ G_{\mathrm{A:B}}^{ord\bullet}$

$G^{\circ}(T) - 0.5\ H_{\mathrm{A}}^{\circ,\mathrm{ref}}(298.15\ \mathrm{K}) - 0.5\ H_{\mathrm{B}}^{\circ,\mathrm{ref}}(298.15\ \mathrm{K}) = \mathrm{G(B{:}A)} = 2.0\ G_{\mathrm{A:B}}^{ord\bullet}$

$G^{\circ}(T) - H_{\mathrm{B}}^{\circ,\mathrm{ref}}(298.15\ \mathrm{K}) = \mathrm{G(B{:}B)} = 0.0$

Phase bcc–$A2$

$G^{\circ}(T) - H_{\mathrm{A}}^{\circ,\mathrm{ref}}(298.15\ \mathrm{K}) = \mathrm{GREF_A}$

$G^{\circ}(T) - H_{\mathrm{B}}^{\circ,\mathrm{ref}}(298.15\ \mathrm{K}) = \mathrm{GREF_B}$

$L_{\mathrm{A,B:\square}}^{0,\mathrm{dis}} = 4\ L_{\mathrm{A,B}}^{0}$
$L_{\mathrm{A,B:\square}}^{1,\mathrm{dis}} = 8\ L_{\mathrm{A,B}}^{1}$
$L_{\mathrm{A,B:\square}}^{2,\mathrm{dis}} = 16\ L_{\mathrm{A,B}}^{2}$

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BINARY SYSTEMS

System Al–B

Solution Phases:

Liquid, fcc-$A1$

Compounds:

AlB_2, AlB_{12}-L, AlB_{12}-H

Modelling:

Liquid : Substitutional, Redlich-Kister
fcc-$A1$: Substitutional, Redlich-Kister
AlB_2 : Stoichiometric, $(Al)(B)_2$
AlB_{12}-L : Stoichiometric, $(Al)(B)_{12}$
AlB_{12}-H : Stoichiometric, $(Al)(B)_{12}$

Assessor and Date:

H.L. Lukas 1992

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase AlB_2

$$G^{\circ}(T) - H_{Al}^{o,fcc-A1}(298.15\ K) - 2.0\ H_{B}^{o,\beta-rhombo-B}(298.15\ K) = \\ -85808.76 + 45.46923\ T + GHSER_{Al} + 2.0\ GHSER_{B}$$

Phase AlB_{12}–L

$$G^{\circ}(T) - H_{Al}^{o,fcc-A1}(298.15\ K) - 12.0\ H_{B}^{o,\beta-rhombo-B}(298.15\ K) = \\ -198290.69 + 33.68638\ T + GHSER_{Al} + 12.0\ GHSER_{B}$$

Phase AlB_{12}–H

$$G^{\circ}(T) - H_{Al}^{o,fcc-A1}(298.15\ K) - 12.0\ H_{B}^{o,\beta-rhombo-B}(298.15\ K) = \\ -75292.23 - 33.66376\ T + GHSER_{Al} + 12.0\ GHSER_{B}$$

Phase fcc–$A1$

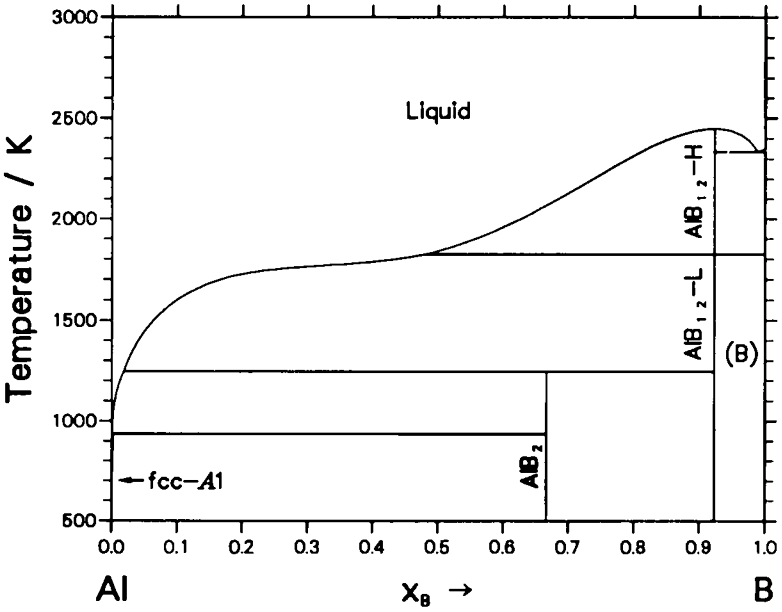
$$L_{Al,B:\square}^{0,fcc-A1} = 12242.44 - 1.74891\ T$$

Phase liquid

$$L^{0,\text{liquid}}_{\text{Al,B}} = -12671.16 + 1.81016\ T$$

$$L^{1,\text{liquid}}_{\text{Al,B}} = 31988.28$$

$$L^{2,\text{liquid}}_{\text{Al,B}} = -15873.74$$



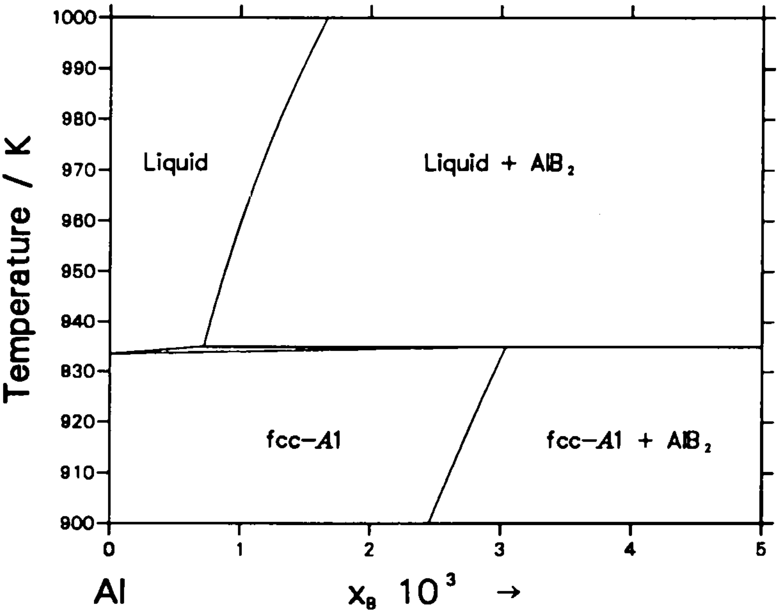


Table I - Invariant Reactions.

Reaction	Type	Compositions x_B			T / K
Liquid + AlB_2 ⇌ fcc-*A1*	Peritectic	.003	.667	.0007	935.0
Liquid + AlB_{12}-L ⇌ AlB_2	Peritectic	.019	.923	.667	1245.8
AlB_{12}-L ⇌ AlB_{12}-H	Polymorphic	.923	.923	....	1826.2
Liquid ⇌ AlB_{12}-H + β-rhombo-B	Eutectic	.988	.923	1.000	2336.0
AlB_{12}-H ⇌ Liquid	Congruent	.923	.923	.....	2448.0

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-B	(Al)	Cu	*cF4* $Fm\bar{3}m$	M 4	
	(B)	β-rhombo-B			
	AlB_{10}	AlB_{10}	*oC88* *Cmcm*		not assessed
	AlB_{12}-L	AlB_{12}	*oP384* $P2_12_12_1$		AlB_{12}-α in [90Mas]
	AlB_{12}-H	AlB_{12}	*tP216* $P4_12_12$		AlB_{12}-β in [90Mas]
	AlB_2	AlB_2	*hP3* *P6/mmm*	Al 1 B 2	

System Al–C

Solution Phases:

Liquid, fcc–$A1$

Compound:

Al_4C_3

Modelling:

Liquid	:	Substitutional, Redlich-Kister
fcc–$A1$	:	Sublattice model , (Al)(C,□)
Al_4C_3	:	Stoichiometric, $(Al)_4(C)_3$

Assessor and Date:

J. Gröbner, H. L. Lukas, and F. Aldinger.

Publication:

Calphad, **20**, 2 (1996) 247-254.

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase Al_4C_3

$$G^{\circ}(T) - 4.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{C}}^{\mathrm{o,graphite}}(298.15\ \mathrm{K}) = - 286002.0 + 1030.273\ T - 161.709142\ T \cdot \ln T - 0.011523\ T^2 + 2450000\ T^{-1} + 7\mathrm{E}{-}07\ T^3$$

Phase fcc–A1

$$G^{\circ}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{C}}^{\mathrm{o,graphite}}(298.15\ \mathrm{K}) = 80\ T + \mathrm{GHSER}_{\mathrm{Al}} + \mathrm{GHSER}_{\mathrm{C}}$$

$$L_{\mathrm{Al:C,\square}}^{0,\mathrm{fcc}-A1} = 80\ T$$

Phase graphite

$$L_{\mathrm{Al,C}}^{0,\mathrm{graphite}} = 80\ T$$

Phase liquid

$$L_{\mathrm{Al,C}}^{0,\mathrm{liquid}} = 40861.02 - 33.21138\ T$$

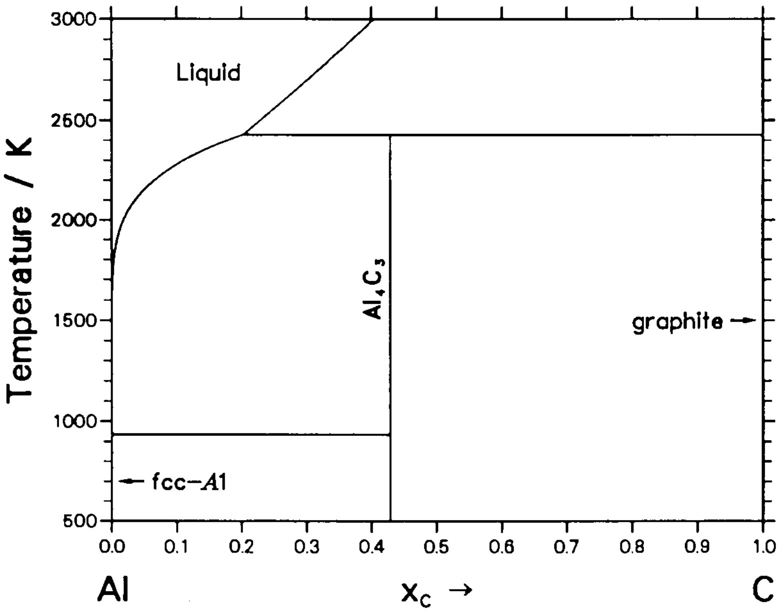


Table I - Invariant Reactions.

Reaction	Type	Compositions x_C			T / K
Liquid + graphite $\rightleftharpoons$ Al_4C_3	Peritectic	.198	1.000	.429	2429.0
Liquid $\rightleftharpoons$ fcc-$A1$ + Al_4C_3	Degenerate	.000	.000	.429	933.5

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	
Al-C	(Al)	Cu	*cF4* $Fm\bar{3}m$	M	4
	(C)	graphite			
	Al_4C_3	Al_4C_3	*hR7* $R\bar{3}m$	Al_1 Al_2 C_1 C_2	2 2 1 2

System Al–Ce

Solution Phases:

Liquid, bcc–$A2$, fcc–$A1$

Compounds:

$Al_{11}Ce_3$, Al_3Ce, AlCe, $AlCe_2$, Al_2Ce

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc–$A2$: Substitutional, Redlich-Kister
fcc–$A1$: Substitutional, Redlich-Kister
$Al_{11}Ce_3$: Stoichiometric, $(Al)_{11}(Ce)_3$
Al_3Ce : Stoichiometric, $(Al)_3(Ce)$
Al_2Ce : Stoichiometric, $(Al)_2(Ce)$
AlCe : Stoichiometric, (Al)(Ce)
$AlCe_2$: Stoichiometric, $(Al)(Ce)_2$

Assessor and Date:

G. Cacciamani, G. Borzone, R. Ferro

Publication:

revised 1997

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase $Al_{11}Ce_3$

$$G^\circ(T) - 11.0\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Ce}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) = - 574000 + 179.3087\ T + 11.0\ \mathrm{GHSER}_{\mathrm{Al}} + 3.0\ \mathrm{GHSER}_{\mathrm{Ce}}$$

Phase Al_3Ce

$$G^\circ(T) - 3.0\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Ce}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) = - 176000 + 54.97964\ T + 3.0\ \mathrm{GHSER}_{\mathrm{Al}} + \mathrm{GHSER}_{\mathrm{Ce}}$$

Phase AlCe

$$G^\circ(T) - H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Ce}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) = - 92000 + 33.90118\ T + \mathrm{GHSER}_{\mathrm{Al}} + \mathrm{GHSER}_{\mathrm{Ce}}$$

Phase AlCe$_3$

$$G^{\circ}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 3.0\ \ H_{\mathrm{Ce}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \\ -\ 108000 + 41.3726\ \ T + \mathrm{GHSER_{Al}} + 3.0\ \ \mathrm{GHSER_{Ce}}$$

Phase Laves–C15

$$G^{\circ}(T) - 2.0\ \ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Ce}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \\ -\ 150000.0 + 45.66405\ \ T + 2.0\ \ \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Ce}}$$

Phase bcc–$A2$

$$L_{\mathrm{Al,Ce:\square}}^{0,\mathrm{bcc}-A2} = 80\ \ T$$

Phase fcc–$A1$

$$L_{\mathrm{Al,Ce:\square}}^{0,\mathrm{fcc}-A1} = 80\ \ T$$

Phase Liquid

$$L_{\mathrm{Al,Ce}}^{0,\mathrm{liquid}} = -\ 167593.1 + 84.87628\ \ T$$

$$L_{\mathrm{Al,Ce}}^{1,\mathrm{liquid}} = -\ 36060 + 5.89346\ \ T$$

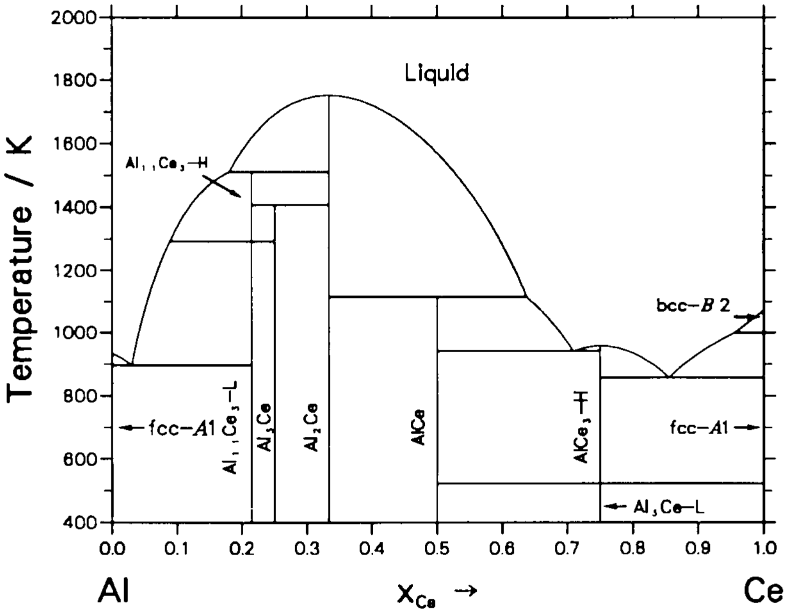


Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Ce}			T / K
Liquid $\rightleftharpoons$ fcc-$A1$ + $Al_{11}Ce_3$	Eutectic	.028	.000	.214	902.6
Liquid + Laves-$C15^*$ $\rightleftharpoons$ $Al_{11}Ce_3$	Peritectic	.179	.333	.214	1497.1
Liquid + Laves-$C15^*$ $\rightleftharpoons$ AlCe	Peritectic	.619	.333	.500	1116.9
Liquid $\rightleftharpoons$ AlCe + $AlCe_3$	Eutectic	.704	.500	.750	911.3
Liquid $\rightleftharpoons$ $AlCe_3$ + fcc-$A1$	Eutectic	.854	.750	1.000	852.2
Liquid $\rightleftharpoons$ bcc-$A2$ + fcc-$A1$	Polymorphic	.956	1.000	1.000	1000.0
$Al_{11}Ce_3$ + Laves-$C15^*$ $\rightleftharpoons$ Al_3Ce	Peritectoid	.214	.333	.250	1408.0
Laves-$C15^*$ $\rightleftharpoons$ Liquid	Congruent	.333	.333	.....	1752.0

* Laves-$C15 \equiv Al_2Ce$

Table II - Crystal Structure and Phase Description.

System	Phase	Structural Type	Pearson Symbol Space Group	Sub-lattices		Comments
Al Ce	(Al)	Cu	$cF4$ $Fm\bar{3}m$	M	4	
	(Ce)	Cu	$cF4$ $Fm\bar{3}m$	M	4	
	(Ce)	W	$cI2$ $Im\bar{3}m$	M	2	
	$Al_{11}Ce_3 - \alpha$	$Al_{11}La_3$	$Immm$ $oI28$			polymorphic trans. not considered
	$Al_{11}Ce_3 - \beta$	Al_4Ba	I_4/mmm tI10			
	Al_3Ce	Ni_3Sn	$hP8$ $P6_3/mmc$			
	Al_2Ce	Cu_2Mg	$cF24$ $Fd\bar{3}m$	Ce Al	8 16	
	AlCe	AlCe	$oC16$ $Cmcm$	Al_1 Al_2 Ce	4 4 8	
	$AlCe_3 - \alpha$	Ni_3Sn	$hP8$ $P6_3/mmc$	Al Ce	2 6	polymorphic trans. not considered
	$AlCe_3 - \beta$	$AuCu_3$	$cP4$ $Pm\bar{3}m$	Al Ce	1 3	

System Al–Cr

Solution Phases:

Liquid, bcc-*A*2, fcc-*A*1

Compounds:

$AlCr_2$, Al_4Cr, Al_8Cr_5-L, Al_8Cr_5-H, Al_9Cr_4-L, Al_9Cr_4-H, $Al_{11}Cr_2$, $Al_{13}Cr_2$

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-*A*2 : Substitutional, Redlich-Kister
fcc-*A*1 : Substitutional, Redlich-Kister
$AlCr_2$: Stoichiometric, $(Al)(Cr)_4$
Al_4Cr : Stoichiometric, $(Al)_4(Cr)$
Al_8Cr_5-L : Stoichiometric, $(Al)_8(Cr)_5$-L
Al_8Cr_5-H : Stoichiometric, $(Al)_8(Cr)_5$-H
Al_9Cr_4-L : Stoichiometric, $(Al)_9(Cr)_4$-L
Al_9Cr_4-H : Stoichiometric, $(Al)_9(Cr)_4$-H
$Al_{11}Cr_2$: Stoichiometric, $(Al)_{11}(Cr)_2$
$Al_{13}Cr_2$: Stoichiometric, $(Al)_{13}(Cr)_2$

Assessor and Date:

N. Saunders, 1991

Publication:

based on the publication of N. Saunders and V.G. Rivlin in Z. für Metallkde, 78, (11) 795-801 (1987).

Thermodynamic properties of the solution and compound phases ($J.mol^{-1}$)

Phase $AlCr_2$

$$G^{\circ}(T) - H_{Al}^{o,fcc-A1}(298.15\ K) - 2.0\ H_{Cr}^{o,bcc-A2,para}(298.15\ K) =$$
$$-\ 32700.0 - 8.79\ T + GHSER_{Al} + 2.0\ GHSER_{Cr}$$

Phase Al_4Cr

$$G^{\circ}(T) - 4.0\ H_{Al}^{o,fcc-A1}(298.15\ K) - H_{Cr}^{o,bcc-A2,para}(298.15\ K) =$$
$$-\ 89025.0 + 19.05\ T + 4.0\ GHSER_{Al} + GHSER_{Cr}$$

Phase Al_8Cr_5–L

$$G^\circ(T) - 8.0 \ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15 \ \mathrm{K}) - 5.0 \ H_{\mathrm{Cr}}^{\mathrm{o,bcc-}A2\mathrm{,para}}(298.15 \ \mathrm{K}) = \\ - 229515.0 + 8.0 \ \mathrm{GHSER}_{\mathrm{Al}} + 5.0 \ \mathrm{GHSER}_{\mathrm{Cr}}$$

Phase Al_8Cr_5–H

$$G^\circ(T) - 8.0 \ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15 \ \mathrm{K}) - 5.0 \ H_{\mathrm{Cr}}^{\mathrm{o,bcc-}A2\mathrm{,para}}(298.15 \ \mathrm{K}) = \\ - 147732.0 - 58.5 \ T + 8.0 \ \mathrm{GHSER}_{\mathrm{Al}} + 5.0 \ \mathrm{GHSER}_{\mathrm{Cr}}$$

Phase Al_9Cr_4–L

$$G^\circ(T) - 9.0 \ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15 \ \mathrm{K}) - 4.0 \ H_{\mathrm{Cr}}^{\mathrm{o,bcc-}A2\mathrm{,para}}(298.15 \ \mathrm{K}) = \\ - 230750.0 + 16.094 \ T + 9.0 \ \mathrm{GHSER}_{\mathrm{Al}} + 4.0 \ \mathrm{GHSER}_{\mathrm{Cr}}$$

Phase Al_9Cr_4 – H

$$G^\circ(T) - 9.0 \ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15 \ \mathrm{K}) - 4.0 \ H_{\mathrm{Cr}}^{\mathrm{o,bcc-}A2\mathrm{,para}}(298.15 \ \mathrm{K}) = \\ - 134433.0 - 56.16 \ T + 9.0 \ \mathrm{GHSER}_{\mathrm{Al}} + 4.0 \ \mathrm{GHSER}_{\mathrm{Cr}}$$

Phase $Al_{11}Cr_2$

$$G^\circ(T) - 11.0 \ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15 \ \mathrm{K}) - 2.0 \ H_{\mathrm{Cr}}^{\mathrm{o,bcc-}A2\mathrm{,para}}(298.15 \ \mathrm{K}) = \\ - 175500.0 + 25.805 \ T + 11.0 \ \mathrm{GHSER}_{\mathrm{Al}} + 2.0 \ \mathrm{GHSER}_{\mathrm{Cr}}$$

Phase $Al_{13}Cr_2$

$$G^\circ(T) - 13.0 \ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15 \ \mathrm{K}) - 2.0 \ H_{\mathrm{Cr}}^{\mathrm{o,bcc-}A2\mathrm{,para}}(298.15 \ \mathrm{K}) = \\ - 174405.0 + 22.2 \ T + 13.0 \ \mathrm{GHSER}_{\mathrm{Al}} + 2.0 \ \mathrm{GHSER}_{\mathrm{Cr}}$$

Phase bcc–$A2$

$$L_{\mathrm{Al,Cr:}\square}^{0,\mathrm{bcc-}A2} = - 54900 + 10 \ T$$

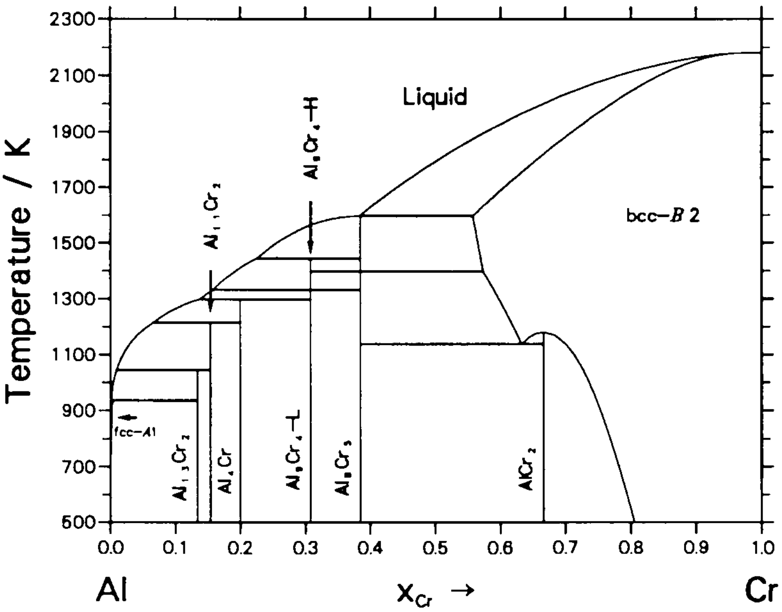
Phase fcc–$A1$

$$L_{\mathrm{Al,Cr:}\square}^{0,\mathrm{fcc-}A1} = - 45900 + 6.0 \ T$$

Phase liquid

$$L_{\mathrm{Al,Cr}}^{0,\mathrm{liquid}} = - 29000.0$$

$$L_{\mathrm{Al,Cr}}^{1,\mathrm{liquid}} = - 11000.0$$


2300
2100
1900
1700
1500
1300
1100
900
700
500
Temperature / K
Liquid
Al$_9$Cr$_4$–H
Al$_{11}$Cr$_2$
bcc–$B2$
fcc–$A1$
Al$_{13}$Cr$_2$
Al$_4$Cr
Al$_9$Cr$_4$–L
Al$_8$Cr$_5$
AlCr$_2$
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
Al
x_{Cr} →
Cr

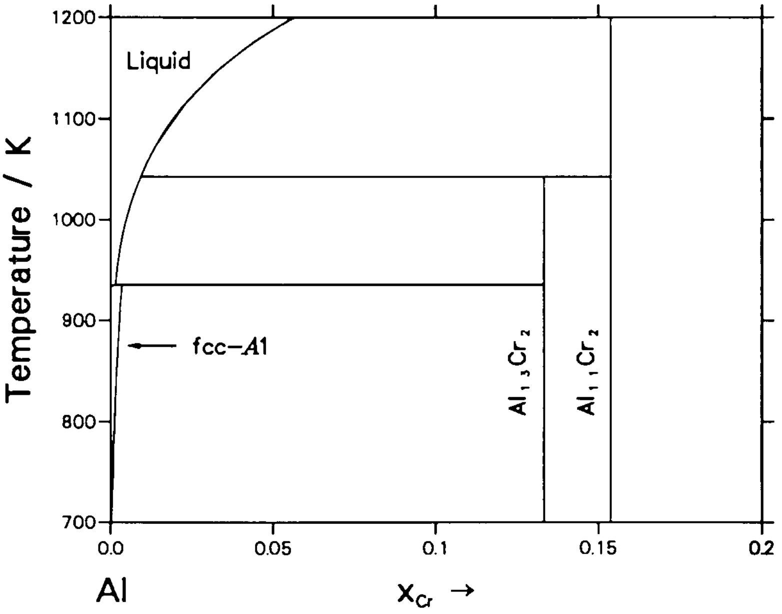

1200
1100
1000
900
800
700
Temperature / K
Liquid
fcc–$A1$
Al$_{13}$Cr$_2$
Al$_{11}$Cr$_2$
0.0
0.05
0.1
0.15
0.2
Al
x_{Cr} →

Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Cr}			T / K
Liquid + $Al_{13}Cr_2 \rightleftharpoons$ fcc-$A1$	Peritectic	.002	.133	.003	934.8
Liquid + $Al_{11}Cr_2 \rightleftharpoons Al_{13}Cr_2$	Peritectic	.009	.154	.133	1042.9
Liquid + $Al_4Cr \rightleftharpoons Al_{11}Cr_2$	Peritectic	.066	.200	.154	1214.6
Liquid + Al_9Cr_4-L $\rightleftharpoons Al_4Cr$	Peritectic	.137	.308	.200	1298.1
Al_9Cr_4-H $\rightleftharpoons Al_9Cr_4$-L	Polymorphic	.158	.158	...	1333.0
Liquid + Al_8Cr_5-H $\rightleftharpoons Al_9Cr_4$-H	Peritectic	.225	.385	.307	1443.1
Liquid $\rightleftharpoons Al_8Cr_5$-H + bcc-$A2$	Eutectic	.385	.383	.558	1597.0
Al_8Cr_5-H $\rightleftharpoons Al_8Cr_5$-L	Polymorphic	.385	.385	...	1398.0
bcc-$A2 \rightleftharpoons Al_8Cr_5$-L + $AlCr_2$	Eutectoid	.633	.385	.667	1139.3
$AlCr_2 \rightleftharpoons$ bcc-$A2$	Congruent	.667	.667	...	1181.0

Table II:a - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-Cr	(Al)	Cu	$cF4$ $Fm\bar{3}m$	M 4	
	(Cr)	W	$cI2$ $Im\bar{3}m$	M 2	
	$AlCr_2$	$MoSi_2$	$tI6$ I4/mmm	Al 2 Cr 4	
	Al_4Cr	Al_4Cr	$mP180$ $P2/m$		
	$Al_{11}Cr_2$	Al_5Cr	$mP48$ P2		also designated by Al_5Cr in [90Mas]
	Al_8Cr_5-L	Al_8Cr_5	$hR26$ $R\bar{3}m$		
	Al_8Cr_5-H	Al_8Cr_5	$hR26$		indicated in [90Mas]
	Al_9Cr_4-L		$cI52$ $I\bar{4}3m$		
	Al_9Cr_4-H				indicated in [90Mas]

Table II:b - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices		Comments
	$Al_{13}Cr_2$-β	$Al_{45}V_7$	$mC104$ $C2/m$	Al_1	2	also designated by by Al_7Cr in [90Mas]
				Al_2	4	
				Al_3	4	
				Al_4	4	
				Al_5	4	
				Al_6	4	
				Al_7	4	
				Al_8	4	
				Al_9	4	
				Al_{10}	8	
				Al_{11}	8	
				Al_{12}	8	
				Al_{13}	8	
				Al_{14}	8	
				Al_{15}	4	
				Al_{16}	4	
				Cr_1	2	
				Cr_2	4	
				Cr_3	8	

System Al–Cu

Solution Phases:

(stable)	Liquid, bcc-*A*2, fcc-*A*1
(metastable)	hcp-*A*3

Compounds:

(stable)	AlCu-δ, AlCu-ϵ, AlCu-η, AlCu-θ, AlCu-γ($D8_3$) AlCu-γ(H), AlCu-ζ
(metastable)	Laves-*C*14, Laves-*C*15, Laves-*C*36

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-*A*2 : Substitutional, Redlich-Kister
fcc-*A*1 : Substitutional, Redlich-Kister
hcp-*A*3 : Substitutional, Redlich-Kister
AlCu-δ : Sublattice model, $(Al,Cu)_2(Cu)_3$
AlCu-ϵ : Sublattice model, (Al,Cu)(Cu)
AlCu-η : Sublattice model, (Al,Cu)(Cu)
AlCu-θ : Sublattice model, $(Al)(Al,Cu)_2$
AlCu-γ($D8_3$) : Sublattice model, $(Al)_4(Al,Cu)(Cu)_8$
AlCu-γ(H) : Sublattice model, $(Al)_4(Al,Cu)(Cu)_8$
AlCu-ζ : Stoichiometric, $(Al)_9(Cu)_{11}$
Laves-*C*14 : Sublattice model, $(Al,Cu)_2(Al,Cu)$
Laves-*C*15 : Sublattice model, $(Al,Cu)_2(Al,Cu)$
Laves-*C*36 : Sublattice model, $(Al,Cu)_2(Al,Cu)$

Assessor and Date:

N. Saunders, 1991
Data relative to the Laves phases evaluated in Round II.

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase AlCu-δ

$$G^{\circ}(T) - 2.0\ \ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 3.0\ \ H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = - 106700.0 + 3.0\ \ T + 2.0\ \ \mathrm{GHSER_{Al}} + 3.0\ \ \mathrm{GHSER_{Cu}}$$

Phase AlCu-ϵ

$$G^{\circ}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Cu)} = - 36976 + 1.2\ \ T + \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Cu}}$$

$$G^{\circ}(T) - 2.0\ \ H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Cu)} = 2.0\ \ \mathrm{GBCC_{Cu}}$$

$$L_{\mathrm{Al,Cu:Cu}}^{0,\mathrm{AlCu}-\epsilon} = 7600 - 24\ \ T$$

$$L_{\mathrm{Al,Cu:Cu}}^{1,\mathrm{AlCu}-\epsilon} = - 72000$$

Phase AlCu-η

$$G^{\circ}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Cu)} = - 40560.0 + 3.14\ \ T + \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Cu}}$$

$$G^{\circ}(T) - 2.0\ \ H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Cu)} = 2.0\ \ \mathrm{GBCC_{Cu}}$$

$$L_{\mathrm{Al,Cu:Cu}}^{0,\mathrm{AlCu}-\eta} = - 25740 - 20\ \ T$$

Phase AlCu-θ

$$G^{\circ}(T) - 3.0\ \ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Al)} = 3.0\ \ \mathrm{GBCC_{Al}}$$

$$G^{\circ}(T) - 2.0\ \ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Cu)} = - 47406.0 + 6.75\ \ T + 2.0\ \ \mathrm{GHSER_{Al}} + 1.0\ \ \mathrm{GHSER_{Cu}}$$

$$L_{\mathrm{Al:Al:Cu}}^{0,\mathrm{AlCu}-\theta} = 2211$$

Phase AlCu-ζ

$$G^{\circ}(T) - 9.0\ \ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 11.0\ \ H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = - 420000.0 + 18.0\ \ T + 9.0\ \ \mathrm{GHSER_{Al}} + 11.0\ \ \mathrm{GHSER_{Cu}}$$

Phase AlCu-$\gamma(D8_3)$

$$G^{\circ}(T) - 5.0\ \ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 8.0\ \ H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Al{:}Cu)} = - 300716.0 + 390.0\ \ T - 52\ \ T \cdot \ln T + 5.0\ \ \mathrm{GHSER_{Al}} + 8.0\ \ \mathrm{GHSER_{Cu}}$$

$$G^{\circ}(T) - 4.0\ \ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 9.0\ \ H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Cu{:}Cu)} = - 280501.0 + 379.6\ \ T - 52\ \ T \cdot \ln T + 4.0\ \ \mathrm{GHSER_{Al}} + 9.0\ \ \mathrm{GHSER_{Cu}}$$

Phase AlCu–γ(H)

$$G^\circ(T) - 5.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 8.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Al{:}Cu)} = $$
$$- 219258.0 - 45.5\ T + 5.0\ \mathrm{GHSER}_{\mathrm{Al}} + 8.0\ \mathrm{GHSER}_{\mathrm{Cu}}$$

$$G^\circ(T) - 4.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 9.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Cu{:}Cu)} = $$
$$- 200460.0 - 58.5\ T + 4.0\ \mathrm{GHSER}_{\mathrm{Al}} + 9.0\ \mathrm{GHSER}_{\mathrm{Cu}}$$

Phase Laves-$C14$

$$G^\circ(T) - 3.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Al)} = $$
$$15000.0 + 3.0\ \mathrm{GHSER}_{\mathrm{Al}}$$

$$G^\circ(T) - 2.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Cu)} = $$
$$15000.0 + 2.0\ \mathrm{GHSER}_{\mathrm{Al}} + \mathrm{GHSER}_{\mathrm{Cu}}$$

$$G^\circ(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Al)} = $$
$$15000.0 + \mathrm{GHSER}_{\mathrm{Al}} + 2.0\ \mathrm{GHSER}_{\mathrm{Cu}}$$

$$G^\circ(T) - 3.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Cu)} = $$
$$15000.0 + 3.0\ \mathrm{GHSER}_{\mathrm{Cu}}$$

$$L_{\mathrm{Al,Cu:Al}}^{0,\mathrm{Laves}-C14} = - 24000 + 2.44\ T$$

$$L_{\mathrm{Al,Cu:Cu}}^{0,\mathrm{Laves}-C14} = - 24000 + 2.44\ T$$

Phase Laves-$C15$

$$G^\circ(T) - 3.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Al)} = $$
$$15000.0 + 3.0\ \mathrm{GHSER}_{\mathrm{Al}}$$

$$G^\circ(T) - 2.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Cu)} = $$
$$15000.0 + 2.0\ \mathrm{GHSER}_{\mathrm{Al}} + \mathrm{GHSER}_{\mathrm{Cu}}$$

$$G^\circ(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Al)} = $$
$$15000.0 + \mathrm{GHSER}_{\mathrm{Al}} + 2.0\ \mathrm{GHSER}_{\mathrm{Cu}}$$

$$G^\circ(T) - 3.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Cu)} = $$
$$15000.0 + 3.0\ \mathrm{GHSER}_{\mathrm{Cu}}$$

$$L_{\mathrm{Al,Cu:Al}}^{0,\mathrm{Laves}-C15} = - 105000 - 1.615\ T$$

$$L_{\mathrm{Al,Cu:Cu}}^{0,\mathrm{Laves}-C15} = - 105000 - 1.615\ T$$

Phase Laves-$C36$

$$G^\circ(T) - 3.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Al)} = $$
$$15000.0 + 3.0\ \mathrm{GHSER}_{\mathrm{Al}}$$

$$G^\circ(T) - 2.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Cu)} = $$
$$15000.0 + 2.0\ \mathrm{GHSER}_{\mathrm{Al}} + \mathrm{GHSER}_{\mathrm{Cu}}$$

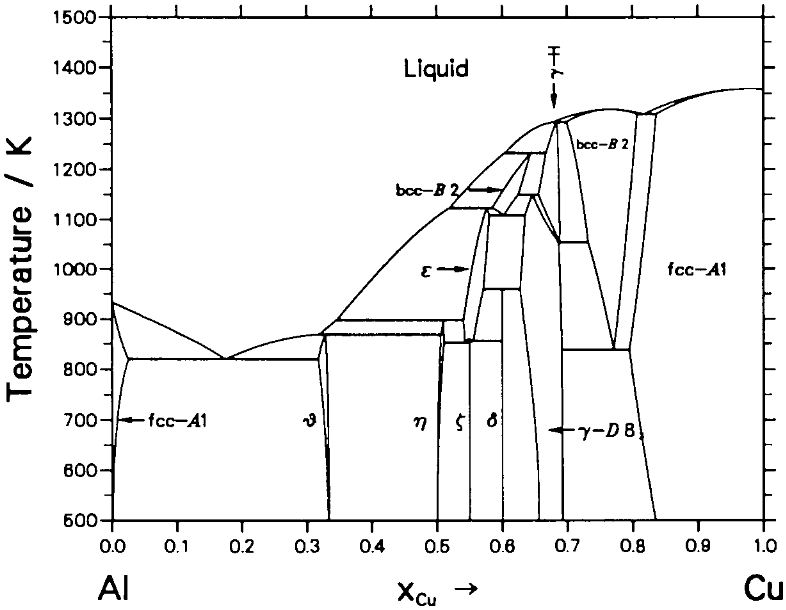
$$G^\circ(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Al)} = $$
$$15000.0 + \mathrm{GHSER}_{\mathrm{Al}} + 2.0\ \mathrm{GHSER}_{\mathrm{Cu}}$$

$$G^\circ(T) - 3.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Cu)} = $$

$$15000.0 + 3.0\ \mathrm{GHSER_{Cu}}$$

$$L^{0,\mathrm{Laves}-C36}_{\mathrm{Al,Cu:Al}} = -126169 + 14.61\ T$$

$$L^{0,\mathrm{Laves}-C36}_{\mathrm{Al,Cu:Cu}} = -126169 + 14.61\ T$$



Phase bcc–A2

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Al,Cu:\square}} = -73554 + 4.0\ T$$

$$L^{1,\mathrm{bcc}-A2}_{\mathrm{Al,Cu:\square}} = 51500 - 11.84\ T$$

Phase fcc–A1

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Al,Cu:\square}} = -53520 + 2\ T$$

$$L^{1,\mathrm{fcc}-A1}_{\mathrm{Al,Cu:\square}} = 38590 - 2\ T$$

$$L^{2,\mathrm{fcc}-A1}_{\mathrm{Al,Cu:\square}} = 1170$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Al,Cu}} = -\,66622 + 8.1\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Al,Cu}} = 46800 - 90.8\ T + 10\ T \cdot \ln T$$

$$L^{2,\mathrm{liquid}}_{\mathrm{Al,Cu}} = -\,2812$$

Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Cu}			T / K
Liquid ⇌ fcc-$A1$ + AlCu-θ	Eutectic	.175	.025	.318	820.7
Liquid + AlCu-η ⇌ AlCu-θ	Peritectic	.319	.506	.329	869.0
Liquid + AlCu-ϵ ⇌ AlCu-η	Peritectic	.345	.541	.510	898.0
Liquid + bcc-$A2$ ⇌ AlCu-ϵ	Peritectic	.519	.585	.576	1124.0
Liquid + AlCu-γ(H) ⇌ bcc-$A2$	Peritectic	.604	.667	.644	1232.4
Liquid + bcc-$A2$ ⇌ AlCu-γ(H)	Peritectic	.678	.698	.684	1293.4
Liquid ⇌ bcc-$A2$ + fcc-$A1$	Eutectic	.817	.807	.837	1309.3
bcc-$A2$ ⇌ AlCu-γ($D8_3$) + fcc-$A1$	Eutectoid	.771	.691	.795	837.9
AlCu-γ(H) ⇌ AlCu-γ($D8_3$) + bcc-$A2$	Eutectoid	.688	.686	.732	1054.2
bcc-$A2$ + AlCu-γ(H) ⇌ AlCu-γ($D8_3$)	Peritectoid	.625	.656	.647	1150.5
bcc-$A2$ ⇌ AlCu-ϵ + AlCu-γ($D8_3$)	Eutectoid	.602	.580	.635	1109.3
AlCu-ϵ + AlCu-γ($D8_3$) ⇌ AlCu-δ	Peritectoid	.572	.628	.600	959.7
AlCu-ϵ ⇌ AlCu-ζ + AlCu-δ	Eutectoid	.555	.550	.600	855.8
AlCu-ϵ ⇌ AlCu-η + AlCu-ζ	Eutectoid	.543	.511	.550	852.4
AlCu-ζ ⇌ AlCu-ϵ	Congruent	.550	.550	...	861.0

Table II:a – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-Cu	(Al)	Cu	*cF4* $Fm\bar{3}m$	M 4	
	(Cu)	Cu	*cF4* $Fm\bar{3}m$	M 4	
	β	W	*cI2* $Im\bar{3}m$	M 2	
	β_0				not considered

Table II:b – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
	AlCu-δ		.... $R3m$		
	AlCu-η_1		$Pban$ or $Cmmm$ $oP16$ or $oC16$		high T phase
	AlCu-η_2	AlCu	$mC20$ $C2/m$		low T phase
	AlCu-θ	Al_2Cu	$tI12$ $I4/mcm$	Al 8 Cu 4	
	AlCu-δ	.....	..... $R\bar{3}m$		
	AlCu-ϵ_1	NiAs	$hP4$ $P6_3/mmc$		low T phase
	AlCu-ϵ_2	.....	.....		not considered
	AlCu-γ($D8_3$)	Al_4Cu_9	$cP52$ $P\bar{4}3m$	Al_1 4 Al_2 12 Cu_1 4 Cu_2 4 Cu_3 4 Cu_4 6 Cu_5 6 Cu_6 12	
	AlCu-γ(II)	.....	....		
	AlCu-ζ_1	.....	$hP42$ $C2/m$		ζ_1
	AlCu-ζ_2	.....			ζ_2 not considered

System Al–Fe

Solution Phases:

(stable) : Liquid, fcc–*A*1, bcc–*A*2, bcc–*B*2,$\mathrm{Al_5Fe_4}$
(metastable) : cbcc–*A*12, cub–*A*13, hcp–*A*3

Compounds:

stable : $\mathrm{Al_2Fe}$, $\mathrm{Al_5Fe_2}$,$\mathrm{Al_{13}Fe_4}$,
metastable : $\mathrm{Al_{11}Mn_4}$, $\mathrm{Al_{12}Mn}$, $\mathrm{Al_6Mn}$

Modelling:

Liquid : Substitutional, Redlich–Kister
cbcc–*A*12 : Substitutional, Redlich–Kister
cub-A13 : Substitutional, Redlich–Kister
fcc–*A*1 : Substitutional, Redlich–Kister
hcp–*A*3 : Substitutional, Redlich–Kister
bcc–*A*2 : see below
bcc–*B*2 : Sublattice model, $(\mathrm{Al,Fe})_{0.5}(\mathrm{Al,Fe})_{0.5}(\square)_3$
Two descriptions of the bcc–*A*2:bcc–*B*2 order-disorder transformation are given: one which includes the parameters of the order and disordered phases in a single description (equation 21 in the thermodynamic modelling chapter), and a second one where the order and disorder contributions are expressed by equation 23. For the second case, the parameters are in a frame.
$\mathrm{Al_5Fe_4}$: Substitutional, Redlich–Kister
$\mathrm{Al_{13}Fe_4}$: Sublattice model , $(\mathrm{Al})_{0.6275}(\mathrm{Fe})_{0.235}(\mathrm{Al},\square)_{0.1375}$
$\mathrm{Al_2Fe}$: Stoichiometric, $(\mathrm{Al})_2(\mathrm{Fe})$
$\mathrm{Al_5Fe_2}$: Stoichiometric, $(\mathrm{Al})_5(\mathrm{Fe})_2$
$\mathrm{Al_{11}Mn_4}$: Stoichiometric, $(\mathrm{Al})_{11}(\mathrm{Mn})_4$
$\mathrm{Al_{12}Mn}$: Stoichiometric, $(\mathrm{Al})_{12}(\mathrm{Mn})$
$\mathrm{Al_6Mn}$: Stoichiometric, $(\mathrm{Al})_6(\mathrm{Mn})$

Assessor and Date:

M. Seierstein, 1991

Comments:

$\mathrm{Al_{11}Mn_4}$, $\mathrm{Al_{12}Mn}$ and $\mathrm{Al_6Mn}$ and the hcp–*A*3 phase have been evaluated by Å. Jansson and T.G.Chart (1995) in the assessment of the Al-Fe-Mn system.

Thermodynamic properties of the solution and compound phases ($J.mol^{-1}$)

Phase fcc–*A*1

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Al,Fe}:\square} = -76066.1 + 18.6758\ T$$

$$L^{1,\mathrm{fcc}-A1}_{\mathrm{Al,Fe}:\square} = 21167.4 + 1.3398\ T$$

Phase hcp–*A*3

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Al,Fe}:\square} = -106903.0 + 20.0\ T$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Al,Fe}} = -91976.5 + 22.1314\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Al,Fe}} = -5672.58 + 4.8728\ T$$

$$L^{2,\mathrm{liquid}}_{\mathrm{Al,Fe}} = 121.9$$

Phase Al_2Fe

$$G^{\circ}(T) - 2.0\ H^{\mathrm{o,fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - H^{\mathrm{o,bcc}-A2,\mathrm{para}}_{\mathrm{Fe}}(298.15\ \mathrm{K}) = -98097.0 + 18.7503\ T + 2.0\ \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Fe}}$$

Phase $Al_{13}Fe_4$

$$G^{\circ}(T) - 0.765\ H^{\mathrm{o,fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 0.235\ H^{\mathrm{o,bcc}-A2,\mathrm{para}}_{\mathrm{Fe}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Fe{:}Al)} = -30714.4 + 7.44\ T + 0.765\ \mathrm{GHSER_{Al}} + 0.235\ \mathrm{GHSER_{Fe}}$$

$$G^{\circ}(T) - 0.6275\ H^{\mathrm{o,fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 0.235\ H^{\mathrm{o,bcc}-A2,\mathrm{para}}_{\mathrm{Fe}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Fe{:}}\square) = -27781.3 + 7.2566\ T + 0.6275\ \mathrm{GHSER_{Al}} + 0.235\ \mathrm{GHSER_{Fe}}$$

Phase Al_5Fe_2

$$G^{\circ}(T) - 5.0\ H^{\mathrm{o,fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 2.0\ H^{\mathrm{o,bcc}-A2,\mathrm{para}}_{\mathrm{Fe}}(298.15\ \mathrm{K}) = -228576 + 48.99503\ T + 5.0\ \mathrm{GHSER_{Al}} + 2.0\ \mathrm{GHSER_{Fe}}$$

Phase $\mathbf{Al_5Fe_4}$

$$G^{\circ}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = 12178.90 - 4.813\ T + \mathrm{GHSER}_{\mathrm{Al}}$$

$$G^{\circ}(T) - H_{\mathrm{Fe}}^{\mathrm{o,bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) = 5009.03 + \mathrm{GHSER}_{\mathrm{Fe}}$$

$$L_{\mathrm{Al,Fe}}^{0,\mathrm{Al_5Fe_4}} = -131649 + 29.4833\ T$$

$$L_{\mathrm{Al,Fe}}^{1,\mathrm{Al_5Fe_4}} = -18619.5$$

Phase bcc–$B2$

$$G^{\circ}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Al{:}\square)} = \mathrm{GBCC}_{\mathrm{Al}}$$

$$G^{\circ}(T) - 0.5\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 0.5\ H_{\mathrm{Fe}}^{\mathrm{o,bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) = \mathrm{G(Fe{:}All{:}\square)} = - 37890.5 + 7.9972\ T + 0.5\ \mathrm{GBCC}_{\mathrm{Al}} + 0.5\ \mathrm{GHSER}_{\mathrm{Fe}}$$

$$T_{\mathrm{c,Fe:Al:\square}}^{\mathrm{bcc}-B2} = 521.5 \qquad \beta_{\mathrm{Fe:Al::\square}}^{\mathrm{bcc}-B2} = 1.11$$

$$G^{\circ}(T) - 0.5\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 0.5\ H_{\mathrm{Fe}}^{\mathrm{o,bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Fe{:}\square)} = - 37890.5 + 7.9972\ T + 0.5\ \mathrm{GBCC}_{\mathrm{Al}} + 0.5\ \mathrm{GHSER}_{\mathrm{Fe}}$$

$$T_{\mathrm{c,Al:Fe:\square}}^{\mathrm{bcc}-B2} = 521.5 \qquad \beta_{\mathrm{c,Al:Fe:\square}}^{\mathrm{bcc}-B2} = 1.11$$

$$G^{\circ}(T) - H_{\mathrm{Fe}}^{\mathrm{o,bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) = \mathrm{G(Fe{:}Fe{:}\square)} = \mathrm{GHSER}_{\mathrm{Fe}}$$

$$T_{\mathrm{c,Fe:Fe:\square}}^{\mathrm{bcc}-B2} = 1043\mathrm{K} \qquad \beta_{\mathrm{c,Al:Fe:\square}}^{\mathrm{bcc}-B2} = 2.22$$

$$L_{\mathrm{Al,Fe:Al:\square}}^{0,\mathrm{bcc}-B2} = L_{\mathrm{Al:Al,Fe:\square}}^{0,\mathrm{bcc}-B2} = -22485.07 + 7.9772\ T$$

$$L_{\mathrm{Al,Fe:Al:\square}}^{1,\mathrm{bcc}-B2} = L_{\mathrm{Al:Al,Fe:\square}}^{1,\mathrm{bcc}-B2} = 368.15$$

$$T_{\mathrm{c,Al,Fe:Al:\square}}^{0,\mathrm{bcc}-B2} = T_{\mathrm{c,Al:Al,Fe:\square}}^{0,\mathrm{bcc}-B2} = 189.0$$

$$T_{\mathrm{c,Al,Fe:Al:\square}}^{1,\mathrm{bcc}-B2} = T_{\mathrm{c,Al:Al,Fe:\square}}^{1,\mathrm{bcc}-B2} = 63.0$$

$$\beta_{\mathrm{Al,Fe:Al:\square}}^{0,\mathrm{bcc}-B2} = \beta_{\mathrm{Al:Al,Fe:\square}}^{0,\mathrm{bcc}-B2} = 0.0$$

$$T_{\mathrm{c,Al,Fe:Fe:\square}}^{0,\mathrm{bcc}-B2} = T_{\mathrm{c,Fe:Al,Fe:\square}}^{0,\mathrm{bcc}-B2} = -189.0$$

$$T_{\mathrm{c,Al,Fe:Fe:\square}}^{1,\mathrm{bcc}-B2} = T_{\mathrm{c,Fe:Al,Fe:\square}}^{1,\mathrm{bcc}-B2} = 63.0$$

$$\beta_{\mathrm{Al,Fe:Fe:\square}}^{0,\mathrm{bcc}-B2} = \beta_{\mathrm{Fe:Al,Fe:\square}}^{0,\mathrm{bcc}-B2} = 0.0$$

$$L_{\mathrm{Fe:Al,Fe:\square}}^{0,\mathrm{bcc}-B2} = L_{\mathrm{Al,Fe:Fe:\square}}^{0,\mathrm{bcc}-B2} = -24694.0 + 7.9772\ T$$

$$L_{\mathrm{Fe:Al,Fe:\square}}^{1,\mathrm{bcc}-B2} = L_{\mathrm{Al,Fe:Fe:\square}}^{1,\mathrm{bcc}-B2} = 368.15$$

$G^{*}_{\mathrm{Al:Fe:\Box}} = -\ 860\ R \qquad (R = 8.31451)$

$L^{0}_{\mathrm{Al,Fe}} = -\ 30740 + 7.9972\ T$

$L^{1}_{\mathrm{Al,Fe}} = 386.15$

Phase bcc–$B2$

$G^{\circ}(T) - H^{\mathrm{o,fcc-}A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) = \mathrm{G(Al:Al:\Box)} = 0.0$

$G^{\circ}(T) - 0.5\ H^{\mathrm{o,fcc-}A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 0.5\ H^{\mathrm{o,fcc-}A1\mathrm{,para}}_{\mathrm{Fe}}(298.15\ \mathrm{K}) = \mathrm{G(Al:Fe:\Box)} = 2.0\ G^{*}_{\mathrm{Al:Fe:\Box}}$

$G^{\circ}(T) - 0.5\ H^{\mathrm{o,fcc-}A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 0.5\ H^{\mathrm{o,fcc-}A1\mathrm{,para}}_{\mathrm{Fe}}(298.15\ \mathrm{K}) = \mathrm{G(Fe:Al:\Box)} = 2.0\ G^{*}_{\mathrm{Al:Fe:\Box}}$

$G^{\circ}(T) - H^{\mathrm{o,fcc-}A1\mathrm{,para}}_{\mathrm{Fe}}(298.15\ \mathrm{K}) = \mathrm{G(Fe:Fe:\Box)} = 0.0$

Phase bcc–$A2$

$L^{0,\mathrm{bcc-}A2}_{\mathrm{Al,Fe:\Box}} = 4.0\ L^{0}_{\mathrm{Al,Fe}}$

$L^{1,\mathrm{bcc-}A2}_{\mathrm{Al,Fe:\Box}} = 8.0\ L^{1}_{\mathrm{Al,Fe}}$

$T^{1,\mathrm{bcc-}A2}_{\mathrm{C,Al,Fe:\Box}} = 504$

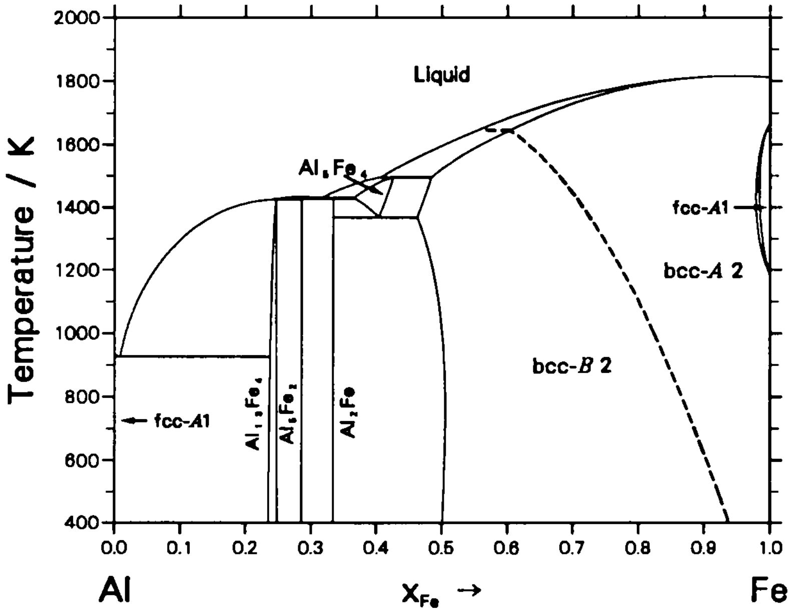


Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Fe}			T / K
$Al_5Fe_4 \rightleftharpoons$ bcc-$B2$ + Al_2Fe	Eutectoid	.403	.462	.333	1368.2
$Al_5Fe_2 \rightleftharpoons$ Liquid	Congruent	.286	.286	....	1434.5
Liquid $\rightleftharpoons Al_5Fe_2 + Al_5Fe_4$	Eutectic	.316	.286	.365	1430.0
Liquid + $Al_5Fe_2 \rightleftharpoons Al_{13}Fe_4$	Peritectic	.242	.286	.247	1424.4
Liquid $\rightleftharpoons$ fcc-$A1$ + $Al_{13}Fe_4$	Eutectic	.009	.000	.237	927.1
Liquid + bcc-$B2 \rightleftharpoons Al_5Fe_4$	Peritectic	.405	.483	.425	1495.5
$Al_5Fe_2 + Al_5Fe_4 \rightleftharpoons Al_2Fe$	Peritectoid	.286	.366	.333	1428.1

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-Fe	(Al)	Cu	*cF4* $Fm\bar{3}m$	M 4	
	(Fe)	Cu	*cF4* $Fm\bar{3}m$	M 4	
	(Fe)	W	*cI2* $Im\bar{3}m$	M 2	
	AlFe	CsCl	*cP2* $Pm\bar{3}m$	M_1 1 M_2 1	
	$AlFe_3$	BiF_3	*cF16* $Fm\bar{3}m$	Al 4 Fe_1 4 Fe_2 8	not considered
	Al_2Fe	Al_2Fe	*aP18* $P1$		
	Al_3Fe		*mC102* $C2/m$		designated by $Al_{13}Fe_4$
	Al_5Fe_2		*oC** $Cmcm$		
	ϵ		*cI16?*		designated by Al_5Fe_4
	Al_6Fe	Al_6Fe	*oC28* $Cmc2_1$	Al_1 4 Al_2 4 Al_3 8 Al_4 8 Fe 4	metastable
	Al_9Fe_2	Al_9Co_2	*mP22* $P2_1/c$		metastable

System Al–Li

Solution Phases:

(stable) : Liquid, bcc–$A2$, fcc–$A1$
(metastable) : hcp–$A3$

Compounds:

(stable) AlLi, Al_2Li_3, Al_4Li_9
(metastable) AlMg–β, Al_2Zr, Al_3Zr, Al_3Zr_2,$Al_{12}Mg_{17}$

Modelling:

bcc–$A2$: Substitutional, Redlich-Kister
fcc–$A1$: Substitutional, Redlich-Kister
hcp–$A3$: Substitutional, Redlich-Kister
Liquid : Substitutional, Redlich-Kister
AlLi : Sublattice model, $(Al,Li)(Li,\square)$
Al_2Li_3 : Stoichiometric, $(Al)_2(Li)_3$
Al_4Li_9 : Stoichiometric, $(Al)_4(Li)_9$
$Al_{12}Mg_{17}$: Sublattice model, $(Li)_{24}(Al,Li)_{10}(Al)_{24}$
Al_2Zr : Sublattice model, $(Al)_2(Zr)$
Al_3Zr : Sublattice model, $(Al)_3(Zr)$
Al_3Zr_2 : Sublattice model, $(Al)_3(Zr)_2$

Assessor and Date:

N. Saunders

Publication:

Calphad, **1**, (3), 237-251 (1977)

Comments:

Data below used to calculate the Al-Li-Mg and Al-Li-Zr systems.

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase hcp–$A3$

$$L^{0,hcp-A3}_{Al,Li:\square} = -27000.0 + 8.0\ T$$

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Al,Li:\square}} = -\ 27000.0 + 8.0\ T$$

$$L^{1,\mathrm{bcc}-A2}_{\mathrm{Al,Li:\square}} = 1.0\mathrm{E}{-06}$$

$$L^{2,\mathrm{bcc}-A2}_{\mathrm{Al,Li:\square}} = 3000.0$$

Phase fcc–$A1$

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Al,Li:\square}} = -\ 27000.0 + 8.0\ T$$

$$L^{1,\mathrm{fcc}-A1}_{\mathrm{Al,Li:\square}} = 1.0\mathrm{E}{-06}$$

$$L^{2,\mathrm{fcc}-A2}_{\mathrm{Al,Li:\square}} = 3000.0 + 0.1\ T$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Al,Li}} = -\ 41500.0 + 20.96\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Al,Li}} = 10000.0 - 5.8\ T$$

$$L^{2,\mathrm{liquid}}_{\mathrm{Al,Li}} = 15902.0 - 9.368\ T$$

$$L^{3,\mathrm{liquid}}_{\mathrm{Al,Li}} = -\ 250.0$$

Phase AlLi

$$G^{\circ}(T) - H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Li}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Li)} = -\ 41300.0 + 16.86\ T + \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Li}}$$

$$G^{\circ}(T) - 2.0\ H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Li}}(298.15\ \mathrm{K}) = \mathrm{G(Li{:}Li)} = 2.0\ \ \mathrm{GHSER_{Li}}$$

$$G^{\circ}(T) - H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}\square)} = 24000.0 + \mathrm{GHSER_{Al}}$$

$$G^{\circ}(T) - H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Li}}(298.15\ \mathrm{K}) = \mathrm{G(Li{:}\square)} = 50000.0 + \mathrm{GHSER_{Li}}$$

$$L^{0,\mathrm{AlLi}}_{\mathrm{Al,Li:Li}} = 20000.0$$

$$L^{1,\mathrm{AlLi}}_{\mathrm{Al,Li:Li}} = -\ 26000.0$$

$$L^{0,\mathrm{AlLi}}_{\mathrm{Al,Li:\square}} = 2000.0$$

$$L^{0,\mathrm{AlLi}}_{\mathrm{Al:Li,\square}} = -\ 24000.0 + 10.0\ T$$

Phase Al_2Li_3

$$\begin{aligned}G^{\circ}(T) - 2.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\mathrm{K}) - 3.0\ H_{\mathrm{Li}}^{\mathrm{o,bcc-}A2}(298.15\ \mathrm{K}) &= \\ - 89640.0 + 32.79\ T + 2.0\ \mathrm{GHSER_{Al}} + 3.0\ \mathrm{GHSER_{Li}}\end{aligned}$$

Phase Al_4Li_9

$$\begin{aligned}G^{\circ}(T) - 4.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 9.0\ H_{\mathrm{Li}}^{\mathrm{o,bcc-}A2}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Li)} &= \\ - 185250.0 + 67.8\ T + 4.0\ \mathrm{GHSER_{Al}} + 9.0\ \mathrm{GHSER_{Li}}\end{aligned}$$

Phase $Al_{12}Mg_{17}$

$$\begin{aligned}G^{\circ}(T) - 34.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 24.0\ H_{\mathrm{Li}}^{\mathrm{o,bcc-}A2}(298.15\ \mathrm{K}) = \mathrm{G(Li{:}Al{:}Al)} &= \\ - 800000 + 405\ T + 34.0\ \mathrm{GHSER_{Al}} + 24.0\ \mathrm{GHSER_{Li}} \\ G^{\circ}(T) - 24.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 34.0\ H_{\mathrm{Li}}^{\mathrm{o,bcc-}A2}(298.15\ \mathrm{K}) = \mathrm{G(Li{:}Li{:}Al)} &= \\ - 750000 + 405\ T + 24.0\ \mathrm{GHSER_{Al}} + 34.0\ \mathrm{GHSER_{Li}}\end{aligned}$$

Phase Al_2Zr

$$\begin{aligned}G^{\circ}(T) - 2.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - H_{\mathrm{Li}}^{\mathrm{o,bcc-}A2}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Li)} &= \\ - 24240 + 16.869\ T + 2.0\ \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Li}}\end{aligned}$$

Phase Al_3Zr

$$\begin{aligned}G^{\circ}(T) - 3.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - H_{\mathrm{Li}}^{\mathrm{o,bcc-}A2}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Li)} &= \\ - 24400 + 16.88\ T + 3.0\ \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Li}}\end{aligned}$$

Phase Al_3Zr_2

$$\begin{aligned}G^{\circ}(T) - 3.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Li}}^{\mathrm{o,bcc-}A2}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Li)} &= \\ - 46625 + 33.25\ T + 3.0\ \mathrm{GHSER_{Al}} + 2.0\ \mathrm{GHSER_{Li}}\end{aligned}$$

Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Li}			T / K
Liquid $\rightleftharpoons$ fcc-$A1$ + AlLi	Eutectic	.256	.155	.462	868.8
Liquid + AlLi $\rightleftharpoons$ Al_2Li_3	Peritectic	.775	.555	.600	793.6
Liquid + Al_2Li_3 $\rightleftharpoons$ Al_4Li_9	Peritectic	.912	.600	.692	607.6
Liquid $\rightleftharpoons$ Al_4Li_9 + bcc-$A2$	Eutectic	.989	.692	.999	447.8
AlLi $\rightleftharpoons$ Liquid	Congruent	.500	.500	....	978.0

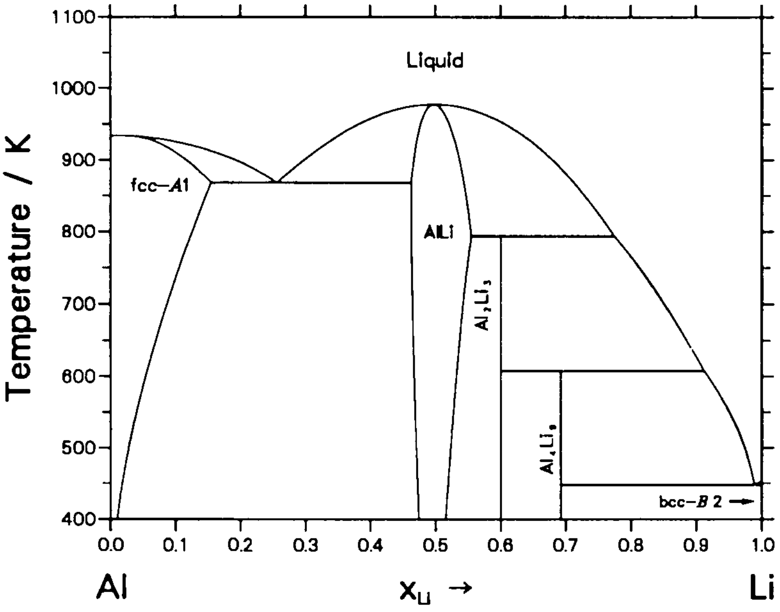


Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-Li	(Al)	Cu	cF4 $Fm\bar{3}m$	M 4	
	(Li)	W	cI2 $Im\bar{3}m$	M 2	
	AlLi	NaTl	cF16 $Fd\bar{3}m$	M_1 8 M_2 8	
	Al_2Li_3	Ga_2Te_3	hR15 $R\bar{3}m$	Al 6 Li_1 3 Li_2 6	
	Al_3Li	$AuCu_3$	cP4 $Pm\bar{3}m$	Al 3 Li 1	metast.
	Al_4Li_9	Al_4Li_9	mC26 C2/m		

System Al–Mg

Version I

Solution Phases:

(stable)	Liquid, fcc–$A1$, hcp–$A3$
(metastable)	bcc-$A2$

Compounds:

(stable)	AlMg-β , AlMg-ϵ , Al-Mg-ζ,$Al_{12}Mg_{17}$
(metastable)	AlLi

Modelling:

Liquid	:	Substitutional, Redlich-Kister
bcc–$A2$	:	Substitutional, Redlich-Kister
fcc–$A1$	:	Substitutional, Redlich-Kister
hcp–$A3$	:	Substitutional, Redlich-Kister
$Al_{12}Mg_{17}$	:	Sublattice model, $Mg_{24}(Al,Mg)_{10}(Al,Mg)_{24}$
AlMg-β	:	Stoichiometric, $(Al)_{0.615}(Mg)_{0.385}$
AlMg-ϵ	:	Stoichiometric, $(Al)_{0.56}(Mg)_{0.44}$
AlMg-ζ	:	Stoichiometric, $(Al)_{0.525}(Mg)_{0.475}$
AlLi	:	Sublattice model $(Al,Mg)(Mg,\square)$

Assessor and Date:

N. Saunders, 1991

Comments:

The data below were used for the thermodynamic assessment of the Al-Li-Mg system in COST507 Round I .

Thermodynamic properties of the solution and compound phases(J.mol^{-1})

Phase AlMg-β

$$G^{\circ}(T) - 0.615\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - 0.385\ H_{\mathrm{Mg}}^{\circ,\mathrm{hcp}-A3}(298.15\ \mathrm{K}) = - 1000.0 - 3.017\ T + 0.615\ \mathrm{GHSER_{Al}} + 0.385\ \mathrm{GHSER_{Mg}}$$

Phase AlMg-ϵ

$$G^{\circ}(T) - 14.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 11.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) =$$
$$-9275.0 - 104.0\ T + 14.0\ \mathrm{GHSER}_{\mathrm{Al}} + 11.0\ \mathrm{GHSER}_{\mathrm{Mg}}$$

Phase AlMg-ζ

$$G^{\circ}(T) - 21.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 19.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) =$$
$$-21040.0 - 163.76\ T + 21.0\ \mathrm{GHSER}_{\mathrm{Al}} + 19.0\ \mathrm{GHSER}_{\mathrm{Mg}}$$

Phase $\mathrm{Al}_{12}\mathrm{Mg}_{17}$

$$G^{\circ}(T) - 34.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 24.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Al{:}Al)} =$$
$$-36800.0 - 140.0\ T + 34.0\ \mathrm{GHSER}_{\mathrm{Al}} + 24.0\ \mathrm{GHSER}_{\mathrm{Mg}}$$

$$G^{\circ}(T) - 24.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 34.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Mg{:}Al)} =$$
$$-123200.0 - 56.26\ T + 24.0\ \mathrm{GHSER}_{\mathrm{Al}} + 34.0\ \mathrm{GHSER}_{\mathrm{Mg}}$$

$$G^{\circ}(T) - 10.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 48.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Al{:}Mg)} =$$
$$151000.0 + 10.0\ \mathrm{GHSER}_{\mathrm{Al}} + 48.0\ \mathrm{GHSER}_{\mathrm{Mg}}$$

$$G^{\circ}(T) - 58.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Mg{:}Mg)} =$$
$$290000 + 58.0\ \mathrm{GHSER}_{\mathrm{Mg}}$$

$$L_{\mathrm{Mg{:}Al,Mg{:}Al}}^{0,\mathrm{Al}_{12}\mathrm{Mg}_{17}} = -17000$$

$$L_{\mathrm{Mg{:}Al,Mg{:}Mg}}^{0,\mathrm{Al}_{12}\mathrm{Mg}_{17}} = -17000$$

Phase AlLi

$$G^{\circ}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}\square)} =$$
$$24000 + \mathrm{GHSER}_{\mathrm{Al}}$$

$$G^{\circ}(T) - H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}\square)} =$$
$$50000 + \mathrm{GBCC}_{\mathrm{Mg}}$$

$$G^{\circ}(T) - 2.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Mg)} =$$
$$2.0\ \mathrm{GBCC}_{\mathrm{Mg}}$$

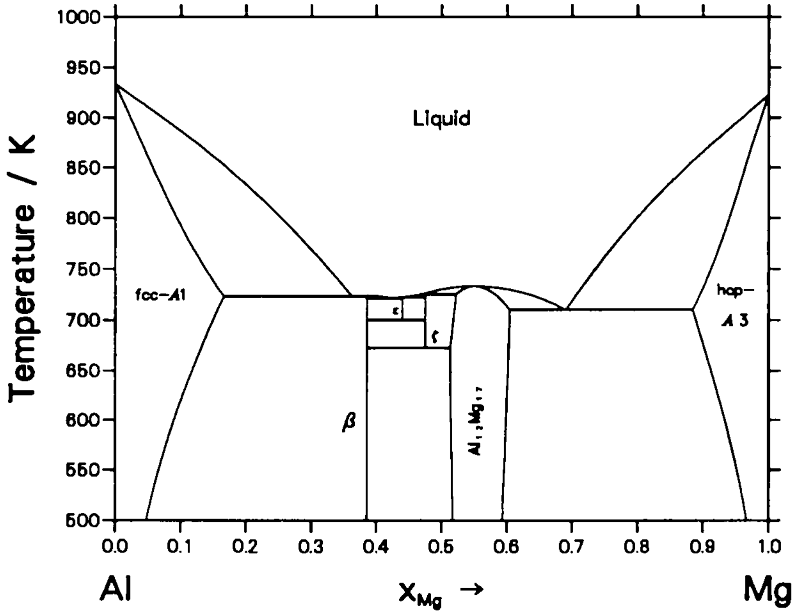
$$G^{\circ}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Mg)} =$$
$$2486 - 1.75\ T + \mathrm{GBCC}_{\mathrm{Al}} + \mathrm{GBCC}_{\mathrm{Mg}}$$

Phase bcc-$A2$

$$L_{\mathrm{Al,Mg{:}\square}}^{0,\mathrm{bcc}-A2} = 4971.0 - 3.5\ T$$

$$L_{\mathrm{Al,Mg{:}\square}}^{1,\mathrm{bcc}-A2} = 900.0 + 0.423\ T$$

$$L_{\mathrm{Al,Mg{:}\square}}^{2,\mathrm{bcc}-A2} = 950.0$$



Phase fcc–$A1$

$$L^{0,\text{fcc}-A1}_{\text{Al,Mg}:\square} = 4971.0 - 3.5\ T$$

$$L^{1,\text{fcc}-A1}_{\text{Al,Mg}:\square} = 900.0 + 0.423\ T$$

$$L^{2,\text{fcc}-A1}_{\text{Al,Mg}:\square} = 950.0$$

Phase hcp–$A3$

$$L^{0,\text{hcp}-A3}_{\text{Al,Mg}:\square} = 1950.0 - 2.0\ T$$

$$L^{1,\text{hcp}-A3}_{\text{Al,Mg}:\square} = 1480.0 - 2.08\ T$$

$$L^{2,\text{hcp}-A3}_{\text{Al,Mg}:\square} = 3500.0$$

Phase liquid

$$L^{0,\text{liquid}}_{\text{Al,Mg}} = -\ 12000.0 + 8.566\ T$$

$$L^{1,\text{liquid}}_{\text{Al,Mg}} = 1894.0 - 3.0\ T$$

$$L^{2,\text{liquid}}_{\text{Al,Mg}} = 2000.0$$

Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Mg}			T / K
Liquid $\rightleftharpoons$ fcc-$A1$ + AlMg-β	Eutectic	.363	.166	.385	723.3
Liquid $\rightleftharpoons$ AlMg-β + AlMg-ϵ	Eutectic	.423	.385	.440	721.5
Liquid + AlMg-ζ $\rightleftharpoons$ + AlMg-ϵ	Peritectic	.436	.475	.440	722.0
Liquid + $Al_{12}Mg_{17}$ $\rightleftharpoons$ AlMg-ζ	Peritectic	.468	.522	.475	725.0
AlMg-ϵ $\rightleftharpoons$ AlMg-β + AlMg-ζ	Eutectoid	.440	.385	.475	700.0
AlMg-ζ $\rightleftharpoons$ AlMg-β + $Al_{12}Mg_{17}$	Eutectoid	.475	.385	.513	673.0
Liquid $\rightleftharpoons$ $Al_{12}Mg_{17}$ + hcp-$A3$	Eutectic	.690	.604	.884	710.0
AlMg-β $\rightleftharpoons$ Liquid	Congruent	.385	.385	....	724.1
$Al_{12}Mg_{17}$ $\rightleftharpoons$ Liquid	Congruent	.556	.556	....	733.3

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-Mg	(Al)	Cu	$cF4$ $Fm\bar{3}m$	M 4	
	(Mg)	Mg	$hP2$ $P6_3/mmc$	M 2	
	$Al_{12}Mg_{17}$	α–Mn cbcc-$A12$	$cI58$ $I\bar{4}3m$	Al 24 Mg_1 2 Mg_2 8 Mg_3 24	γ in Masl
	Al_3Mg_2	Cd_2Na	$cF112$ $Fd\bar{3}m$		$cF1832$ in [91Vil] designated as AlMg-β
	$Al_{30}Mg_{23}$	$Co_5Cr_2Mo_3$ ($Mn_{44}Si_9$)	$hR53$ $R\bar{3}$	Al_1 18 Al_2 18 Al_3 18 Al_4 18 Al_5 18 Mg_1 3 Mg_2 6 Mg_3 6 Mg_4 18 Mg_5 18 Mg_6 18	ϵ
	$Al_{49}Mg_{32}$	$Al_6Mg_{11}Zn_{11}$	$cI162$ $Im\bar{3}$		ζ

System Al–Mg

Version II

Solution Phases:

(stable) Liquid, fcc-$A1$, hcp-$A3$

(metastable) bcc-$A2$,hcp-Zn

Compounds:

(stable) AlMg-β , AlMg-ϵ, AlMg-γ

(metastable) Laves-$C14$, Laves-$C15$, Laves-$C36$, Mg_2Zn_{11}, Mg_2Zn_3, MgZn, φ-phase, τ-phase

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-$A2$: Substitutional, Redlich-Kister
fcc-$A1$: Substitutional, Redlich-Kister
hcp-$A3$: Substitutional, Redlich-Kister
hcp-Zn : Substitutional, Redlich-Kister
AlMg-β : Stoichiometric, $(Al)_{0.615}(Mg)_{0.385}$
AlMg-ϵ : Stoichiometric, $(Al)_{0.56}(Mg)_{0.44}$
MgZn : Stoichiometric, $(Al)_{13}(Mg)_{12}$
Mg2Zn3 : Stoichiometric, $(Al)_3(Mg)_2$
φ-phase : Stoichiometric, $(Al)_5(Mg)_6$
Mg2Zn11 : Stoichiometric, $(Al)_{11}(Mg)_2$
AlMg-γ : Sublattice model, $Mg_5(Al,Mg)_{12}(Al,Mg)_{12}$
Laves-$C14$: Sublattice model $(Al,Mg)_2(Al,Mg)$
Laves-$C15$: Sublattice model $(Al,Mg)_2(Al,Mg)$
Laves-$C36$: Sublattice model $(Al,Mg)_2(Al,Mg)$
τ-phase : Sublattice model $(Mg)_{26}(Al,Mg)_6(Al,Mg)_{48}(Al)$

Assessor and Date:

H.-L. Lukas

Comments:

The data for the Laves-$C15$ phase were evaluated by T. Bühler for the thermodynamic assessment of the Al-Cu-Mg system

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase liquid

$$L^{0,\text{liquid}}_{\text{Al,Mg}} = -12000 + 8.566\ T$$

$$L^{1,\text{liquid}}_{\text{Al,Mg}} = 1894 - 3\ T$$

$$L^{2,\text{liquid}}_{\text{Al,Mg}} = 2000$$

Phase AlMg-β

$$G^{\circ}(T) - 140.0\ H^{\circ,\text{fcc}-A1}_{\text{Al}}(298.15\ \text{K}) - 89.0\ H^{\circ,\text{hcp}-A3}_{\text{Mg}}(298.15\ \text{K}) = -246175 - 675.55\ T + 140.0\ \text{GHSER}_{\text{Al}} + 89.0\ \text{GHSER}_{\text{Mg}}$$

Phase AlMg-ϵ

$$G^{\circ}(T) - 30.0\ H^{\circ,\text{fcc}-A1}_{\text{Al}}(298.15\ \text{K}) - 23.0\ H^{\circ,\text{hcp}-A3}_{\text{Mg}}(298.15\ \text{K}) = -52565.4 - 173.1775\ T + 30.0\ \text{GHSER}_{\text{Al}} + 23.0\ \text{GHSER}_{\text{Mg}}$$

Phase AlMg-γ

$$G^{\circ}(T) - 24.0\ H^{\circ,\text{fcc}-A1}_{\text{Al}}(298.15\ \text{K}) - 5.0\ H^{\circ,\text{hcp}-A3}_{\text{Mg}}(298.15\ \text{K}) = G(\text{Mg:Al:Al}) = 97875 - 101.5\ T + 24.0\ \text{GHSER}_{\text{Al}} + 5.0\ \text{GHSER}_{\text{Mg}}$$

$$G^{\circ}(T) - 12.0\ H^{\circ,\text{fcc}-A1}_{\text{Al}}(298.15\ \text{K}) - 17.0.\ H^{\circ,\text{hcp}-A3}_{\text{Mg}}(298.15\ \text{K}) = G(\text{Mg:Mg:Al}) = -52780 - 50.75\ T + 12.0\ \text{GHSER}_{\text{Al}} + 17.0\ \text{GHSER}_{\text{Mg}}$$

$$G^{\circ}(T) - 12.0\ H^{\circ,\text{fcc}-A1}_{\text{Al}}(298.15\ \text{K}) - 17.0\ H^{\circ,\text{hcp}-A3}_{\text{Mg}}(298.15\ \text{K}) = G(\text{Mg:Al:Mg}) = 284124.6 - 138.069\ T + 12.0\ \text{GHSER}_{\text{Al}} + 17.0\ \text{GHSER}_{\text{Mg}}$$

$$G^{\circ}(T) - 29.0\ H^{\circ,\text{hcp}-A3}_{\text{Mg}}(298.15\text{K}) = G(\text{Mg:Mg:Mg}) = 133469.6 - 87.319\ T + 29.0\ \text{GHSER}_{\text{Mg}}$$

$$L^{0,\text{Al}_{12}\text{Mg}_{17}}_{\text{Mg:Al:Al,Mg}} = 113100 - 14.5\ T$$

$$L^{0,\text{Al}_{12}\text{Mg}_{17}}_{\text{Mg:Mg:Al,Mg}} = 113100 - 14.5\ T$$

Phase fcc-$A1$

$$L^{0,\text{fcc}-A1}_{\text{Al,Mg:}\square} = 4971 - 3.5\ T$$

$$L^{1,\text{fcc}-A1}_{\text{Al,Mg:}\square} = 900 + 0.423\ T$$

$$L^{2,\text{fcc}-A1}_{\text{Al,Mg:}\square} = 950$$

Phase hcp–$A3$

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Al,Mg:\square}} = 1950 - 2\ T$$

$$L^{1,\mathrm{hcp}-A3}_{\mathrm{Al,Mg:\square}} = 1480 - 2.08\ T$$

$$L^{2,\mathrm{hcp}-A3}_{\mathrm{Al,Mg:\square}} = 3500$$

Phase hcp–Zn

$$L^{0,\mathrm{hcp}-Zn}_{\mathrm{Al,Mg:\square}} = 1950 - 2\ T$$

$$L^{1,\mathrm{hcp}-Zn}_{\mathrm{Al,Mg:\square}} = 1480 - 2.08\ T$$

$$L^{2,\mathrm{hcp}-Zn}_{\mathrm{Al,Mg:\square}} = 3500$$

Phase Laves-$C14$

$$G^{\circ}(T) - 3.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Al)} = $$
$$15000 + 3.0\ \mathrm{GHSER_{Al}}$$
$$G^{\circ}(T) - H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 2.0\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Al)} = $$
$$17329 - 16.8\ T + \mathrm{GHSER_{Al}} + 2.0\ \mathrm{GHSER_{Mg}}$$
$$G^{\circ}(T) - 2.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Mg)} = $$
$$12671.1 + 16.8\ T + 2.0\ \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Mg}}$$
$$G^{\circ}(T) - 3.0\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Mg)} = $$
$$15000 + 3.0\ \mathrm{GHSER_{Mg}}$$

$$L^{0,\mathrm{Laves}-C14}_{\mathrm{Al,Mg:Al}} = 15000$$

$$L^{0,\mathrm{Laves}-C14}_{\mathrm{Al:Al,Mg}} = 8000$$

$$L^{0,\mathrm{Laves}-C14}_{\mathrm{Mg:Al,Mg}} = 8000$$

$$L^{0,\mathrm{Laves}-C14}_{\mathrm{Al,Mg:Mg}} = 15000$$

Phase Laves-$C15$

$$G^{\circ}(T) - 3.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Al)} = $$
$$15000 + 3.0\ \mathrm{GHSER_{Al}}$$
$$G^{\circ}(T) - H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 2.0\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Al)} = $$
$$104970.96 - 16.46448\ T + \mathrm{GHSER_{Al}} + 2.0\ \mathrm{GHSER_{Mg}}$$
$$G^{\circ}(T) - 2.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Mg)} = $$
$$30000 + 4.0\ T + 2.0\ \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Mg}}$$
$$G^{\circ}(T) - 3.0\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Mg)} = 15000 + 3.0\ \mathrm{GHSER_{Mg}}$$

$$L^{0,\mathrm{Laves}-C15}_{\mathrm{Al,Mg:Al}} = 15000$$

$$L^{0,\mathrm{Laves}-C15}_{\mathrm{Al:Al,Mg}} = 8000$$

$$L^{0,\mathrm{Laves}-C15}_{\mathrm{Mg:Al,Mg}} = 8000$$

$$L^{0,\mathrm{Laves}-C15}_{\mathrm{Al,Mg:Mg}} = 15000$$

Phase Laves-$C36$

$$G^{\circ}(T) - 3.0\ H^{\mathrm{o,fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) = \mathrm{G(Al:Al)} = \\ 15000 + 3.0\ \mathrm{GHSER_{Al}}$$

$$G^{\circ}(T) - H^{\mathrm{o,fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 2.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Mg:Al)} = \\ 84970.96 - 16.46448\ T + \mathrm{GHSER_{Al}} + 2\ \mathrm{GHSER_{Mg}}$$

$$G^{\circ}(T) - 2.0\ H^{\mathrm{o,fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - H^{\mathrm{o,hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Al:Mg)} = \\ 21734 + 11.02\ T + 2.0\ \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Mg}}$$

$$G^{\circ}(T) - 3.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Mg:Mg)} = \\ 15000 + 3.0\ \mathrm{GHSER_{Mg}}$$

$$L^{0,\mathrm{Laves}-C36}_{\mathrm{Al,Mg:Al}} = 15000$$

$$L^{0,\mathrm{Laves}-C36}_{\mathrm{Al:Al,Mg}} = 8000$$

$$L^{0,\mathrm{Laves}-C36}_{\mathrm{Mg:Al,Mg}} = 8000$$

$$L^{0,\mathrm{Laves}-C36}_{\mathrm{Al,Mg:Mg}} = 15000$$

Phase $\mathrm{Mg_2Zn_{11}}$

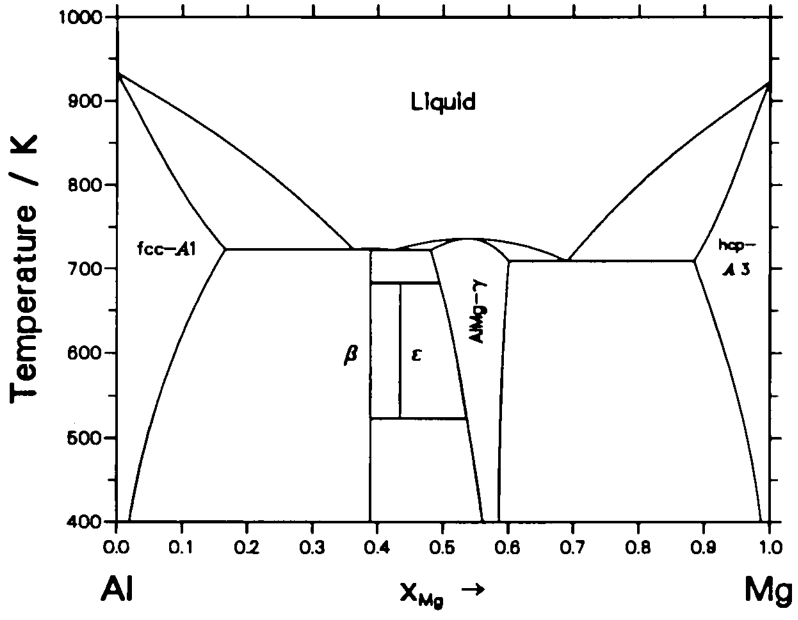
$$G^{\circ}(T) - 11.0\ H^{\mathrm{o,fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 2.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \\ +\ 130000 - 26.0\ T + 11.0\ \mathrm{GHSER_{Al}} + 2.0\ \mathrm{GHSER_{Mg}}$$

Phase $\mathrm{Mg_2Zn_3}$

$$G^{\circ}(T) - 3.0\ H^{\mathrm{o,fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 2.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \\ 1000 - 0.2\ T + 3.0\ \mathrm{GHSER_{Al}} + 2.0\ \mathrm{GHSER_{Mg}}$$

Phase MgZn

$$G^{\circ}(T) - 13.0\ H^{\mathrm{o,fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 12.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \\ -\ 10000 + 2.5\ T + 13.0\ \mathrm{GHSER_{Al}} + 12.0\ \mathrm{GHSER_{Mg}}$$



Phase φ–phase

$$G^\circ(T) - 5.0.\ H^{\circ,fcc-A1}_{Al}(298.15\ K) - 6.0\ H^{\circ,hcp-A3}_{Mg}(298.15\ K) =$$
$$-\ 15400 - 16.5\ T + 5.0\ GHSER_{Al} + 6.0\ GHSER_{Mg}$$

Phase τ–phase

$$G^\circ(T) - 55.0\ H^{\circ,fcc-A1}_{Al}(298.15\ K) - 26.0\ H^{\circ,hcp-A3}_{Mg}(298.15\ K) =$$
$$G(Mg{:}Al{:}Al{:}Al) = -\ 105.3\ T + 55.0\ GHSER_{Al} + 26.0\ GHSER_{Mg}$$

$$G^\circ(T) - 49.0\ H^{\circ,fcc-A1}_{Al}(298.15\ K) - 32.0\ H^{\circ,hcp-A3}_{Mg}(298.15\ K) =$$
$$G(Mg{:}Mg{:}Al{:}Al) = -\ 81000 - 186.3\ T + 49.0\ GHSER_{Al} + 32.0\ GHSER_{Mg}$$

$$G^\circ(T) - 7.0\ H^{\circ,fcc-A1}_{Al}(298.15\ K) - 74.0\ H^{\circ,hcp-A3}_{Mg}(298.15\ K) =$$
$$G(Mg{:}Al{:}Mg{:}Al) = 1053000 + 405\ T + 7.0\ GHSER_{Al} + 74.0\ GHSER_{Mg}$$

$$G^\circ(T) - H^{\circ,fcc-A1}_{Al}(298.15\ K) - 80.0\ H^{\circ,hcp-A3}_{Mg}(298.15\ K) =$$
$$G(Mg{:}Mg{:}Mg{:}Al) = 405000 + 243\ T + GHSER_{Al} + 80.0\ GHSER_{Mg}$$

$$L^{0,\tau-phase}_{Mg:Al:Al,Mg:Al} = -\ 202500 - 40.5\ T$$

$$L^{0,\tau-phase}_{Mg:Mg:Al,Mg:Al} = -\ 202500 - 40.5\ T$$

Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Mg}			T / K
Liquid ⇌ fcc-$A1$ + AlMg-β	Eutectic	.363	.166	.389	723.6
Liquid ⇌ AlMg-β + AlMg-γ	Eutectic	.424	.389	.480	722.7
AlMg-β+ AlMg-γ ⇌ AlMg-ϵ	Peritectoid	.389	.494	.434	682.9
AlMg-ϵ ⇌ AlMg-β + AlMg-γ	Eutectoid	.434	.389	.536	523.2.0
Liquid ⇌ AlMg-γ + hcp-$A3$	Eutectic	.690	.601	.884	709.4
AlMg-β ⇌ Liquid	Congruent	.385	.385	....	724.7
$Al_{12}Mg_{17}$ ⇌ Liquid	Congruent	.523	.523	....	736.3

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-Mg	(Al)	Cu	$cF4$ $Fm\bar{3}m$	M 4	
	(Mg)	Mg	$hP2$ $P6_3/mmc$	M 2	
	AlMg-γ	α-Mn cbcc-$A12$	$cI58$ $I\bar{4}3m$	Al 24 Mg_1 2 Mg_2 8 Mg_3 24	designated as $Al_{12}Mg_{17}$
	Al_3Mg_2	Cd_2Na	$cF112$ $Fd\bar{3}m$		$cF1832$ in [91Vil] designated as AlMg-β
	AlMg-ϵ	$Co_5Cr_2Mo_3$ ($Mn_{44}Si_9$)	$hR53$ $R\bar{3}$	Al_1 18 Al_2 18 Al_3 18 Al_4 18 Al_5 18 Mg_1 3 Mg_2 6 Mg_3 6 Mg_4 18 Mg_5 18 Mg_6 18	R phase in [Masl]

System Al–Mn

Solution Phases:

Liquid, bcc-*A*2, cbcc-*A*12,
cub-*A*13,fcc-*A*1, hcp-*A*3

Stoichiometric Compounds:

(stable) $Al_{11}Mn_4$, Al_6Mn, Al_4Mn, Al_8Mn_5-*D*8_{10}
(metastable) Al_2Fe, Al_5Fe_2, $Al_{13}Fe_4$

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-*A*2 : Substitutional, Redlich-Kister
cbcc-*A*12 : Substitutional, Redlich-Kister
cub-*A*13 : Substitutional, Redlich-Kister
fcc-*A*1 : Substitutional, Redlich-Kister
hcp-*A*3 : Substitutional, Redlich-Kister
Al_8Mn_5 -*D*8_{10} : Sublattice model, $(Al)_{12}(Mn)_4(Al,Mn)_{10}$
Al_2Fe : Stoichiometric, $(Al)_2(Fe)_1$
Al_5Fe_2 : Stoichiometric, $(Al)_5(Fe)_2$
$Al_{13}Fe_4$: Sublattice model, $(Al)_{.6275}(Fe)_{.235}(Al,\square)_{.1375}$

Assessor and Date:

Å. Jansson

Publication:

Trita-Mac-0462, May 1991, Materials Research Center,
The Royal Institute of Technology, Stockholm

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase $Al_{11}Mn_4$

$$G^{\circ}(T) - 11.0\ H_{Al}^{o,fcc-A1}(298.15\ K) - 4.0\ H_{Mn}^{o,cbcc-A12,para}(298.15\ K) = - 354690.0 + 103.031\ T + 11.0\ GHSER_{Al} + 4.0\ GHSER_{Mn}$$

Phase $Al_{12}Mn$

$$G^{\circ}(T) - 12.0\ H_{Al}^{o,fcc-A1}(298.15\ K) - H_{Mn}^{o,cbcc-A12,para}(298.15\ K) = - 125730.0 + 54.98103\ T + 12.0\ GHSER_{Al} + GHSER_{Mn}$$

Phase Al_4Mn

$$G^\circ(T) - 4.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Mn}}^{\mathrm{o,cbcc}-A12,\mathrm{para}}(298.15\ \mathrm{K}) =$$
$$-\ 100005.0 + 30.0\ T + 4.0\ \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Mn}}$$

Phase Al_6Mn

$$G^\circ(T) - 6.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Mn}}^{\mathrm{o,cbcc}-A12,\mathrm{para}}(298.15\ \mathrm{K}) =$$
$$-\ 124561.3 + 53.6593\ T + 6.0\ \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Mn}}$$

Phase $Al_8Mn_5-D8_{10}$

$$G^\circ(T) - 22.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 4.0\ H_{\mathrm{Mn}}^{\mathrm{o,cbcc}-A12,\mathrm{para}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Mn{:}Al)} =$$
$$-\ 308671 + 56.6488\ T + 22.0\ \mathrm{GHSER_{Al}} + 4.0\ \mathrm{GHSER_{Mn}}$$
$$G^\circ(T) - 12.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 14.0\ H_{\mathrm{Mn}}^{\mathrm{o,cbcc}-A12,\mathrm{para}}(298.15\ \mathrm{K}) =$$
$$\mathrm{G(Al{:}Mn{:}Mn)} = -\ 596867 + 94.612\ T + 12.0\ \mathrm{GHSER_{Al}} + 14.0\ \mathrm{GHSER_{Mn}}$$
$$L_{\mathrm{Al:Mn:Al,Mn}}^{0,\mathrm{Al_8Mn_5}-D8_{10}} = -\ 546234 + 387.348\ T$$

Phase Al_2Fe

$$G^\circ(T) - 2.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Mn}}^{\mathrm{o,cbcc}-A12,\mathrm{para}}(298.15\ \mathrm{K}) =$$
$$-\ 14065.0\ T + 2.0\ \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Mn}}$$

Phase Al_5Fe_2

$$G^\circ(T) - 5.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Mn}}^{\mathrm{o,cbcc}-A12,\mathrm{para}}(298.15\ \mathrm{K}) =$$
$$5.0\ \mathrm{GHSER_{Al}} + 2.0\ \mathrm{GHSER_{Mn}}$$

Phase $Al_{13}Fe_4$

$$G^\circ(T) - 0.765\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 0.235\ H_{\mathrm{Mn}}^{\mathrm{o,cbcc}-A12,\mathrm{para}}(298.15\ \mathrm{K}) =$$
$$-20000.0 + 10.0\ T + 0.765\ \mathrm{GHSER_{Al}} + 0.235\ \mathrm{GHSER_{Mn}}$$
$$G^\circ(T) - 0.6275\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 0.235\ H_{\mathrm{Mn}}^{\mathrm{o,cbcc}-A12,\mathrm{para}}(298.15\ \mathrm{K}) =$$
$$-\ 17000.0 + 10.0\ T + 0.6275\ \mathrm{GHSER_{Al}} + 0.235\ \mathrm{GHSER_{Mn}}$$

Phase bcc–$A2$

$$L_{\mathrm{Al,Mn:\square}}^{0,\mathrm{bcc}-A2} = -\ 120077 + 52.851\ T \qquad L_{\mathrm{Al,Mn:\square}}^{1,\mathrm{bcc}-A2} = -\ 40652 + 29.2764\ T$$

Phase cbcc–$A12$

$$L_{\mathrm{Al,Mn:\square}}^{0,\mathrm{cbcc}-A12} = -\ 101410 + 43.0\ T$$

Phase cub–$A13$

$$L_{\mathrm{Al,Mn:\square}}^{0,\mathrm{cub}-A13} = -\ 119022 + 52.507\ T \qquad L_{\mathrm{Al,Mn:\square}}^{1,\mathrm{cub}-A13} = -\ 1763$$

Phase fcc-$A1$

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Al,Mn:\square}} = -69300 + 25.0\ T \qquad L^{1,\mathrm{fcc}-A1}_{\mathrm{Al,Mn:\square}} = 8800$$

Phase hcp-$A3$

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Al,Mn:\square}} = -108066 + 43.83\ T \qquad L^{1,\mathrm{hcp}-A3}_{\mathrm{Al,Mn:\square}} = -54519.8 + 40\ T$$

Phase liquid

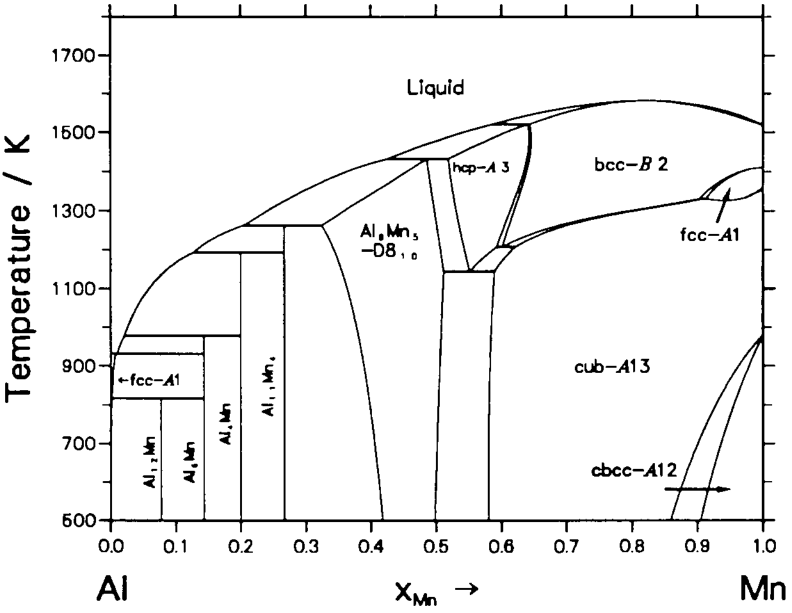
$$L^{0,\mathrm{liquid}}_{\mathrm{Al,Mn}} = -66174 + 27.0988\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Al,Mn}} = -7509 + 5.4836\ T$$

$$L^{2,\mathrm{liquid}}_{\mathrm{Al,Mn}} = -2639$$

Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Mn}			T / K
Liquid + $Al_4Mn \rightleftharpoons Al_6Mn$	Peritectic	.021	.200	.143	978.0
Liquid $\rightleftharpoons$ fcc-A1 + Al_6Mn	Eutectic	.010	.007	.143	931.1
fcc-A1 + $Al_6Mn \rightleftharpoons Al_{12}Mn$	Peritectoid	.002	.143	.077	817.0
Liquid + $Al_{11}Mn_4 \rightleftharpoons Al_4Mn$	Peritectic	.127	.266	.200	1193.1
Liquid + Al_8Mn_5-$D8_{10} \rightleftharpoons Al_{11}Mn_4$	Peritectic	.205	.324	.266	1262.4
Liquid + hcp-A3 $\rightleftharpoons$ Al_8Mn_5-$D8_{10}$	Peritectic	.425	.519	.486	1433.3
hcp-A3 $\rightleftharpoons$ Al_8Mn_5-$D8_{10}$ + cub-A13	Eutectoid	.551	.511	.590	1143.7
bcc-A2 $\rightleftharpoons$ hcp-A3 + cub-A13	Eutectoid	.601	.592	.621	1207.0
fcc-A1 + bcc-A2 $\rightleftharpoons$ cub-A13	Pertitectoid	.913	.903	.910	1330.9
Liquid + bcc-A2 $\rightleftharpoons$ hcp-A3	Peritectic	.588	.644	.641	1522.3
bcc-A2 $\rightleftharpoons$ Liquid	Congruent	.816	.816	....	1582.0


Temperature / K
1700
1500
1300
1100
900
700
500
Liquid
hcp-A3
bcc-B2
Al8Mn5
-D8₁₀
fcc-A1
←fcc-A1
cub-A13
cbcc-A12
Al12Mn
Al6Mn
Al4Mn
Al11Mn4
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
Al
xMn →
Mn

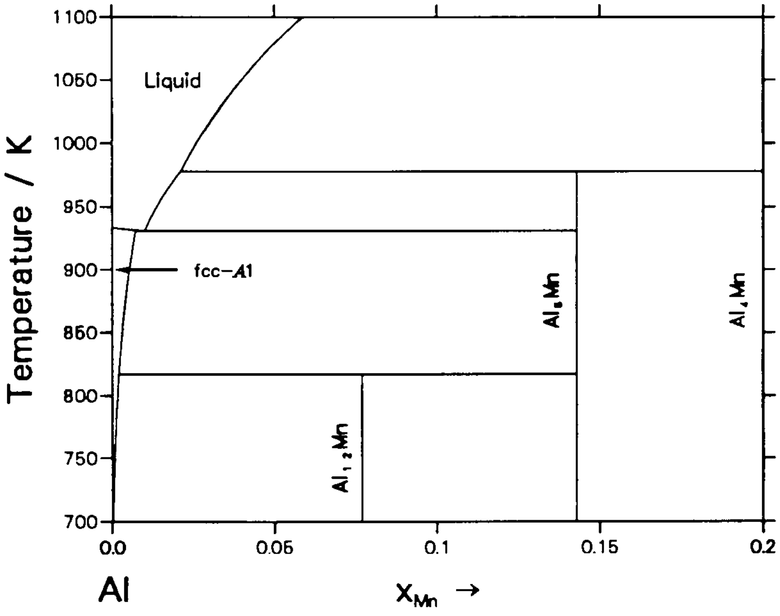

Temperature / K
1100
1050
1000
950
900
850
800
750
700
Liquid
fcc-A1
Al6Mn
Al4Mn
Al12Mn
0.0
0.05
0.1
0.15
0.2
Al
xMn →

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-Mn	(Al)	Cu	$cF4$ $Fm\bar{3}m$	M_1 4	
	α-Mn	α-Mn	$c58$ $I\bar{4}3m$		cbcc-$A1$
	β-Mn	β-Mn	$cP20$ $P4_132$		cub-$A13$
	γ-Mn	Cu	$cF4$ $Fm3m$		fcc-$A1$
	δ-Mn	W	$cI2$ $Im\bar{3}m$		bcc-$A2$
	AlMn	AuCu-$L1_0$	$tP2$ $P4/mmm$	M_1 1 M_2 1	metast.
	λ	Al_4Mn	$oP60$ $Pnnn$		reported as Al_4Mn
	Al_6Mn	Al_6Mn	$oC28$ $Cmcm$	Al_1 8 Al_2 8 Al_3 8 Mn 4	
	$Al_{10}Mn_3$	Al_5Mn_2	$hP28$ $P6_3/mmc$	Al_1 2 Al_2 6 Al_3 12 Mn 6	
	$Al_{11}Mn_4$-L	$Al_{11}Mn_4$	$aP30$ $P\bar{1}$		transformation not taken into account reported as $aP15$ in [91Vil]
	$Al_{11}Mn_4$-H	.....	$oP160$ $Pnma$		not in [90Mas] metast.
	$Al_{12}Mn$	$Al_{12}W$	$cI26$ $Im\bar{3}$		not quoted in [90Mas] metast.
	Al_8Mn_5	Al_8Cr_5	$hR26$ $R3m$		Al_8Mn_5-$D0_8$

System Al-Mo

Solution Phases:

(stable)	Liquid, bcc-$A2$, fcc-$A1$
(metastable)	bcc-$B2$, hcp-$A3$

Compounds:

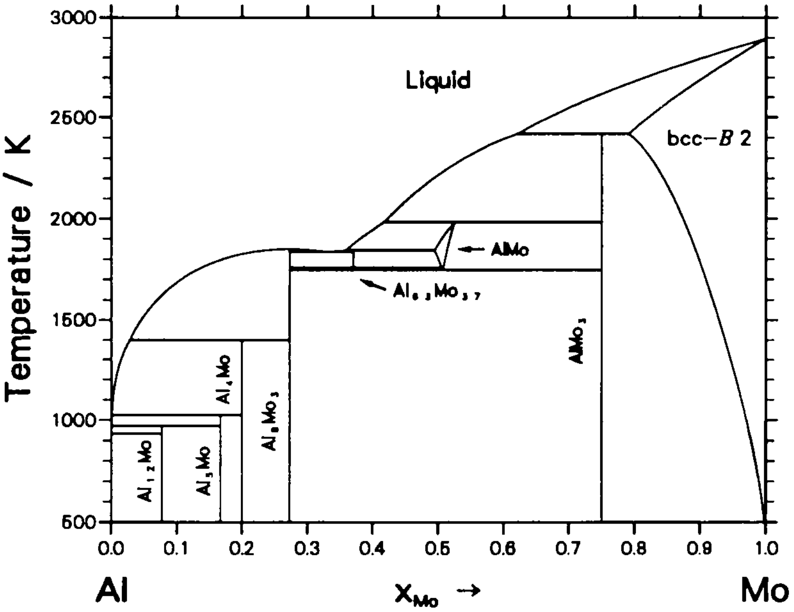
(stable)	$Al_{12}Mo$, Al_4Mo, Al_5Mo, $Al_{63}Mo_{37}$, Al_8Mo_3, AlMo, cub-$A15$
(metastable)	AlM-$D0_{19}$, AlTi-$L1_0$

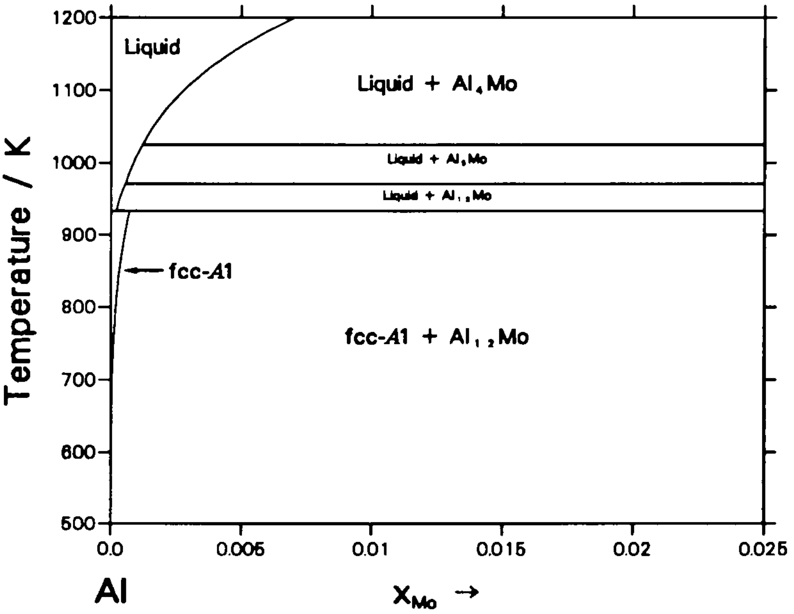
Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-$A2$: Substitutional, Redlich-Kister
fcc-$A1$: Substitutional, Redlich-Kister
hcp-$A3$: Substitutional, Redlich-Kister
$Al_{12}Mo$: Stoichiometric, $(Al)_{12}(Mo)$
Al_5Mo : Stoichiometric, $(Al)_5(Mo)$
Al_4Mo : Stoichiometric, $(Al)_4(Mo)$
$Al_{63}Mo_{37}$: Stoichiometric, $(Al)_{63}(Mo)_{37}$
Al_8Mo_3 : Stoichiometric, $(Al)_8(Mo)_3$
cub-$A15$: Stoichiometric, $(Al)(Mo)_3$
AlMo : Sublattice model, (Al,Mo)(Al,Mo)
bcc-$B2$: Sublattice model, $(Al,Mo)_{0.5}(Al,Mo)_{0.5}(\square)_3$
The thermodynamic description of the bcc-B2 takes into account the ordering reaction bcc-$A2$ $\rightleftharpoons$ bcc-$B2$.
Two descriptions are given:
one using equations 23 and 27,
the other using equations 23 and 28.
For the latter, the parameters are given in a frame.
AlM-$D0_{19}$: Sublattice model, $(Al,Mo)_3(Al,Mo)(\square)_{0.5}$
AlTi-$L1_0$: Sublattice model, (Al,Mo)(Al,Mo)

Assessor and Date:

N. Saunders (1996)


Liquid
bcc-B 2
AlMo
Al8Mo3
Al63Mo37
AlMo3
Al4Mo
Al12Mo
Al5Mo
Temperature / K
3000
2500
2000
1500
1000
500
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
Al
XMo →
Mo


Liquid
Liquid + Al4Mo
Liquid + Al5Mo
Liquid + Al12Mo
fcc-A1
fcc-A1 + Al12Mo
Temperature / K
1200
1100
1000
900
800
700
600
500
0.0
0.005
0.01
0.015
0.02
0.025
Al
XMo →

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase $Al_{12}Mo$

$$G^\circ(T) - 12.0\ H_{Al}^{o,fcc-A1}(298.15\ K) - H_{Mo}^{o,bcc-A2}(298.15\ K) =$$
$$-\ 139100 + 26.975\ T + 12.0\ GHSER_{Al} + GHSER_{Mo}$$

Phase Al_4Mo

$$G^\circ(T) - 4.0\ H_{Al}^{o,fcc-A1}(298.15\ K) - H_{Mo}^{o,bcc-A2}(298.15\ K) =$$
$$-\ 137570 + 29.69\ T + 4.0\ GHSER_{Al} + GHSER_{Mo}$$

Phase Al_5Mo

$$G^\circ(T) - 5.0\ H_{Al}^{o,fcc-A1}(298.15\ K) - H_{Mo}^{o,bcc-A2}(298.15\ K) =$$
$$-139104 + 30.156\ T + 5.0\ GHSER_{Al} + GHSER_{Mo}$$

Phase $Al_{63}Mo_{37}$

$$G^\circ(T) - 63.0\ H_{Al}^{o,fcc-A1}(298.15\ K) - 37.0\ H_{Mo}^{o,bcc-A2}(298.15\ K) =$$
$$-\ 2268100 + 167.2\ T + 63.0\ GHSER_{Al} + 37.0\ GHSER_{Mo}$$

Phase Al_8Mo_3

$$G^\circ(T) - 8.0\ H_{Al}^{o,fcc-A1}(298.15\ K) - 3.0\ H_{Mo}^{o,bcc-A2}(298.15\ K) =$$
$$-\ 412500 + 105.05\ T + 8.0\ GHSER_{Al} + 3.0\ GHSER_{Mo}$$

Phase cub–$A15$

$$G^\circ(T) - H_{Al}^{o,fcc-A1}(298.15\ K) - 3.0\ H_{Mo}^{o,bcc-A2}(298.15\ K) =$$
$$-\ 89000 + 20\ T - 0.003\ T^2 + GHSER_{Al} + 3.0\ GHSER_{Mo}$$

Phase AlMo

$$G^\circ(T) - 2.0\ H_{Al}^{o,fcc-A1}(298.15\ K) = G(Al{:}Al) =$$
$$2.0\ GBCC_{Al}$$
$$G^\circ(T) - H_{Al}^{o,fcc-A1}(298.15\ K) - H_{Mo}^{o,bcc-A2}(298.15\ K) = G(Al{:}Mo) =$$
$$-\ 36850 + T + GHSER_{Al} + GHSER_{Mo}$$
$$G^\circ(T) - H_{Al}^{o,fcc-A1}(298.15\ K) - H_{Mo}^{o,bcc-A2}(298.15\ K) = G(Mo{:}Al) =$$
$$-\ 36850 + T + GHSER_{Al} + GHSER_{Mo}$$
$$G^\circ(T) - 2.0\ H_{Mo}^{o,bcc-A2}(298.15\ K) = G(Mo{:}Mo) =$$
$$2.0\ + GHSER_{Mo}$$

$$L^{0,\mathrm{AlMo}}_{\mathrm{Al,Mo:Al}} = L^{0,\mathrm{AlMo}}_{\mathrm{Al:Al,Mo}} = -\ 5000$$

$$L^{0,\mathrm{AlMo}}_{\mathrm{Mo:Al,Mo}} = L^{0,\mathrm{AlMo}}_{\mathrm{Al,Mo:Mo}} = 25000$$

$$L^{1,\mathrm{AlMo}}_{\mathrm{Mo:Al,Mo}} = L^{1,\mathrm{AlMo}}_{\mathrm{Al,Mo:Mo}} = -\ 10000$$

Phase AlM–$D0_{19}$

$$G^{\circ}(T) - 4.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Al)} = 4.0\ \mathrm{GHCP_{Al}}$$

$$G^{\circ}(T) - H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 3.0\ H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Mo}}(298.15\ \mathrm{K}) = \mathrm{G(Mo{:}Al)} = -\ 64000 + 15.32\ T + \mathrm{GHCP_{Al}} + 3.0\ \mathrm{GHCP_{Mo}}$$

$$G^{\circ}(T) - 3.0\ \mathrm{GHCP_{Al}} - H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Mo}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Mo)} = -\ 64000 + 15.32\ T + 3.0\ \mathrm{GHCP_{Al}} + \mathrm{GHCP_{Mo}}$$

$$G^{\circ}(T) - 4.0\ H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Mo}}(298.15\ \mathrm{K}) = \mathrm{G(Mo{:}Mo)} = 4.0\ \mathrm{GHSER_{Mo}}$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Al,Mo}} = -\ 100000 + 35\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Al,Mo}} = -\ 15000 + 6.3\ T$$

Phase fcc–$A1$

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Al,Mo:}\square} = -\ 92220 + 20\ T$$

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Al,Mo:}\square} = -\ 75000 + 25\ T$$

Phase bcc–$B2$

$$G^{\circ}(T) - H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Al{:}}\square) = 0.0$$

$$G^{\circ}(T) - 0.5\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 0.5\ H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Mo}}(298.15\ \mathrm{K}) = \mathrm{G(Mo{:}Al{:}}\square) = -\ 7050 + T$$

$$G^{\circ}(T) - 0.5\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 0.5\ H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Mo}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Mo{:}}\square) = -\ 7050 + T$$

$$G^{\circ}(T) - H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Mo}}(298.15\ \mathrm{K}) = \mathrm{G(Mo{:}Mo{:}}\square) = 0.0$$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Al:Al,Mo:}\square} = 7050 - T$$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Mo:Al,Mo:}\square} = 7050 - T$$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Al,Mo:Al:}\square} = 7050 - T$$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Al,Mo:Al:}\square} = 7050 - T$$

Phase bcc–$B2$

$$G^{*}_{\mathrm{Al:Mo:\square}} = -\ 7050 + T$$

$$G^{\circ}(T) - {}^{\mathrm{o,fcc-}A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) = \mathrm{G(Al:Al:\square)} = 0.0$$

$$G^{\circ}(T) - 0.5\ H^{\mathrm{o,fcc-}A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 0.5\ H^{\mathrm{o,bcc-}A2}_{\mathrm{Mo}}(298.15\ \mathrm{K}) = \mathrm{G(Al:Mo:\square)} = 2.0\ \ \mathrm{G}^{*}_{\mathrm{Al:Mo:\square}}$$

$$G^{\circ}(T) - 0.5\ H^{\mathrm{o,fcc-}A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - 0.5\ H^{\mathrm{o,bcc-}A2}_{\mathrm{Mo}}(298.15\ \mathrm{K}) = \mathrm{G(Mo:Al:\square)} = 2.0\ \ \mathrm{G}^{*}_{\mathrm{Al:Mo:\square}}$$

$$G^{\circ}(T) - H^{\mathrm{o,bcc-}A2}_{\mathrm{Mo}}(298.15\ \mathrm{K}) = \mathrm{G(Mo:Mo:\square)} = 0.0$$

Phase bcc–$A2$

$$L^{\mathrm{0,bcc-}A2}_{\mathrm{Al,Mo:\square}} = -\ 75000 + 25\ \ T$$

Phase hcp–$A3$

$$L^{\mathrm{0,hcp-}A3}_{\mathrm{Al,Mo:\square}} \quad = \quad -\ 85570 + 25\ \ T$$

Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Mo}			T / K
AlMo $\rightleftharpoons$ $\mathrm{Al_8Mo_3}$ + cub–$A15$	Eutectoid	.507	.273	.750	1745.6
$\mathrm{Al_{63}Mo_{37}}$ $\rightleftharpoons$ $\mathrm{Al_8Mo_3}$ + AlMo	Eutectoid	.370	.273	.505	1759.6
Liquid $\rightleftharpoons$ $\mathrm{Al_8Mo_3}$ + $\mathrm{Al_{63}Mo_{37}}$	Eutectic	.333	.273	.370	1836.4
Liquid + AlMo $\rightleftharpoons$ $\mathrm{Al_{63}Mo_{37}}$	Peritectic	.358	.4955	.370	1844.7
Liquid + cub–$A15$ $\rightleftharpoons$ AlMo	Peritectic	.417	.750	.525	1983.6
Liquid + bcc–$A2$ $\rightleftharpoons$ cub–$A15$	Peritectic	.621	.791	.750	2418.9
Liquid + $\mathrm{Al_4Mo}$ $\rightleftharpoons$ $\mathrm{Al_5Mo}$	Peritectic	.0012	.200	.166	1025.2
Liquid + $\mathrm{Al_5Mo}$ $\rightleftharpoons$ $\mathrm{Al_{12}Mo}$	Peritectic	.0005	.167	.077	971.6
Liquid + $\mathrm{Al_{12}Mo}$ $\rightleftharpoons$ fcc–$A1$	Peritectic	.0002	.077	.0007	933.8
Liquid + $\mathrm{Al_8Mo_3}$ $\rightleftharpoons$ $\mathrm{Al_4Mo}$	Peritectic	.028	.273	.200	1397.7
$\mathrm{Al_8Mo_3}$ $\rightleftharpoons$ Liquid	Congruent	.273	.273	...	1850.5

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-Mo	(Al)	Cu	*cF4* $Fm\bar{3}m$	M 4	
	(Mo)	W	*cI2* $Im\bar{3}m$	M 2	
	$Al_{12}Mo$	$Al_{12}W$	*cI26* $Im\bar{3}$	Al 24 Mo 2	
	Al_5Mo	Al_5W	*hP12* $P6_3$		
	Al_4Mo	Al_4W	*mC30* *Cm*	Al_1 2 Al_2 2 Mo_1 2 Al_3 4 Al_4 4 Al_5 4 Al_6 4 Al_7 4 Mo_2 4	
	Al_8Mo_3	Al_8Mo_3	*mC22* *C2/m*	Mo_1 2 Al_1 48 Al_2 4 Al_3 4 Al_4 4 Mo_2 4	
	$Al_{23}V_4$	$Al_{23}V_4$	*hP54* $P6_3/mmc$		
	$Al_{63}Mo_{37}$				
	AlMo	W	*cI2* $Im\bar{3}m$	M 2	
	$AlMo_3$	Cr_3Si	*cP8* $Pm\bar{3}n$	Al 2 Mo 6	cub-*A15*

System Al–N

Solution Phases:

(stable)	Liquid, fcc–*A*1
(metastable)	bcc–*A*2, hcp–*A*3

Compound:

AlN

Modelling:

Liquid	:	Substitutional, Redlich–Kister
bcc–*A*2	:	Sublattice model, (Al)(C,□)$_3$
fcc–*A*1	:	Sublattice model, (Al)(C,□)
hcp–*A*3	:	Sublattice model, (Al)(C,□)$_{0.5}$
gas	:	ideal (Al,Al2,N,N_2,N_3)
AlN	:	Stoichiometric, (Al)(N)

Assessor and Date:

H.L. Lukas 1992
Data relative for the bcc–*A*2 and hcp–3 phases were evaluated by R. Fetzer and K. Zeng for the Al-N-Ti system.

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase AlN

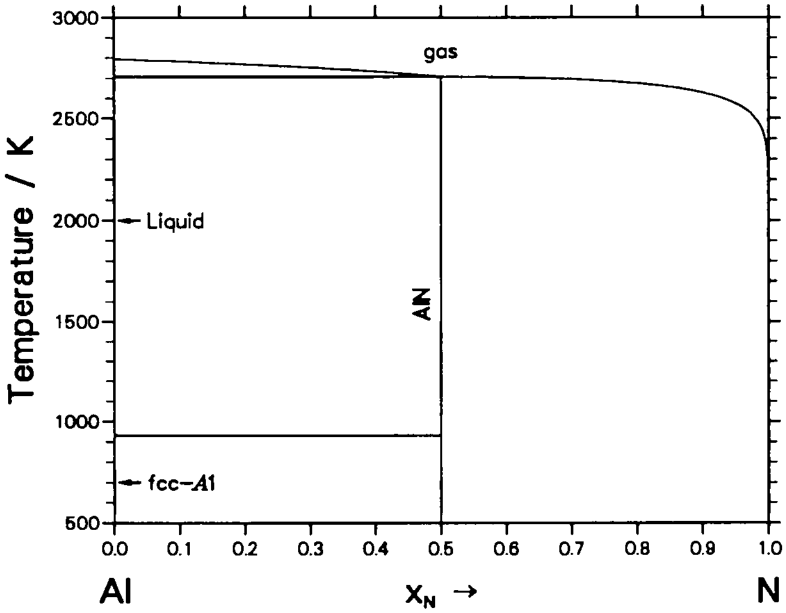
$$G^{\circ}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 2.0\ H_{0.5\mathrm{N}_2}^{\mathrm{o,gas}}(298.15\ \mathrm{K}) = - 338005.5 + 305.211\ T - 46.94867\ T\cdot \ln T - 0.00189068\ T^2 + 874528\ T^{-1} + 1.3756\mathrm{E}{-07}\ T^3$$

Phase bcc–*A*2

$$G^{\circ}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 3.0\ H_{0.5\mathrm{N}_2}^{\mathrm{o,gas}}(298.15\ \mathrm{K}) = 23000 + 10\ T + \mathrm{GHSER}_{\mathrm{Al}} + 3.0\ \mathrm{GHSER}_{\mathrm{N}}$$

Phase fcc–*A*1

$$G^{\circ}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - H_{0.5\mathrm{N}_2}^{\mathrm{o,gas}}(298.15\ \mathrm{K}) = 80\ T + \mathrm{GHSER}_{\mathrm{Al}} + \mathrm{GHSER}_{\mathrm{N}}$$



Phase hcp-$A3$

$$\begin{aligned} G^{\circ}(T) - H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - 0.5\ H_{0.5\mathrm{N}_2}^{\circ,\mathrm{gas}}(298.15\ \mathrm{K}) &= \\ 80000\ T + \mathrm{GHSER}_{\mathrm{Al}} + 0.5\ \mathrm{GHSER}_{\mathrm{N}} \end{aligned}$$

Phase liquid

$$L_{\mathrm{Al,N}}^{0,\mathrm{liquid}} = -\ 336826.61 + 103.22478\ T$$

Phase gas(Al,Al$_2$,N,N$_2$,N$_3$) (P = 0.1 MPa)

$$G_{\mathrm{Al}}^{\circ,\mathrm{gas}}(T) - H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) = RT\ \ln P +$$

$$\begin{array}{lcrl} 298.15 & < T < & 4300.00 & : 323947.58 - 25.1480948\ T - 20.859\ T\cdot\ln T \\ & & & \quad + 4.5665\mathrm{E}{-05}\ T^2 - 3.942\mathrm{E}{-09}\ T^3 - 24275.5\ T^{-1} \\ 4300.00 & < T < & 8200.00 & : 342017.234 - 54.0526114\ T - 17.7891\ T\cdot\ln T \\ & & & \quad + 6.822\mathrm{E}{-05}\ T^2 - 1.9111\mathrm{E}{-08}\ T^3 \\ & & & \quad - 14782200\ T^{-1} \\ 8200.00 & < T < & 10000.00 & : 542396.07 - 411.214335\ T + 22.2419\ T\cdot\ln T \\ & & & \quad - 0.00349619\ T^2 + 4.0491\mathrm{E}{-08}\ T^3 \\ & & & \quad - 2.0366965\mathrm{E}{+08}\ T^{-1} \end{array}$$

$$G^{\mathrm{o,gas}}_{\mathrm{Al}_2}(T) - 2.0\ H^{\mathrm{o,fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) = RT\ \ln P +$$

$$\begin{array}{rcrcl}
298.15 & < T < & 900.00 & : & 496408.232 + 35.4797382\ T - 41.6397\ T\cdot\ln T \\
 & & & & + 0.00249636\ T^2 - 4.9050\mathrm{E}{-07}\ T^3 \\
 & & & & + 85390.3\ T^{-1} \\
900.00 & < T < & 10000.00 & : & + 497613.221 + 17.3681302\ T - 38.85476\ T\cdot\ln T \\
 & & & & - 2.249805\mathrm{E}{-04}\ T^2 - 9.49003167\mathrm{E}{-09}\ T^3 \\
 & & & & - 5287.23\ T^{-1}
\end{array}$$

$$G^{\mathrm{o,gas}}_{\mathrm{N}}(T) - H^{\mathrm{o,gas}}_{0.5\mathrm{N}_2}(298.15\ \mathrm{K}) = RT\ \ln P +$$

$$\begin{array}{rcrcl}
298.15 & < T < & 2950.00 & : & 466446.153 + 2788.78662\ T^{-1} - 13.2660528\ T \\
 & & & & - 20.8939295\ T\cdot\ln T + 8.4552092\mathrm{E}{-05}\ T^2 \\
 & & & & - 1.00186856\mathrm{E}{-08}\ T^3 \\
2950.00 & < T < & 6000.00 & : & 481259.023 - 7559107.28\ T^{-1} - 52.4348889\ T \\
 & & & & - 16.3761342\ T\cdot\ln T - 2.28373808\mathrm{E}{-04}\ T^2 \\
 & & & & - 2.78997209\mathrm{E}{-08}\ T^3
\end{array}$$

$$G^{\mathrm{o,gas}}_{\mathrm{N}_2}(T) - 2.0\ H^{\mathrm{o,gas}}_{0.5\mathrm{N}_2}(298.15\ \mathrm{K}) = 2.0\ \mathrm{GHSER}_{\mathrm{N}} + RT\ \ln P$$

$$G^{\mathrm{o,gas}}_{\mathrm{N}_3}(T) - 3.0\ H^{\mathrm{o,gas}}_{0.5\mathrm{N}_2}(298.15\ \mathrm{K}) = RT\ \ln P +$$

$$\begin{array}{rcrcl}
298.15 & < T < & 800.00 & : & 403075.636 - 14.3245228\ T - 29.5595416\ \mathrm{T}\cdot\ln T \\
 & & & & - 0.02413122\ T^2 + 3.6156036\mathrm{E}{-06}\ T^3 \\
 & & & & + 55714.144\ T^{-1} \\
800.00 & < T < & 2000.00 & : & 388937.207 + 158.809275\ T - 55.404528\ \mathrm{T}\cdot\ln T \\
 & & & & - 0.0026570492\ T^2 + 1.9365644\mathrm{E}{-07}\ T^3 \\
 & & & & + 1536448.48\ T^{-1} \\
2000.00 & < T < & 6000.00 & : & 380898.006 + 210.207464\ T - 62.295576\ \mathrm{T}\cdot\ln T \\
 & & & & + 6.5726456\mathrm{E}{-06}\ T^2 - 7.868012\mathrm{E}{-10}\ T^3 \\
 & & & & + 3336949.2\ T^{-1}
\end{array}$$

Table I - Invariant Reactions.

Reaction	Type	Compositions x_{N}			T / K
Liquid ⇌ fcc-$A1$ + AlN	Degenerate	.000	.000	.500	933.3
Liquid + gas ⇌ AlN	Peritectic-like	.001	.503	.500	2707.7

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Comments
Al-N	(Al)	Cu	$cF4$ $Fm\bar{3}m$	
	AlN	ZnS	$hP4$ $P6_3mc$	Wurtzite

System Al-Nb

Solution Phases:

(stable)	Liquid, bcc–*A*2, fcc–*A*1
(metastable)	bcc–*B*2, hcp–*A*3

Compounds :

(stable)	AlM-$D0_{22}$, σ, $AlNb_3$–*A*15
(metastable)	AlTi-$L1_0$,AlM-$D0_{19}$

Modelling:

Liquid : Substitutional, Redlich-Kister

bcc–*A*2 : Substitutional, Redlich-Kister

fcc–*A*1 : Substitutional, Redlich-Kister

hcp–*A*3 : Substitutional, Redlich-Kister

bcc–*B*2 : Sublattice model, $(Al,Nb)_{0.5}(Al,Nb)_{0.5}(\square)_3$
The thermodynamic description of the bcc–B2 takes into account the ordering reaction bcc–*A*2 $\rightleftharpoons$ bcc–*B*2.
Two descriptions are given:
one using equations 23 and 27,
the other using equations 23 and 28.
For the latter, the parameters are given in a frame.

AlM-$D0_{22}$: Sublattice model, $(Al)_3(Nb)$

$AlNb_3$–*A*15 : Sublattice model, $(Al,Nb)(Nb)_3$

σ : Sublattice model , $(Al)_8(Nb)_4(Al,Nb)_{18}$

AlTi-$L1_0$: Sublattice model, (Al)(Nb)

AlM-$D0_{19}$: Sublattice model, $(Al,Nb)_3(Al,Nb)(\square)$

Assessor and Date:

N. Saunders, 1997.

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase AlM–$D0_{22}$

$$G^\circ(T) - 3.0\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) = -136000 + 24\ T + 3.0\ \mathrm{GHSER}_{\mathrm{Al}} + \mathrm{GHSER}_{\mathrm{Nb}}$$

Phase AlM–$D0_{19}$

$$G^\circ(T) - 4.0\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Al{:}\square)} = 4.0\ \mathrm{GHCP}_{\mathrm{Al}}$$

$$G^\circ(T) - 3.0\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Nb}}^{\circ,\mathrm{bcc}-A2}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Nb{:}\square)} = -98000 + 22\ T + 3.0\ \mathrm{GHCP}_{\mathrm{Al}} + \mathrm{GHCP}_{\mathrm{Nb}}$$

$$G^\circ(T) - H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Nb}}^{\circ,\mathrm{bcc}-A2}(298.15\ \mathrm{K}) = \mathrm{G(Nb{:}Al{:}\square)} = -98000 + 10\ T + \mathrm{GHCP}_{\mathrm{Al}} + 3.0\ \mathrm{GHCP}_{\mathrm{Nb}}$$

$$G^\circ(T) - 4.0\ H_{\mathrm{Nb}}^{\circ,\mathrm{bcc}-A2}(298.15\ \mathrm{K}) = \mathrm{G(Nb{:}Nb{:}\square)} = 4.0\ \mathrm{GHCP}_{\mathrm{Nb}}$$

$$L^{0,\mathrm{AlM-D0_{19}}}_{\mathrm{Al,Nb:Al:\square}} = -137400 + 60\ T$$

$$L^{0,\mathrm{AlM-D0_{19}}}_{\mathrm{Al:Al,Nb:\square}} = -45760 + 20\ T$$

$$L^{0,\mathrm{AlM-D0_{19}}}_{\mathrm{Nb:Al,Nb:\square}} = 4000$$

$$L^{0,\mathrm{AlM-D0_{19}}}_{\mathrm{Al,Nb:Nb:\square}} = 12000$$

Phase AlNb$_3$–$A15$

$$G^\circ(T) - H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Nb}}^{\circ,\mathrm{bcc}-A2}(298.15\ \mathrm{K}) = \mathrm{G(Nb{:}Al)} = -77920 + 4.88\ T + \mathrm{GHSER}_{\mathrm{Al}} + 3.0\ \mathrm{GHSER}_{\mathrm{Nb}}$$

$$G^\circ(T) - 4.0\ H_{\mathrm{Nb}}^{\circ,\mathrm{bcc}-A2}(298.15\ \mathrm{K}) = \mathrm{G(Nb{:}Nb)} = 20000 + 10\ T + 4.0\ \mathrm{GHSER}_{\mathrm{Nb}}$$

$$L^{0,\mathrm{AlNb_3-A15}}_{\mathrm{Nb:Al,Nb}} = -68000 + 20\ T$$

$$L^{1,\mathrm{AlNb_3-A}A15}_{\mathrm{Nb:Al,Nb}} = 1.0\mathrm{E}{-04}$$

$$L^{2,\mathrm{AlNb_3-A}A15}_{\mathrm{Nb:Al,Nb}} = -12000$$

Phase σ

$$G^\circ(T) - 26.0\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - 4.0\ H_{\mathrm{Nb}}^{\circ,\mathrm{bcc}-A2}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Nb{:}Al)} = -150000 + 96\ T + 26.0\ \mathrm{GHSER}_{\mathrm{Al}} + 4.0\ \mathrm{GHSER}_{\mathrm{Nb}}$$

$$G^\circ(T) - 8.0\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - 22.0\ H_{\mathrm{Nb}}^{\circ,\mathrm{bcc}-A2}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Nb{:}Nb)} = -635250 + 60\ T + 8.0\ \mathrm{GHSER}_{\mathrm{Al}} + 22.0\ \mathrm{GHSER}_{\mathrm{Nb}}$$

$$L^{0,\sigma}_{\mathrm{Al:Nb:Al,Nb}} = -990000 + 270\ T$$

$$L^{1,\sigma}_{\mathrm{Al:Nb:Al,Nb}} = 420000$$

Phase AlTi-$L1_0$

$G^\circ(T)$ - 2.0 $H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Al)} = 4 + 2.0\ \mathrm{GHSER_{Al}}$

$G^\circ(T) - H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Nb}}^{\circ,\mathrm{bcc}-A2}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Nb)} =$
$- 44400 + 5.5\ T + \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Nb}}$

$G^\circ(T) - H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Nb}}^{\circ,\mathrm{bcc}-A2}(298.15\ \mathrm{K}) = \mathrm{G(Nb{:}Al)} =$
$- 44400 + 5.5\ T + \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Nb}}$

$G^\circ(T) - 2.0\ H_{\mathrm{Nb}}^{\circ,\mathrm{bcc}-A2}(298.15\ \mathrm{K}) = \mathrm{G(Nb{:}Nb)} = 2.0\ \mathrm{GFCC_{Nb}}$

$L_{\mathrm{Al,Nb:Al}}^{0,\mathrm{AlTi}-L1_0} = - 80800 + 30\ T$

$L_{\mathrm{Al:Al,Nb}}^{0,\mathrm{AlTi}-L1_0} = - 80800 + 30\ T$

$L_{\mathrm{Nb:Al,Nb}}^{0,\mathrm{AlTi}-L1_0} = - 37600$

$L_{\mathrm{Al,Nb:Nb}}^{0,\mathrm{AlTi}-L1_0} = - 37600$

Phase bcc–$A2$

$L_{\mathrm{Al,Nb:\square}}^{0,\mathrm{bcc}-A2} = - 104050 + 30\ T$

$L_{\mathrm{Al,Nb:\square}}^{1,\mathrm{bcc}-A2} = 9140 - 4\ T$

$L_{\mathrm{Al,Nb:\square}}^{2,\mathrm{bcc}-A2} = 12000$

Phase bcc–$B2$

$G^\circ(T) - H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Al)} = 0$

$G^\circ(T) - 0.5\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - 0.5\ H_{\mathrm{Nb}}^{\circ,\mathrm{bcc}-A2}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Nb)}$
$- 8650 + T$

$G^\circ(T) - 0.5\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - 0.5\ H_{\mathrm{Nb}}^{\circ,\mathrm{bcc}-A2}(298.15\ \mathrm{K}) = \mathrm{G(Nb{:}Al)}$
$- 8650 + T$

$G^\circ(T) - H_{\mathrm{Nb}}^{\circ,\mathrm{bcc}-A2}(298.15\ \mathrm{K}) = \mathrm{G(Nb{:}Nb)} = 0$

$L_{\mathrm{Al:Al,Nb:\square}}^{0,\mathrm{bcc}-B2} = 8650 - T$

$L_{\mathrm{Nb:Al,Nb:\square}}^{0,\mathrm{bcc}-B2} = 8650 - T$

$L_{\mathrm{Al,Nb:Al:\square}}^{0,\mathrm{bcc}-B2} = 8650 - T$

$L_{\mathrm{Al,Nb:Nb:\square}}^{0,\mathrm{bcc}-B2} = 8650 - T$

Phase bcc–*B*2

$$G^{*}_{\mathrm{Al:Nb:\square}} = -\ 8650 + T$$

$$G^{\circ}(T) - {}^{\mathrm{o,fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) = \mathrm{G(Al:Al:\square)} = 0.0$$

$$G^{\circ}(T) - 0.5\ H^{\mathrm{o,fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 0.5\ H^{\mathrm{o,bcc}-A2}_{\mathrm{Nb}}(298.15\ \mathrm{K}) = \mathrm{G(Al:Nb:\square)} = 2.0\ \ \mathrm{G}^{*}_{\mathrm{Al:Nb:\square}}$$

$$G^{\circ}(T) - 0.5\ H^{\mathrm{o,fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - 0.5\ H^{\mathrm{o,bcc}-A2}_{\mathrm{Nb}}(298.15\ \mathrm{K}) = \mathrm{G(Nb:Al:\square)} = 2.0\ \ \mathrm{G}^{*}_{\mathrm{Al:Nb:\square}}$$

$$G^{\circ}(T) - H^{\mathrm{o,bcc}-A2}_{\mathrm{Nb}}(298.15\ \mathrm{K}) = \mathrm{G(Nb:Nb:\square)} = 0.0$$

Phase bcc–*A*2

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Al,Nb:\square}} = -\ 104050 + 30\ \ T$$
$$L^{1,\mathrm{bcc}-A2}_{\mathrm{Al,Nb:\square}} = 9140 - 4\ \ T$$
$$L^{2,\mathrm{bcc}-A2}_{\mathrm{Al,Nb:\square}} = 12000$$

Phase fcc–*A*1

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Al,Nb:\square}} = -\ 113500 + 21.1\ \ T$$

$$L^{1,\mathrm{fcc}-A1}_{\mathrm{Al,Nb:\square}} = 5000$$

$$L^{2,\mathrm{fcc}-A1}_{\mathrm{Al,Nb:\square}} = 10000$$

Phase hcp–*A*3

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Al,Nb:\square}} = -\ 113500 + 21.1\ \ T$$

$$L^{1,\mathrm{hcp}-A3}_{\mathrm{Al,Nb:\square}} = 5000$$

$$L^{2,\mathrm{hcp}-A3}_{\mathrm{Al,Nb:\square}} = 10000$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Al,Nb}} = -\ 91000 + 25\ \ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Al,Nb}} = 6000$$

$$L^{2,\mathrm{liquid}}_{\mathrm{Al,Nb}} = 15000$$

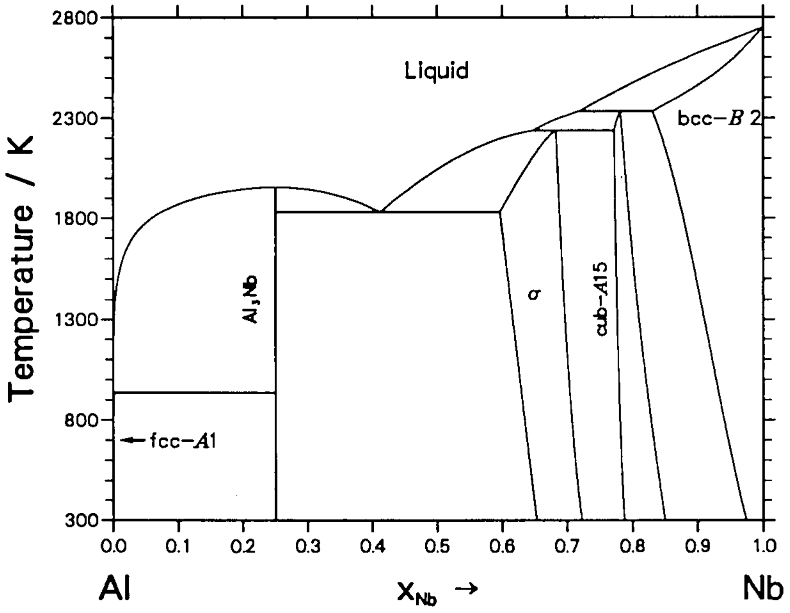


Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Nb}			T / K
Liquid + Al_3Nb^* $\rightleftharpoons$ fcc-$A1$	Peritectic	.000	.250	.001	934.2
Liquid $\rightleftharpoons$ Al_3Nb^* + σ	Eutectic	.412	.250	.596	1832.1
Liquid + $AlNb_3^{**}$ $\rightleftharpoons$ σ	Peritectic	.647	.772	.683	2237.6
Liquid + bcc-$A2$ $\rightleftharpoons$ $AlNb_3^{**}$	Peritectic	.718	.831	.782	2333.7
Al_3Nb^* $\rightleftharpoons$ Liquid	Congruent	.250	.250	...	1955.5

* Al_3Nb-$D0_{22}$
** Cr_3Si-$A15$

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-Nb	(Al)	Cu	$cF4$ $Fm\bar{3}m$	M 4	
	(Nb)	W	$cI2$ $Im\bar{3}m$	M 2	
	$AlNb_3$	Cr_3Si	$cP8$ $Pm\bar{3}n$	Al 2 Nb 6	cub-$A15$
	$AlNb_2$	σ-CrFe	$tP30$ $P4_2/mnm$	Al_1 2 Nb_1 4 Al_2 8 Nb_2 8 Nb_3 8	
	Al_3Nb	Al_3Ti	$tI8$ $I4/mm3m$	Nb 2 Al_1 2 Al_1 42	AlM-$D0_{22}$

System Al–Nd

Solution Phases:

Liquid, bcc–$A2$, dhcp

Compounds:

$Al_{11}Nd_3$-H, $Al_{11}Nd_3$-L, Al_3Nd, AlNd, $AlNd_2$, $AlNd_3$, Laves-$C15$

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-$A2$: Substitutional, Redlich-Kister
dhcp : Substitutional, Redlich-Kister
$Al_{11}Nd_3$-H : Stoichiometric, $(Al)_{11}(Nd)_3$
$Al_{11}Nd_3$-L : Stoichiometric, $(Al)_{11}(Nd)_3$
Al_3Nd : Stoichiometric, $(Al)_3(Nd)$
AlNd : Stoichiometric, (Al)(Nd)
$AlNd_2$: Stoichiometric, $(Al)(Nd)_2$
$AlNd_3$: Stoichiometric, $(Al)(Nd)_3$
Laves-$C15$: Stoichiometric, $(Al)_2(Nd)$

Assessor and Date:

G. Cacciamani, G. Borzone, R. Ferro

Publication:

G. Cacciamani, G. Borzone, R. Ferro, Anales de Fisica 86B, 160-162 (1991)
Revised in 1997.

Thermodynamic properties of the solution and compound phases ($J.mol^{-1}$)

Phase $Al_{11}Nd_3$–H

$$G^\circ(T) - 11.0\ H_{Al}^{o,fcc-A1}(298.15\ K) - 3.0\ H_{Nd}^{o,dhcp}(298.15\ K) =$$
$$- 526776.18 + 114.5827\ T + 11.0\ GHSER_{Al} + 3.0\ GHSER_{Nd}$$

Phase $Al_{11}Nd_3$–L

$$G^\circ(T) - 11.0\ H_{Al}^{o,fcc-A1}(298.15\ K) - 3.0\ H_{Nd}^{o,dhcp}(298.15\ K) =$$
$$- 548308.18 + 132.1646\ T + 11.0\ GHSER_{Al} + 3.0\ GHSER_{Nd}$$

Phase Laves-$C15$

$$G^{\circ}(T) - 2.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - H_{\mathrm{Nd}}^{\mathrm{o,dhcp}}(298.15\ \mathrm{K}) = \\ -\ 158935.47 + 41.37165\ T + 2.0\ \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Nd}}$$

Phase $\mathrm{Al_3Nd}$

$$G^{\circ}(T) - 3.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - H_{\mathrm{Nd}}^{\mathrm{o,dhcp}}(298.15\ \mathrm{K}) = \\ -\ 181169.24 + 47.75868\ T + 3.0\ \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Nd}}$$

Phase $\mathrm{AlNd_2}$

$$G^{\circ}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Nd}}^{\mathrm{o,dhcp}}(298.15\ \mathrm{K}) = \\ -\ 107787.66 + 37.00017\ T + \mathrm{GHSER_{Al}} + 2.0\ \mathrm{GHSER_{Nd}}$$

Phase AlNd

$$G^{\circ}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - H_{\mathrm{Nd}}^{\mathrm{o,dhcp}}(298.15\ \mathrm{K}) = \\ -\ 99854.84 + 34.32248\ T + \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Nd}}$$

Phase $\mathrm{AlNd_3}$

$$G^{\circ}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Nd}}^{\mathrm{o,dhcp}}(298.15\ \mathrm{K}) = \\ -107474.72 + 35.0142\ T + \mathrm{GHSER_{Al}} + 3.0\ \mathrm{GHSER_{Nd}}$$

Phase bcc$-A2$

$$L_{\mathrm{Al,Nd:}\square}^{0,\mathrm{bcc-}A2} = -\ 113226 + 45.05\ T$$

$$L_{\mathrm{Al,Nd:}\square}^{1,\mathrm{bcc-}A2} = 10340 - 15.93\ T$$

Phase fcc$-A1$

$$L_{\mathrm{Al,Nd:}\square}^{0,\mathrm{fcc-}A1} = 0$$

Phase Liquid

$$L_{\mathrm{Al,Nd}}^{0,\mathrm{liquid}} = -\ 125909.87 + 56.16354\ T - 21805836\ T^{-1}$$

$$L_{\mathrm{Al,Nd}}^{1,\mathrm{liquid}} = 35170.81 - 33.34898\ T - 32643234\ T^{-1}$$

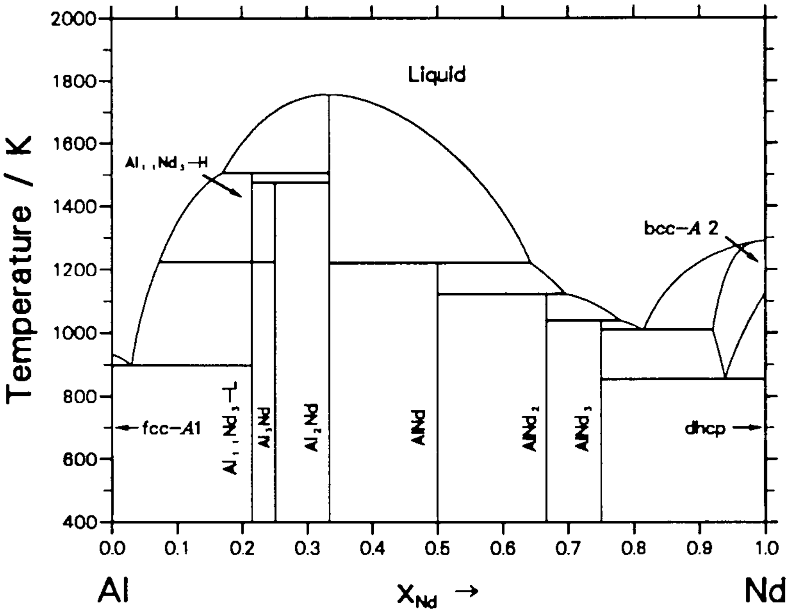


Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Nd}			T / K
Liquid $\rightleftharpoons$ $Al_{11}Nd_3$-L + fcc-$A1$	Eutectic	.030	.000	.214	898.6
Liquid + Laves-$C15$* $\rightleftharpoons$ $Al_{11}Nd_3$-H	Peritectic	.170	.333	.214	1506.6
$Al_1$1Nd_3-H + Al_2Nd * $\rightleftharpoons$ Al_3Nd	Peritectic	.214	.333	.250	1475.8
Liquid + AlNd $\rightleftharpoons$ Al_2Nd	Peritectic	.643	0.500	.333	1220.3
Liquid + AlNd $\rightleftharpoons$ $AlNd_2$	Peritectic	.696	.500	.667	1122.2
Liquid + $AlNd_2$ $\rightleftharpoons$ $AlNd_3$-L	Peritectic	.780	.667	.750	1037.9
Liquid $\rightleftharpoons$ $AlNd_3$-L + bcc-$A2$	Eutectic	.815	.750	.920	1008.9
bcc-$A2$ $\rightleftharpoons$ $AlNd_3$-L + dhcp	Eutectoid	.939	.750	1.000	855.3
Al_2Nd $\rightleftharpoons$ Liquid	Congruent	.333	.333	...	1758.0
$Al_{11}Nd_3$-L $\rightleftharpoons$ $Al_{11}Nd_3$-H	Polymorphic	.214	.214	...	1224.7

* Laves-$C15$ ≡ Al_2Nd

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-Nd	(Al)	Cu	$cF4$ $Fm\bar{3}m$	M 4	
	(Nd)	La-α	$hP4$ $P6_3/mmc$	M 4	
	(Nd)	W	$cI2$ $Im\bar{3}m$	M 2	
	$Al_{11}Nd_3-\alpha$	$Al_{11}La_3-\alpha$	$oI28$ $Immm$		$Al_{11}Nd_3$-L
	$Al_{11}Nd_3-\beta$	Al_4Ba	$tI28$ $I4/mmm$		$Al_{11}Nd_3$-H
	Al_3Nd	Ni_3Sn	$hP8$ $P6_3/mmc$		
	Al_2Nd	Cu_2Mg	$cF24$ $Fd\bar{3}m$	Nd 8 Al 16	Laves-$C15$
	AlNd	AlEr	$oP16$ $Pmmma$	Al 1 Nd 1	
	$AlNd_2$	Co_2Si	$oP12$ $Pnma$	Al 1 Nd 3	
	$AlNd_3$	Ni_3Sn	$hP8$ $P6_3/mmc$	Al 1 Nd 3	

System Al–Si

Solution Phases:

(stable)	Liquid, fcc-*A*1
(metastable)	hcp-*A*3

Modelling:

Liquid	:	Substitutional, Redlich-Kister
fcc-*A*1	:	Substitutional, Redlich-Kister
hcp-*A*3	:	Substitutional, Redlich-Kister
diamond	:	Substitutional, Redlich-Kister

Assessor and Date:

J. Gröbner, H.-L. Lukas, and F. Aldinger.

Publication:

Calphad, **20**, 2 (1996) 247-254.

Thermodynamic properties of the solution phases(J.mol^{-1})

Phase fcc–*A*1

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Al,Si:}\square} = -3143.78 + 0.39297\ T$$

Phase hcp–*A*3

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Al,Si:}\square} = -3143.78 + 0.39297\ T$$

Phase diamond

$$L^{0,\mathrm{diamond}}_{\mathrm{Al,Si}} = 113246.16 - 47.5551\ T$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Al,Si}} = -11340.1 - 1.23394\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Al,Si}} = -3530.93 + 1.35993\ T$$

$$L^{2,\mathrm{liquid}}_{\mathrm{Al,Si}} = 2265.39$$

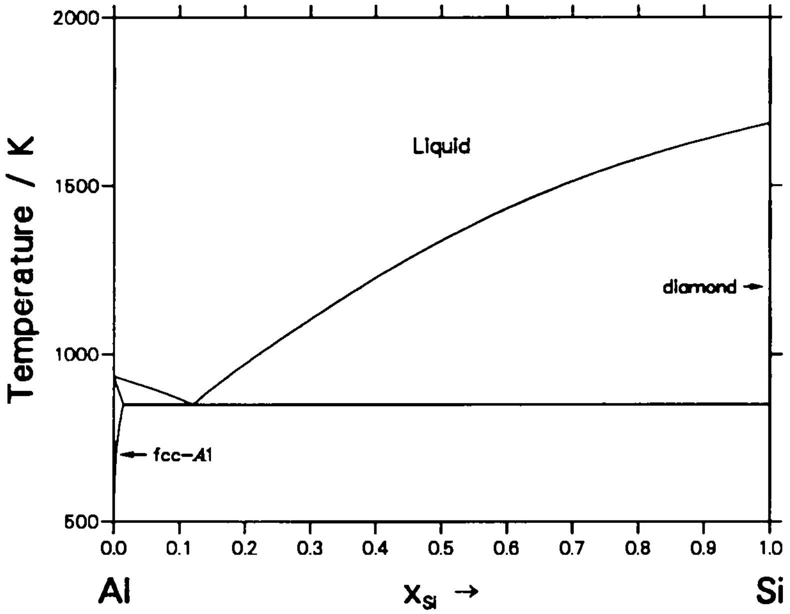


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Si}	T / K
Liquid ⇌ fcc-A1 + diamond	Eutectic	.122 .016 1.000	850.1

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group
Al-Si	(Al)	Cu	cF4 $Fm\bar{3}m$
	(Si)	diamond	cF8 $Fd\bar{3}m$

System Al–Sn

Solution Phases:

(stable) : Liquid, fcc–$A1$, bct–$A5$
(metastable) : hcp–$A3$

Modelling:

Liquid : Substitutional, Redlich–Kister
fcc–$A1$: Substitutional, Redlich–Kister
bct–$A5$: Substitutional, Redlich–Kister
hcp–$A3$: Substitutional, Redlich–Kister

Assessor and Date:

S. Fries, and H.L. Lukas,

Publication:

"Cost507 New Light Alloys", Leuven Proceedings,
Ed. G. Effenberg (1991)

Thermodynamic properties of the solution phases (J.mol^{-1})

Phase bct–$A5$

$$L^{0,\mathrm{bct}-A5}_{\mathrm{Al,Sn}} = 14136.95 - 4.71231\ T$$

Phase fcc–$A1$

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Al,Sn:\square}} = 45297.84 - 8.39814\ T$$

Phase hcp–$A3$

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Al,Sn:\square}} = 0.00001$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Al,Sn}} = 16329.85 - 4.98306\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Al,Sn}} = 4111.97 - 1.15145\ T$$

$$L^{2,\mathrm{liquid}}_{\mathrm{Al,Sn}} = 1765.43 - 0.57390\ T$$

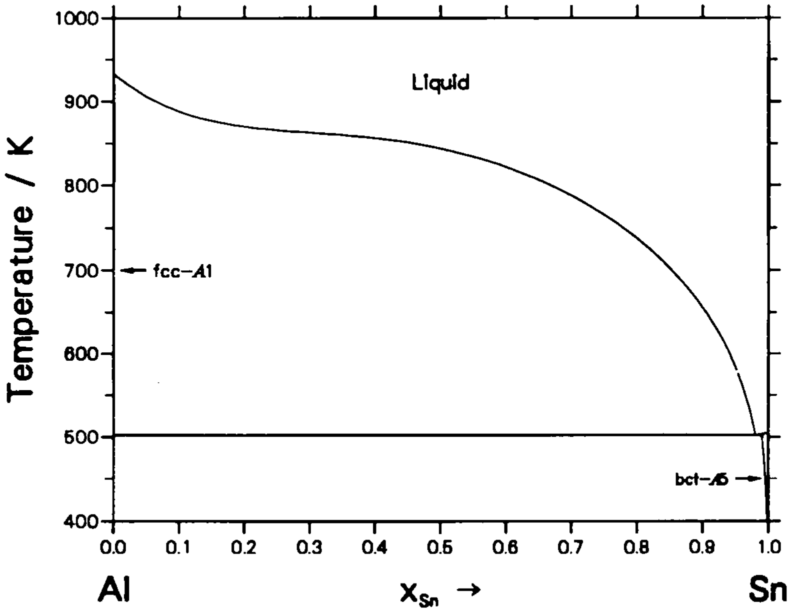


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Sn}	T / K
Liquid ⇌ fcc-$A1$ + bct-$A5$	Eutectic	.980 .000 .990	502.4

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group
Al-Sn	(Al)	Cu	$cF4$ $Fm\bar{3}m$
	(Sn)	β-Sn	$tI4$ $I4_1/amd$

System Al-Ta

Solution Phases:

(stable)	Liquid, bcc-$A2$, fcc-$A1$
(metastable)	bcc-$B2$, hcp-$A3$

Compounds :

(stable)	AlM-$D0_{22}$, σ
(metastable)	AlTi-$L1_0$,AlM-$D0_{19}$

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-$A2$: Substitutional, Redlich-Kister
fcc-$A1$: Substitutional, Redlich-Kister
hcp-$A3$: Substitutional, Redlich-Kister
bcc-$B2$: Sublattice model, $(\mathrm{Al,Ta})_{0.5}(\mathrm{Al,Ta})_{0.5}(\square)_3$
The thermodynamic description of the bcc-B2 takes into account the ordering reaction bcc-$A2$ $\rightleftharpoons$ bcc-$B2$.
Two descriptions are given:
one using equations 23 and 27,
the other using equations 23 and 28.
For the latter, the parameters are given in a frame.
AlM-$D0_{19}$: Sublattice model, $(\mathrm{Al,Ta})_3(\mathrm{Al,Ta})(\square)$
AlM-$D0_{22}$: Sublattice model, $(\mathrm{Al})_3(\mathrm{Ta})$
σ : Sublattice model , $(\mathrm{Al})_8(\mathrm{Ta})_4(\mathrm{Al,Ta})_{18}$
AlTi-$L1_0$: Sublattice model, $(\mathrm{Al,Ta})_{0.5}(\mathrm{,TaTa})_{0.5}$

Assessor and Date:

N. Saunders, 1997.

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase AlM-$D0_{22}$

$$G^{\circ}(T) - 3.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - H_{\mathrm{Ta}}^{\mathrm{o,bcc-}A2}(298.15\ \mathrm{K}) = - 130456 + 23\ T + 3.0\ \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Ta}}$$

Phase Al_3Ta_2–H

$$G^\circ(T) - 3.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Ta}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) = -\ 145000 + 17.325\ T + 3.0\ \mathrm{GHSER}_{\mathrm{Al}} + 2.0\ \mathrm{GHSER}_{\mathrm{Ta}}$$

Phase Al_3Ta_2–L

$$G^\circ(T) - 3.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Ta}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) = -\ 155000 + 24\ T + 3.0\ \mathrm{GHSER}_{\mathrm{Al}} + 2.0\ \mathrm{GHSER}_{\mathrm{Ta}}$$

Phase AlM–$D0_{19}$

$$G^\circ(T) - 4.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = G(\mathrm{Al{:}Al{:}}\square) = 4.0\ \mathrm{GHCP}_{\mathrm{Al}}$$

$$G^\circ(T) - 3.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Ta}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) = G(\mathrm{Al{:}Ta{:}}\square) = -\ 96000 + 22.52\ T + 3\ \mathrm{GHCP}_{Al} + \mathrm{GHCP}_{Ta}$$

$$G^\circ(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Ta}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) = G(\mathrm{Ta{:}Al{:}}\square) = -\ 96000 + 22.52\ T + \mathrm{GHCP}_{\mathrm{Al}} + 3\ \mathrm{GHCP}_{Ta}$$

$$G^\circ(T) - 4\ H_{\mathrm{Ta}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) = G(\mathrm{Ta{:}Ta{:}}\square) = 4 + 4\ \mathrm{GHCP}_{\mathrm{Ta}}$$

$$L_{\mathrm{Al,Ta{:}Al{:}}\square}^{0,\mathrm{AlM}-D0_{19}} = -\ 200000 + 60\ T$$

$$L_{\mathrm{Al{:}Al,Ta{:}}\square}^{0,\mathrm{AlM}-D0_{19}} = -\ 66000 + 20\ T$$

$$L_{\mathrm{Ta{:}Al,Ta{:}}\square}^{0,\mathrm{AlM}-D0_{19}} = 8000$$

$$L_{\mathrm{Al,Ta{:}Ta{:}}\square}^{0,\mathrm{AlM}-D0_{19}} = 20000$$

Phase σ

$$G^\circ(T) - 26\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 4\ H_{\mathrm{Ta}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) = G(\mathrm{Al{:}Ta{:}Al}) = -\ 300000 + 90\ T + 26\ \mathrm{GHSER}_{Al} + 4\ \mathrm{GHSER}_{Ta}$$

$$G^\circ(T) - 8\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 22\ H_{\mathrm{Ta}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) = G(\mathrm{Al{:}Ta{:}Ta}) = -\ 657000 + 90\ T + 8\ \mathrm{GHSER}_{Al} + 22\ \mathrm{GHSER}_{Ta}$$

$$L_{\mathrm{Al{:}Ta{:}Al,Ta}}^{0,\sigma} = -\ 1230000 + 450\ T$$

$$L_{\mathrm{Al{:}Ta{:}Al,Ta}}^{1,\sigma} = 1.0\mathrm{E}{-4}$$

$$L_{\mathrm{Al{:}Ta{:}Al,Ta}}^{2,\sigma} = 300000$$

Phase AlTi-$L1_0$

$$G^{\circ}(T) - 2.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Al)} = 4 + 2.0\ \ \mathrm{GHSER_{Al}}$$
$$G^{\circ}(T) - H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Ta}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Ta)} =$$
$$-\ 71000 + 15.0\ \ T + \ \mathrm{GHSER}_{Al} + \ \mathrm{GHFCC}_{Ta}$$
$$G^{\circ}(T) - H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Ta}}(298.15\ \mathrm{K}) = \mathrm{G(Ta{:}Al)} =$$
$$-\ 71000 + 15.0\ \ T + \ \mathrm{GHSER}_{Al} + \ \mathrm{GHFCC}_{Ta}$$
$$G^{\circ}(T) - 2\ \ H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Ta}}(298.15\ \mathrm{K}) = \mathrm{G(Ta{:}Ta)} = 2\ \ \mathrm{GFCC}_{Ta}$$
$$L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Al,Ta:Al}} = -\ 56000 + 20\ \ T$$

$$L^{1,\mathrm{AlTi}-L1_0}_{\mathrm{Al,Ta:Al}} = 30000$$

$$L^{2,\mathrm{AlTi}-L1_0}_{\mathrm{Al,Ta:Al}} = 20000$$

$$L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Al:Al,Ta}} = -\ 56000 + 20\ \ T$$

$$L^{1,\mathrm{AlTi}-L1_0}_{\mathrm{Al:Al,Ta}} = 30000$$

$$L^{2,\mathrm{AlTi}-L1_0}_{\mathrm{Al:Al,Ta}} = 20000$$

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Al,Ta}:\square} = -\ 89000 + 30\ \ T$$

$$L^{1,\mathrm{bcc}-A2}_{\mathrm{Al,Ta}:\square} = -\ 5000$$

$$L^{2,\mathrm{bcc}-A2}_{\mathrm{Al,Ta}:\square} = 15000$$

Phase bcc–$B2$

$$G^{\circ}(T) - H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Al)} = 0$$
$$G^{\circ}(T) - 0.5\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 0.5\ \ H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Ta}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Ta)}$$
$$-\ 8250 + T$$
$$G^{\circ}(T) - 0.5\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 0.5\ \ H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Ta}}(298.15\ \mathrm{K}) = \mathrm{G(Ta{:}Al)}$$
$$-\ 8250 + T$$
$$G^{\circ}(T) - H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Ta}}(298.15\ \mathrm{K}) = \mathrm{G(Ta{:}Ta)} = 0$$
$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Al:Al,Ta}:\square} = 8250 - T$$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Ta:Al,Ta}:\square} = 8250 - T$$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Al,Ta:Al}:\square} = 8250 - T$$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Al,Ta:Al}:\square} = 8250 - T$$

Phase bcc–$B2$

$G^{\bullet}_{\mathrm{Al:Ta:\square}} = -\ 8250 + T$

$G^{\circ}(T)\ -\ {}^{\mathrm{o,fcc-}A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Al{:}\square)} = 0.0$

$G^{\circ}(T)\ -\ 0.5\ H^{\mathrm{o,fcc-}A1}_{\mathrm{Al}}(298.15\ \mathrm{K})\ -\ 0.5\ H^{\mathrm{o,bcc-}A2}_{\mathrm{Ta}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Ta{:}\square)} = 2.0\ \ \mathrm{G}^{\bullet}_{\mathrm{Al:Ta:\square}}$

$G^{\circ}(T)\ -\ 0.5\ H^{\mathrm{o,fcc-}A1}_{\mathrm{Cu}}(298.15\ \mathrm{K})\ -\ 0.5\ H^{\mathrm{o,bcc-}A2}_{\mathrm{Ta}}(298.15\ \mathrm{K}) = \mathrm{G(Ta{:}Al{:}\square)} = 2.0\ \ \mathrm{G}^{\bullet}_{\mathrm{Al:Ta:\square}}$

$G^{\circ}(T)\ -\ H^{\mathrm{o,bcc-}A2}_{\mathrm{Ta}}(298.15\ \mathrm{K}) = \mathrm{G(Ta{:}Ta{:}\square)} = 0.0$

bcc–$A2$

$L^{0,\mathrm{bcc-}A2}_{\mathrm{Al,Ta:\square}} = -\ 89000 + 30\ \ T$

$L^{1,\mathrm{bcc-}A2}_{\mathrm{Al,Ta:\square}} = -\ 5000$

$L^{2,\mathrm{bcc-}A2}_{\mathrm{Al,Ta:\square}} = 15000$

Phase fcc–$A1$

$L^{0,\mathrm{fcc-}A1}_{\mathrm{Al,Ta:\square}} \quad = \quad -\ 100000 + 30\ \ T$

Phase hcp–$A3$

$L^{0,\mathrm{hcp-}A3}_{\mathrm{Al,Ta:\square}} \quad = \quad -\ 100000 + 30\ \ T$

Phase liquid

$L^{0,\mathrm{liquid}}_{\mathrm{Al,Ta}} \quad = \quad -\ 108000 + 30\ \ T$

$L^{1,\mathrm{liquid}}_{\mathrm{Al,Ta}} \quad = \quad 6000$

$L^{2,\mathrm{liquid}}_{\mathrm{Al,Ta}} \quad = \quad 17000$

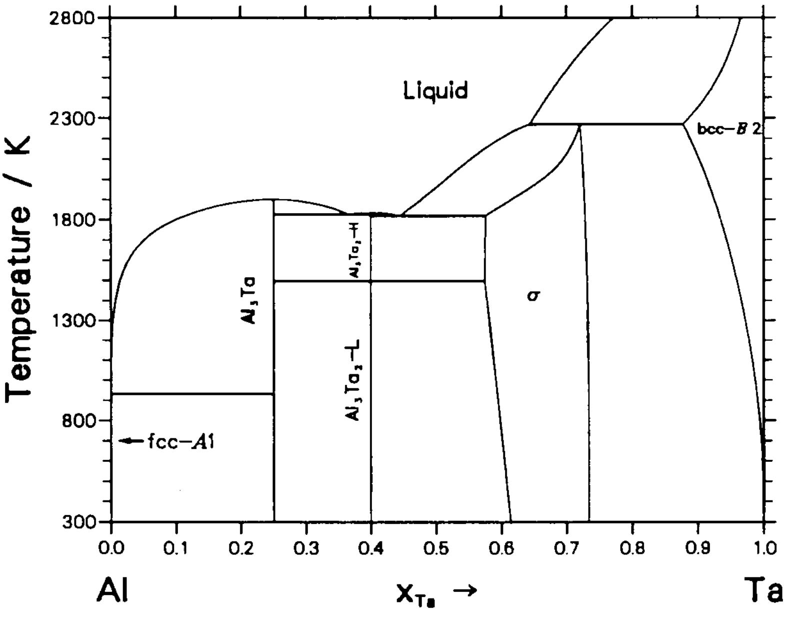


Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Ta}			T / K
Liquid + AlM-$D0^{*}_{22}$ ⇌ fcc-$A1$	Peritectic	.00001	.250	.0008	934.0
Liquid ⇌ + AlM-$D0^{*}_{22}$ + Al_3Ta_2-II	Eutectic	.366	.250	.400	1826.8
Liquid ⇌ Al_3Ta_2-H ⇌ + σ	Eutectic	.444	.400	.576	1819.8
Liquid + bcc-$A2$ ⇌ σ	Peritectic	.643	.877	.720	2270.4
Al_3Ta^{*} ⇌ Liquid	Congruent	.250	.250	...	1901.0
Al_3Ta_2-H ⇌ Al_3Ta_2-II	Polymorphic	.400	.400	...	1498.1

* AlM-$D0_{22}$ ≡ Al_3Ta

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-Ta	(Al)	Cu	$cF4$ $Fm\bar{3}m$	M 4	
	(Ta)	W	$cI2$ $Im\bar{3}m$	M 2	
	$AlTa_2$	σ-CrFe	$tP30$ $P4_2/mnm$	Al_1 2 Ta_1 4 Al_2 8 Ta_2 8 Ta_3 8	
	Al_3Ta	Al_3Ti	$tI8$ $I4/mm3m$	Ta 2 Al_1 2 Al_1 42	AlM-$D0_{22}$
	Al_3Ta_2-L		o^{**}		
	Al_3Ta_2-H		$o^{*}24$		

System Al–Ti

Solution Phases:

(stable) Liquid, bcc-$A2$, fcc-$A1$, hcp-$A3$, AlM-$D0_{19}$, AlTi-$L1_0$
(metastable) bcc-$B2$

Compounds:

AlM-$D0_{22}$, Al_2Ti, $Al_{11}Ti_5$

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-$A2$: Substitutional, Redlich-Kister
fcc-$A1$: Substitutional, Redlich-Kister
bcc-$B2$: Sublattice model, $(Al,Ti)_{0.5}(Al,Ti)_{0.5}(\square)_3$
The thermodynamic description of the bcc-B2 takes into account the ordering reaction bcc-$A2$ $\rightleftharpoons$ bcc-$B2$. Two descriptions are given: one using equations 23 and 27, the other using equations 23 and 28. For the latter, the parameters are given in a frame.
hcp-$A3$: Substitutional, Redlich-Kister
AlM-$D0_{19}$: Sublattice model, $(Al,Ti)(Al,Ti)_3(\square)_{0.5}$
$L1_0$-AlTi : Sublattice model, (Al,Ti)(Al,Ti)
AlM-$D0_{22}$: Stoichiometric, $(Al)_3(Ti)$
Al_2Ti : Stoichiometric, $(Al)_2(Ti)$
$Al_{11}Ti_5$: Stoichiometric, $(Al)_{11}(Ti)_5$

Assessor and Date:

N. Saunders (1992)

Thermodynamic properties of the solution and compound phases ($J.mol^{-1}$)

Phase AlTi-$L1_0$

$$G^\circ(T) - 2.0\ H_{Al}^{\circ,fcc-A1}(298.15\ K) = G(Al{:}Al) = 2.0\ \ GHSER_{Al}$$

$$G^\circ(T) - H_{Al}^{\circ,fcc-A1}(298.15\ K) - H_{Ti}^{\circ,hcp-A3}(298.15\ K) = G(Ti{:}Al) = -79644.0 + 19.2\ T + GHSER_{Al} + GHSER_{Ti}$$

$$G^\circ(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Ti}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Al:Ti)} = -79644.0 + 19.2\ T + \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Ti}}$$

$$G^\circ(T) - 2.0\ H_{\mathrm{Ti}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Ti:Ti)} = 2.0\ \mathrm{GFCCTi}$$

$$L_{\mathrm{Al,Ti:Al}}^{0,\mathrm{AlTi}-L1_0} = -89892 + 44\ T$$

$$L_{\mathrm{Al,Ti:Al}}^{1,\mathrm{AlTi}-L1_0} = 30000$$

$$L_{\mathrm{Al,Ti:Al}}^{2,\mathrm{AlTi}-L1_0} = 20000$$

$$L_{\mathrm{Al:Al,Ti}}^{0,\mathrm{AlTi}-L1_0} = -89892 + 44\ T$$

$$L_{\mathrm{Al:Al,Ti}}^{1,\mathrm{AlTi}-L1_0} = 30000$$

$$L_{\mathrm{Al:Al,Ti}}^{2,\mathrm{AlTi}-L1_0} = 20000$$

$$L_{\mathrm{Ti:Al,Ti}}^{0,\mathrm{AlTi}-L1_0} = -15134 - 2.36\ T$$

$$L_{\mathrm{Al,Ti:Ti}}^{0,\mathrm{AlTi}-L1_0} = -15134 - 2.36\ T$$

Phase AlM$-D0_{19}$

$$G^\circ(T) - 4.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Al:Al:}\square) = 4.0\ \mathrm{GHCPAl}$$

$$G^\circ(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Ti}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Ti:Al:}\square) = -110080 + 23.88\ T + \mathrm{GHSER_{Al}} + 3.0\ \mathrm{GHSER_{Ti}}$$

$$G^\circ(T) - 3.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Ti}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Al:Ti:}\square) = -99120.0 + 32.28\ T + 3.0\ \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Ti}}$$

$$G^\circ(T) - 4.0\ H_{\mathrm{Ti}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Ti:Ti:}\square) = 4.0\ \mathrm{GHSER_{Ti}}$$

$$L_{\mathrm{Al,Ti:Al:}\square}^{0,\mathrm{AlM}-D0_{19}} = -298200 + 100\ T$$

$$L_{\mathrm{Al,Ti:Ti:}\square}^{0,\mathrm{AlM}-D0_{19}} = 32000 - 4\ T$$

$$L_{\mathrm{Al:Al,Ti:}\square}^{0,\mathrm{AlM}-D0_{19}} = -98968 + 33.3\ T$$

$$L_{\mathrm{Ti:Al,Ti:}\square}^{0,\mathrm{AlM}-D0_{19}} = 10656 - 1.332\ T$$

Phase Al$_2$Ti

$$G^\circ(T) - 2.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Ti}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = -121500 + 31.2\ T + 2.0\ \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Ti}}$$

Phase AlM-$D0_{22}$

$G^{\circ}(T) - 3.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Ti}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Ti)} =$
$- 144592.0 + 37.024\ T + 3.0\ \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Ti}}$
$G^{\circ}(T) - 4.0\ H_{\mathrm{Ti}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Ti)} =$
$\mathrm{GFCC_{Ti}}$
$L_{\mathrm{Al,Ti:Ti}}^{0,\mathrm{AlM}-D0_{22}} = - 60000$

Phase "$\mathbf{Al_{11}Ti_5}$"

$G^{\circ}(T) - 17.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 8.0\ H_{\mathrm{Ti}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) =$
$- 971125.0 + 236.4\ T + 17.0\ \mathrm{GHSER_{Al}} + 8.0\ \mathrm{GHSER_{Ti}}$

Phase bcc-$A2$

$L_{\mathrm{Al,Ti:\square}}^{0,\mathrm{bcc}-A2} = - 128500 + 39\ T$

$L_{\mathrm{Al,Ti:\square}}^{1,\mathrm{bcc}-A2} = 6000$

$L_{\mathrm{Al,Ti:\square}}^{2,\mathrm{bcc}-A2} = 21200$

Phase bcc-$B2$

$G^{\circ}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Al{:}\square)} = 0$
$G^{\circ}(T) - 0.5\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 0.5\ H_{\mathrm{Ti}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Ti{:}\square)}$
$- 8750 + 1.25\ T$
$G^{\circ}(T) - 0.5\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 0.5\ H_{\mathrm{Ti}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Al{:}\square)}$
$- 8750 + 1.25\ T$
$G^{\circ}(T) - H_{\mathrm{Ti}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Ti{:}\square)} = 0$
$L_{\mathrm{Al:Al,Ti:\square}}^{0,\mathrm{bcc}-B2} = 8750 - 1.25\ T$

$L_{\mathrm{Ti:Al,Ti:\square}}^{0,\mathrm{bcc}-B2} = 8750 - 1.25\ T$

$L_{\mathrm{Al,Ti:Al:\square}}^{0,\mathrm{bcc}-B2} = 8750 - 1.25\ T$

$L_{\mathrm{Al,Ti:Al:\square}}^{0,\mathrm{bcc}-B2} = 8750 - 1.25\ T$

Phase bcc–$B2$

$G^{\bullet}_{\mathrm{Al:Ti:}\square} = -\ 8750 + 1.25\ T$

$G^{\circ}(T) - H^{\mathrm{o,fcc-}A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) = \mathrm{G(Al:Al:}\square) = 0.0$

$G^{\circ}(T) - 0.5\ H^{\mathrm{o,fcc-}A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 0.5\ H^{\mathrm{o,hcp-}A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Al:Ti:}\square) = 2.0\ \ \mathrm{G}^{\bullet}_{\mathrm{Al:Ti:}\square}$

$G^{\circ}(T) - 0.5\ H^{\mathrm{o,fcc-}A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - 0.5\ \mathrm{H}^{\mathrm{o,hcp-}A3}_{\mathrm{Ti}}(298.15\mathrm{K}) = \mathrm{G(Ti:Al:}\square) = 2.0\ \ \mathrm{G}^{\bullet}_{\mathrm{Al:Ti:}\square}$

$G^{\circ}(T) - H^{\mathrm{o,hcp-}A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti:Ti:}\square) = 0.0$

Phase bcc–$A2$

$L^{0,\mathrm{bcc-}A2}_{\mathrm{Al,Ti:}\square} = -\ 128500 + 39\ \ T$

$L^{1,\mathrm{bcc-}A2}_{\mathrm{Al,Ti:}\square} = \ 6000$

$L^{2,\mathrm{bcc-}A2}_{\mathrm{Al,Ti:}\square} = \ 21200$

Phase fcc–$A1$

$L^{0,\mathrm{fcc-}A1}_{\mathrm{Al,Ti:}\square} = -\ 128970 + 39\ \ T$

$L^{1,\mathrm{fcc-}A1}_{\mathrm{Al,Ti:}\square} = -\ 5000$

$L^{2,\mathrm{fcc-}A1}_{\mathrm{Al,Ti:}\square} = \ 20000$

Phase hcp–$A3$

$L^{0,\mathrm{hcp-}A3}_{\mathrm{Al,Ti:}\square} = -\ 133500 + 39\ \ T$

$L^{1,\mathrm{hcp-}A3}_{\mathrm{Al,Ti:}\square} = \ 750.0$

$L^{2,\mathrm{hcp-}A3}_{\mathrm{Al,Ti:}\square} = \ 17500.0$

Phase liquid

$$L_{\mathrm{Al,Ti}}^{0,\mathrm{liquid}} = -108250 + 38\ T$$

$$L_{\mathrm{Al,Ti}}^{1,\mathrm{liquid}} = -6000 + 5\ T$$

$$L_{\mathrm{Al,Ti}}^{2,\mathrm{liquid}} = 15000$$

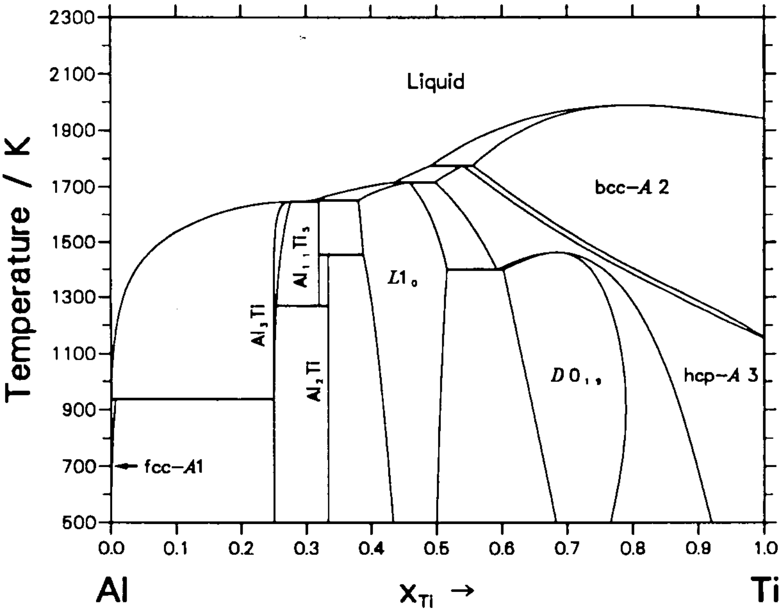


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Ti}			T / K
$Al_{11}Ti_5$ + AlTi-$L1_0$ ⇌ Al_2Ti	Peritectoid	.320	.388	.333	1454.3
$Al_{11}Ti_5$ ⇌ AlM* + Al_2Ti	Eutectoid	.320	.250	.333	1259.8
Liquid + $Al_{11}Ti_5$ ⇌ AlM-$D0^*_{22}$	Peritectic	.247	.320	.250	1627.7
Liquid + AlM-$D0^*_{22}$ ⇌ fcc-$A1$	Degenerate	.001	.250	.000	934.2
Liquid + AlTi-$L1_0$ ⇌ $Al_{11}Ti_5$	Peritectic	.310	.380	.320	1651.9
Liquid + hcp-$A3$ ⇌ AlTi-$L1_0$	Peritectic	.436	.498	.459	1716.7
Liquid + bcc-$A2$ ⇌ hcp-$A3$	Peritectic	.491	.555	.540	1775.9
hcp-$A3$ ⇌ $L1_0$-AlTi + AlM-$D0_{19}$	Eutectoid	.595	.518	.607	1384.4
AlM-$D0_{19}$ ⇌ hcp-$A3$	Congruent	.682	.682	....	1452.0
bcc-$A2$ ⇌ liquid	Congruent	.788	.788	....	1989.0

* AlM-$D0_{22}$ ≡ Al_3Ti

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	
Al-Ti	(Al)	Cu	$cF4$ $Fm\bar{3}m$	M 4	
	(Ti)	Mg	$hP2$ $P6_3/mmc$	M 2	
	(Ti)	W	$cI2$ $Im\bar{3}m$	M 2	
	AlTi	AuCu	$tP4$ $P4/mmm$	Al 2 Ti_1 1 Ti_2 1	AlTi-$L1_0$
	$AlTi_3$	Ni_3Sn	$hP8$ $P6_3/mmc$		AlM-$D0_{19}$
	Al_2Ti	Ga_2Hf	$tI24$ $I4_1/amd$		
	Al_2Ti-α	Ga_2Zr	$oC12$ $Cmmm$		transformation not taken into account in [90Mas]
	Al_3Ti	Al_3Ti	$tI8$ $I4/mmm$	Al_1 2 Al_2 4 Ti 2	AlM-$D0_{22}$
	Al_5Ti_3		$tP32$ $I4/mbm$		
	δ	Al_3Zr	$tI16$		$Al_{11}Ti_5$ from [91Vil]
	Al_5Ti_3		$tP32$ $I4/mbm$		metastable

System Al–V

Solution Phases:

Liquid, bcc–$A2$, fcc–$A1$

Compounds:

$Al_{10}V$,Al_7V, $Al_{23}V_4$, AlM–$D0_{22}$, Al_8V_5

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc–$A2$: Substitutional, Redlich-Kister
fcc–$A1$: Substitutional, Redlich-Kister
$Al_{10}V$: Stoichiometric, $(Al)_{10}(V)$
Al_7V : Stoichiometric, $(Al)_7(V)$
$Al_{23}V_4$: Stoichiometric, $(Al)_{23}(V)_4$
AlM–$D0_{22}$: Stoichiometric, $(Al)_3(V)$
Al_8V_5 : Stoichiometric, $(Al)_8(V)_5$

Assessor and Date:

N. Saunders (1991)

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase $Al_{10}V$

$$G^\circ(T) - 10.0 \; H_{Al}^{o,fcc-A1}(298.15 \text{ K}) - H_{V}^{o,bcc-A2}(298.15 \text{ K}) =$$
$$- 111221 + 18.909 \; T + 10.0 \; GHSER_{Al} + GHSER_{V}$$

Phase $Al_{23}V_4$

$$G^\circ(T) - 23.0 \; H_{Al}^{o,fcc-A1}(298.15 \text{ K}) - 4.0 \; H_{V}^{o,bcc-A2}(298.15 \text{ K}) =$$
$$- 430650 + 64.665 \; T + 23.0 \; GHSER_{Al} + 4.0 \; GHSER_{V}$$

Phase AlM–$D0_{22}$

$$G^\circ(T) - 3.0 \; H_{Al}^{o,fcc-A1}(298.15 \text{ K}) - H_{V}^{o,bcc-A2}(298.15 \text{ K}) =$$
$$- 104308.0 + 15.2 \; T + 3.0 \; GHSER_{Al} + GHSER_{V}$$

Phase Al_7V

$$G^\circ(T) - 7.0\ H_{Al}^{o,fcc-A1}(298.15\ K) - H_V^{o,bcc-A2}(298.15\ K) = \\ -108800.0 + 16.8\ T + 7.0\ GHSER_{Al} + GHSER_V$$

Phase Al_8V_5

$$G^\circ(T) - 8.0\ H_{Al}^{o,fcc-A1}(298.15\ K) - 5.0\ H_V^{o,bcc-A2}(298.15\ K) = \\ -294320.0 - 13.0\ T + 8.0\ GHSER_{Al} + 5.0\ GHSER_V$$

Phase bcc-A2

$$L_{Al,V:\square}^{0,bcc-A2} = -95000 + 20\ T$$

$$L_{Al,V:\square}^{1,bcc-A2} = -6000$$

Phase fcc-A1

$$L_{Al,V:\square}^{0,fcc-A1} = -69800 + 15\ T$$

$$L_{Al,V:\square}^{1,fcc-A1} = -8000$$

Phase liquid

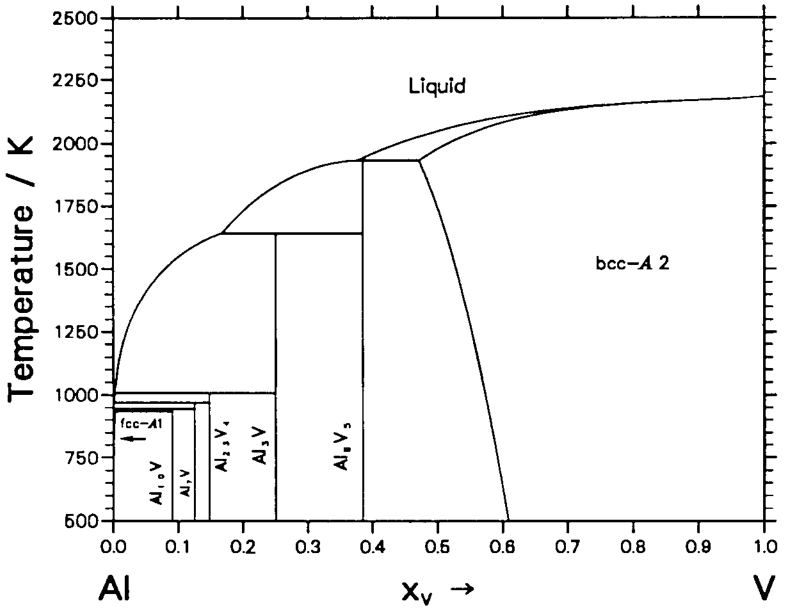
$$L_{Al,V}^{0,liquid} = -50725 + 9\ T$$

$$L_{Al,V}^{1,liquid} = -15000 + 8\ T$$

Table I - Invariant Reactions.

Reaction	Type	Compositions x_V			T / K
Liquid + AlM-$D0_{22}^*$ ⇌ $Al_{23}V_4$	Peritectic	.003	.250	.148	1007.3
Liquid + $Al_{23}V_4$ ⇌ Al_7V	Peritectic	.002	.148	.125	969.0
Liquid + Al_7V ⇌ $Al_{10}V$	Peritectic	.001	.125	.091	945.2
Liquid + $Al_{10}V$ ⇌ fcc-A1	Peritectic	.000	.091	.001	935.3
Liquid + Al_8V_5 ⇌ AlM-$D0_{22}^*$	Peritectic	.167	.384	.250	1640.1
Liquid + bcc-A2 ⇌ Al_8V_5	Peritectic	.376	.471	.384	1932.7

* AlM-$D0_{22}$ ≡ Al_3V


2500
2250
2000
1750
1500
1250
1000
750
500
Temperature / K
Liquid
bcc–A 2
fcc–A1
Al10V
Al7V
Al23V4
Al3V
Al8V5
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
Al
xV →
V

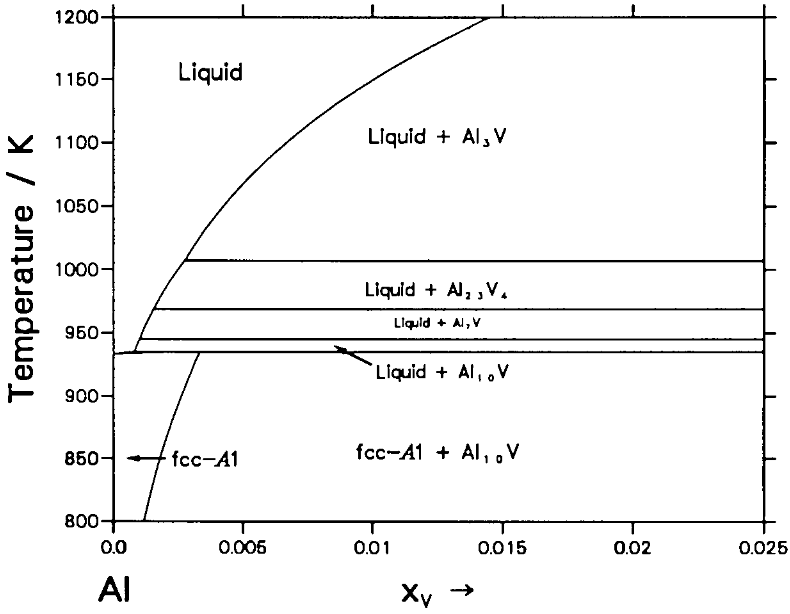

1200
1150
1100
1050
1000
950
900
850
800
Temperature / K
Liquid
Liquid + Al3V
Liquid + Al23V4
Liquid + Al7V
Liquid + Al10V
fcc–A1
fcc–A1 + Al10V
0.0
0.005
0.01
0.015
0.02
0.025
Al
xV →

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-V	(Al)	Cu	$cF4$ $Fm\bar{3}m$	M 4	
	(V)	W	$cI2$ $Im\bar{3}m$	M 2	
	Al_3V	Al_3Ti	$tI8$ $I4/mmm$	Al_1 2 Al_2 4 V 2	AlM-$D0_{22}$
	Al_8V_5	Cu_5Zn_8	$cI52$ $I\bar{4}3m$	A_1 24 M_1 8 M_2 12 V 8	
	$Al_{21}V_2$	$Al_{21}V_2$	$cF176$ $Fd\bar{3}m$	Al_1 16 Al_2 48 Al_3 96 V 16	described as $Al_{10}V$
	$Al_{23}V_4$	$Al_{23}V_4$	$hP54$ $P6_3/mmc$		
	$Al_{45}V_7$	$Al_{45}V_7$	$mC104$ $C2/m$		described as Al_7V
	AlV_3	Cr_3Si	$cP8$ $Pm\bar{3}n$	Al 2 V 6	A_{15} stable?

System Al-Y

Solution Phases:

Liquid, bcc-$A2$, fcc-$A1$, hcp-$A3$

Compounds:

Al_3Y, Al_2Y, AlY, Al_2Y_3, Al_3Y_5, AlY_2

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-$A2$: Substitutional, Redlich-Kister
fcc-$A1$: Substitutional, Redlich-Kister
hcp-$A3$: Substitutional, Redlich-Kister
Al_3Y : Stoichiometric, $(Al)_3(Y)$
Al_2Y : Stoichiometric, $(Al)_2(Y)$
AlY : Stoichiometric, (Al)(Y)
Al_2Y_3 : Stoichiometric, $(Al)_2(Y)_3$
Al_3Y_5 : Stoichiometric, $(Al)_3(Y)_5$
AlY_2 : Stoichiometric, $(Al)(Y)_2$

Assessor and Date:

H.L. Lukas, 1993

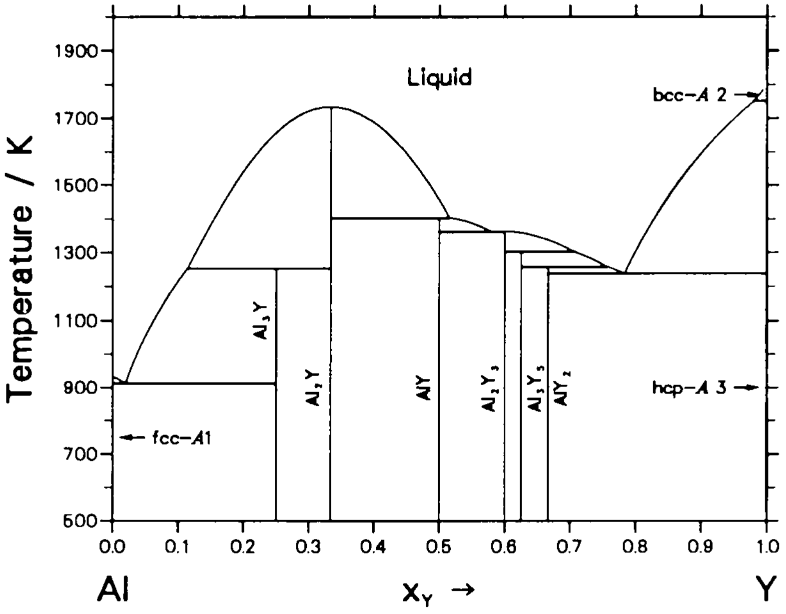
Thermodynamic properties of the solution and compound phases (J.mol⁻)

Phase Al_2Y

$$G^\circ(T) - 2.0\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Y}}^{\circ,\mathrm{hcp}-A3}(298.15\ \mathrm{K}) = - 246018.0 + 35.32809\ T + 2.0\ \mathrm{GHSER}_{\mathrm{Al}} + \mathrm{GHSER}_{\mathrm{Y}}$$

Phase Al_2Y_3

$$G^\circ(T) - 2.0\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Y}}^{\circ,\mathrm{hcp}-A3}(298.15\ \mathrm{K}) = - 373605.0 + 84.410\ T + 2.0\ \mathrm{GHSER}_{\mathrm{Al}} + 3.0\ \mathrm{GHSER}_{\mathrm{Y}}$$



Phase Al_3Y

$$G^\circ(T) - 3.0\ H_{Al}^{o,fcc-A1}(298.15\ K) - H_Y^{o,hcp-A3}(298.15\ K) =$$
$$-\ 267460.0 + 46.48084\ T + 3.0\ GHSER_{Al} + GHSER_Y$$

Phase Al_3Y_5

$$G^\circ(T) - 3.0\ H_{Al}^{o,fcc-A1}(298.15\ K) - 5.0\ H_Y^{o,hcp-A3}(298.15\ K) =$$
$$-\ 564479.2 + 127.7201\ T + 3.0\ GHSER_{Al} + 5.0\ GHSER_Y$$

Phase AlY

$$G^\circ(T) - H_{Al}^{o,fcc-A1}\ (298.15\ K) - H_Y^{o,hcp-A3}(298.15\ K) =$$
$$-\ 173810.0 + 40.86834\ T + GHSER_{Al} + GHSER_Y$$

Phase AlY_2

$$G^\circ(T) - H_{Al}^{o,fcc-A1}\ (298.15\ K) - 2.0\ H_Y^{o,hcp-A3}(298.15\ K) =$$
$$-\ 190908.0 + 44.38629\ T + GHSER_{Al} + 2.0\ GHSER_Y$$

Phase bcc–*A*2

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Al,Y}:\square} = 90\ T$$

Phase hcp–*A*3

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Al,Y}:\square} = 90\ T$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Al,Y}} = -\,202611.28 + 4.63942\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Al,Y}} = -\,54350.11 + 0.28402\ T$$

$$L^{2,\mathrm{liquid}}_{\mathrm{Al,Y}} = 83347.01 - 34.76401\ T$$

$$L^{3,\mathrm{liquid}}_{\mathrm{Al,Y}} = 15488.69 - 0.7988\ T$$

$$L^{4,\mathrm{liquid}}_{\mathrm{Al,Y}} = -\,51205.9 + 30.2161\ T$$

Table I - Invariant Reactions.

Reaction	Type	Compositions x_Y			T / K
Liquid $\rightleftharpoons$ Al_3Y + fcc–*A*1	Eutectic	.020	.000	.250	913.0
Liquid + Al_2Y $\rightleftharpoons$ Al_3Y	Peritectic	.114	.333	.250	1253.0
Liquid + Al_2Y $\rightleftharpoons$ AlY	Peritectic	.516	.330	.500	1403.0
Liquid $\rightleftharpoons$ AlY + Al_2Y_3	Eutectic	.581	.500	.600	1361.2
Liquid + Al_2Y_3 $\rightleftharpoons$ Al_3Y_5	Peritectic	.707	.600	.625	1302.5
Liquid + Al_3Y_5 $\rightleftharpoons$ AlY_2	Peritectic	.757	.625	.666	1258.0
Liquid $\rightleftharpoons$ AlY_2 + hcp–*A*3	Eutectic	.667	.783	1.000	1239.0
hcp–*A*3 $\rightleftharpoons$ bcc–*A*2	Allotropic	1.000	1.000	.....	1752.0
Liquid $\rightleftharpoons$ Al_2Y	Congruent	.333	.333	.....	1734.0
Liquid $\rightleftharpoons$ Al_2Y_3	Congruent	.600	.600	.....	1364.0

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-Y	(Al)	Cu	$cF4$ $Fm\bar{3}m$	M 4	
	(Y)	Mg	$hP2$ $P6_3/mmc$	M 2	
	(Y)	W	$cI2$ $Im\bar{3}m$	M 4	
	Al_3Y-α	Ni_3Sn	$hP8$ $P6_3/mmc$	Al 6 Y 2	
	Al_3Y-β	$BaPb_3$	$hR12$ $R\bar{3}m$	Al_1 9 Al_2 18 Y_1 3 Y_2 6	
	Al_2Y	Cu_2Mg	$cF24$ $Fd\bar{3}m$	Al 16 Y 8	
	AlY	CrB	$oC8$ $Cmcm$	Al 4 Y 4	
	Al_2Y_3	Al_2Zr_3	$tP20$ $P4_2/mnm$	Al 8 Y_1 4 Y_2 4 Y_3 4	
	AlY_2	Co_2Si	$oP12$ $Pnma$	Al 4 Y_1 4 Y_2 4	
	AlY_3	$AuCu_3$	$cP4$ $Pm\bar{3}m$	Al 1 Y 3	$L1_2$ metastable
	Al_3Y_5	Mn_5Si_3	$hP16$ $P6_3/mcm$		impurity stabilized [91Vil]?

System Al-W

Solution Phases:

(stable)	Liquid, bcc-$A2$, fcc-$A1$
(metastable)	bcc-$B2$, hcp-$A3$

Compounds:

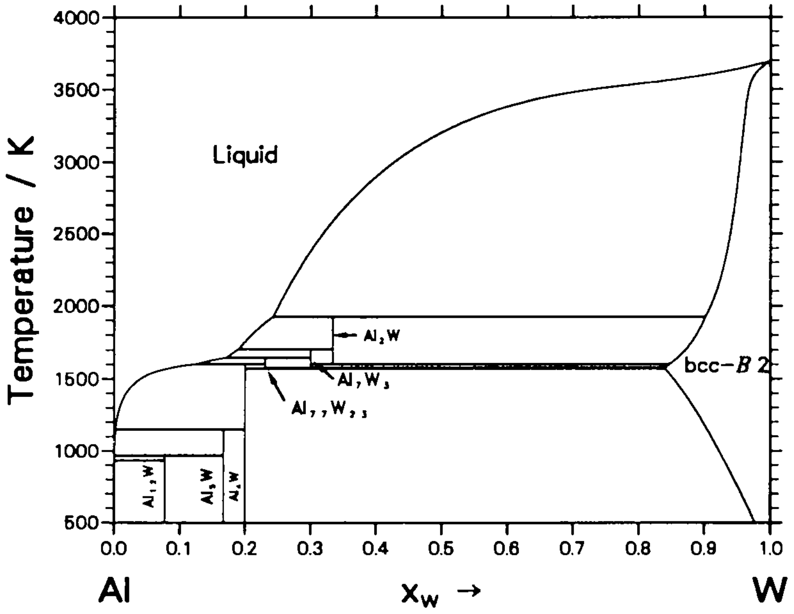
(stable)	$Al_{12}W$, Al_4W, Al_5W, $Al_{77}W_{23}$, Al_7W_3, Al_2W
(metastable)	AlM-$D0_{19}$, AlTi-$L1_0$

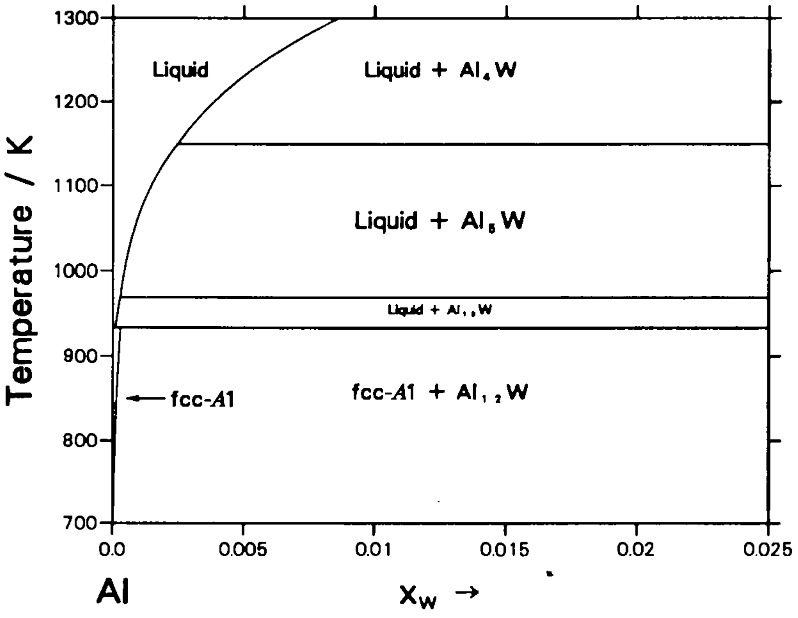
Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-$A2$: Substitutional, Redlich-Kister
fcc-$A1$: Substitutional, Redlich-Kister
hcp-$A3$: Substitutional, Redlich-Kister
$Al_{12}W$: Stoichiometric, $(Al)_{12}(W)$
Al_5W : Stoichiometric, $(Al)_5(W)$
Al_4W : Stoichiometric, $(Al)_4(W)$
$Al_{77}W_{23}$: Stoichiometric, $(Al)_{77}(W)_{23}$
Al_7W_3 : Stoichiometric, $(Al)_7(W)_3$
cub-$A15$: Stoichiometric, $(Al)(W)_3$
Al_2W : Sublattice model, $(Al)_2(W)$
bcc-$B2$: Sublattice model, $(Al,W)_{0.5}(AlW)_{0.5}(\square)_3$
The thermodynamic description of the bcc-B2 takes into account the ordering reaction bcc-$A2$ $\rightleftharpoons$ bcc-$B2$. Two descriptions are given: one using equations 23 and 27, the other using equations 23 and 28. For the latter, the parameters are given in a frame.
AlM-$D0_{19}$: Sublattice model, $(Al,W)_3(Al,W)(\square)_{0.5}$
AlTi-$L1_0$: Sublattice model, $(Al,W)(Al,W)$

Assessor and Date:

N. Saunders, 1996.


Temperature / K
4000
3500
3000
2500
2000
1500
1000
500
Liquid
Al₂W
Al₇W₃
Al₇₇W₂₃
bcc-B2
Al₁₂W
Al₅W
Al₄W
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
Al
x_W →
W


Temperature / K
1300
1200
1100
1000
900
800
700
Liquid
Liquid + Al₄W
Liquid + Al₅W
Liquid + Al₁₂W
fcc-A1
fcc-A1 + Al₁₂W
0.0
0.005
0.01
0.015
0.02
0.025
Al
x_W →

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase Al$_{12}$W

$G^{\circ}(T) - 12.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{W}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$
$-62400 + 9.49\ T + 12.0\ \mathrm{GHSER_{Al}} + \mathrm{GHSER_{W}}$

Phase Al$_4$W

$G^{\circ}(T) - 4.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{W}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$
$-\ 57500 + 9.73\ T + 4.0\ \mathrm{GHSER_{Al}} + \mathrm{GHSER_{W}}$

Phase Al$_5$W

$G^{\circ}(T) - 5.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{W}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$
$-\ 58446 + 8.4\ T + 5.0\ \mathrm{GHSER_{Al}} + \mathrm{GHSER_{W}}$

Phase Al$_2$W

$G^{\circ}(T) - 2.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{W}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$
$13536 - 22.38\ T + 2.0\ \mathrm{GHSER_{Al}} + \mathrm{GHSER_{W}}$

Phase Al$_{77}$W$_{23}$

$G^{\circ}(T) - 77.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 23.0\ H_{\mathrm{W}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$
$-\ 189300 -400\ T + 77.0\ \mathrm{GHSER_{Al}} + 23.0\ \mathrm{GHSER_{W}}$

Phase Al$_7$W$_3$

$G^{\circ}(T) - 7.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{W}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$
$34700 - 70\ T + 7.0\ \mathrm{GHSER_{Al}} + 3.0\ \mathrm{GHSER_{W}}$

Phase AlM-$D0_{19}$

$G^{\circ}(T) - 4.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Al)} =$
$4.0\ \mathrm{GHCP_{Al}}$
$G^{\circ}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{W}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) = \mathrm{G(W{:}Al)} =$
$-\ 12716 + 15.16\ T + \mathrm{GHCP_{Al}} + 3.0\ \mathrm{GHCP_{W}}$
$G^{\circ}(T) - 3.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{W}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}W)} =$
$-\ 12716 + 15.16\ T + 3.0\ \mathrm{GHCP_{Al}} + \mathrm{GHCP_{W}}$
$G^{\circ}(T) - 4.0\ H_{\mathrm{W}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) = \mathrm{G(W{:}W)} =$
$4.0\ \mathrm{GHSER_{W}}$

Phase bcc–$A2$

$L^{0,bcc-A2}_{Al,W:\square} = -\ 27000 + 25\ T$

$L^{1,bcc-A2}_{Al,W:\square} = -\ 10000$

Phase bcc–$B2$

$G^\circ(T) - H^{o,fcc-A1}_{Al}(298.15\ K) = G(Al{:}Al{:}\square) = 0.0$
$G^\circ(T) - 0.5\ H^{o,fcc-A1}_{Al}(298.15\ K) - 0.5\ H^{o,bcc-A2}_{W}(298.15\ K) = G(W{:}Al{:}\square) =$
$1.0E\text{-}4$
$G^\circ(T) - 0.5\ H^{o,fcc-A1}_{Al}(298.15\ K) - 0.5\ H^{o,bcc-A2}_{W}(298.15\ K) = G(Al{:}W{:}\square) =$
$1.0E\text{-}4$
$G^\circ(T) - H^{o,bcc-A2}_{W}(298.15\ K) = G(W{:}W{:}\square) = 0.0$
$L^{0,bcc-B2}_{Al:Al,W:\square} = 1.0E\text{-}4$

$L^{0,bcc-B2}_{Ta:Al,W:\square} = 1.0E\text{-}4$

$L^{0,bcc-B2}_{Al,W:Al:\square} = 1.0E\text{-}4$

$L^{0,bcc-B2}_{Al,W:Al:\square} = 1.0E\text{-}4$

Phase bcc–$B2$

$G^{*}_{Al:W:\square} = 1.0E\text{-}4$

$G^\circ(T) - {}^{o,fcc-A1}_{Al}\ (298.15\ K) = G(Al{:}Al{:}\square) = 0.0$

$G^\circ(T) - 0.5\ H^{o,fcc-A1}_{Al}(298.15\ K) - 0.5\ H^{o,bcc-A2}_{W}(298.15\ K) = G(Al{:}W{:}\square) = 2.0\ G^{*}_{Al:W:\square}$

$G^\circ(T) - 0.5\ H^{o,fcc-A1}_{Cu}(298.15\ K) - 0.5\ H^{o,bcc-A2}_{W}(298.15\ K) = G(W{:}Al{:}\square) = 2.0\ G^{*}_{Al:W:\square}$

$G^\circ(T) - H^{o,bcc-A2}_{W}(298.15\ K) = G(W{:}W{:}\square) = 0.0$

Phase bcc–$A2$

$L^{0,bcc-A2}_{Al,W:\square} = -\ 27000 + 25\ T$

$L^{1,bcc-A2}_{Al,W:\square} = -\ 10000$

Phase fcc–$A1$

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Al,W:\square}} = -19250 + 20.2\ T$$

$$L^{1,\mathrm{fcc}-A1}_{\mathrm{Al,W:\square}} = -10000$$

Phase hcp–$A3$

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Al,W:\square}} = -19250 + 20.2\ T$$

$$L^{1,\mathrm{hcp}-A3}_{\mathrm{Al,W:\square}} = -10000$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Al,W}} = -70000 + 35\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Al,W}} = 1.0\mathrm{E}{-4}$$

$$L^{2,\mathrm{liquid}}_{\mathrm{Al,W}} = 15000$$

Table I - Invariant Reactions.

Reaction	Type	Compositions x_W			T / K
$Al_2W \rightleftharpoons Al_7W_3 + \text{bcc}-A2$	Eutectoid	.333	.300	.847	1602.6
$\text{Liquid} + Al_2W \rightleftharpoons Al_7W_3$	Peritectic	.190	.333	.300	1706.8
$\text{Liquid} + \text{bcc}-A2 \rightleftharpoons Al_2W$	Peritectic	.243	.901	.333	1925.7
$\text{Liquid} + Al_7W_3 \rightleftharpoons Al_{77}W_{23}$	Peritectic	.172	.300	.230	1648.2
$\text{Liquid} + Al_{77}W_{23} \rightleftharpoons Al_4W$	Peritectic	.125	.230	.200	1604.1
$Al_{77}W_{23} \rightleftharpoons Al_4W + \text{bcc}-A2$	Eutectoid	.023	.200	.840	1571.0
$Al_{77}W_{23} + \text{bcc}-A2 \rightleftharpoons Al_7W_3$	Eutectoid	.230	.841	.300	1580.0
$\text{Liquid} + Al_4W \rightleftharpoons Al_5W$	Peritectic	.0025	.200	.167	1149.6
$\text{Liquid} + Al_5W \rightleftharpoons Al_{12}W$	Peritectic	.0003	.167	.077	969.4
$\text{Liquid} + Al_{12}W \rightleftharpoons \text{fcc}-A$	Peritectic	.0002	.077	.0003	933.6
$Al_8W_3 \rightleftharpoons \text{Liquid}$	Congruent	.273	.273	...	1850.5

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-W	(Al)	Cu	*cF4* $Fm\bar{3}m$	M 4	
	(W)	W	*cI2* $Im\bar{3}m$	M 2	
	$Al_{12}W$	$Al_{12}W$	*cI26* $Im\bar{3}$	Al 24 W 2	
	Al_5W	Al_5W	*hP12* $P6_3$		
	Al_4W	Al_4W	*mC30* *Cm*	Al_1 2 Al_2 2 W_1 2 Al_3 4 Al_4 4 Al_5 4 Al_6 4 Al_7 4 W_2 4	
	Al_2W				not quoted in [Mas1] nor in [Vil1]
	Al_7W_3				not quoted in [Mas1] nor in [Vil1]
	$Al_{77}W_{23}$				not quoted in [Mas1] nor in [Vil1]

System Al–Zn

Solution Phases:

(stable) Liquid, fcc-*A*1, hcp-Zn
(metastable) hcp-*A*3

Compounds:

(metastable) AlCu-η, Laves-*C*14

Modelling:

Liquid : Substitutional, Redlich-Kister
fcc-*A*1 : Substitutional, Redlich-Kister
hcp-*A*3 : Substitutional, Redlich-Kister
hcp-Zn : Substitutional, Redlich-Kister
AlCu-η : Stoichiometric, (Al)(Zn)
Laves-*C*14 : Sublattice model, $(Al,Zn)_2(Al,Zn)$

Assessor and Date:

S. an Mey (1991)

Publication:

Z. für Metallkde, 84, 7, 451-455 (1993).

Thermodynamic properties of the solution phases (J.mol^{-1})

Phase fcc-*A*1

$$L^{0,fcc-A1}_{Al,Zn:\square} = 7297.48 + 0.47512\ T$$

$$L^{1,fcc-A1}_{Al,Zn:\square} = 6612.88 - 4.59110\ T$$

$$L^{2,fcc-A1}_{Al,Zn:\square} = -3097.19 + 3.30635\ T$$

Phase hcp–$A3$

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Al,Zn:\Box}} = 18820.95 - 8.95255\ T$$

$$L^{1,\mathrm{hcp}-A3}_{\mathrm{Al,Zn:\Box}} = 1.0\mathrm{E}{-6}$$

$$L^{2,\mathrm{hcp}-A3}_{\mathrm{Al,Zn:\Box}} = 1.0\mathrm{E}\ 6$$

$$L^{3,\mathrm{hcp}-A3}_{\mathrm{Al,Zn:\Box}} = -702.79$$

Phase hcp–Zn

$$L^{0,\mathrm{hcp-Zn}}_{\mathrm{Al,Zn:\Box}} = 18820.95 - 8.95255\ T$$

$$L^{1,\mathrm{hcp-Zn}}_{\mathrm{Al,Zn:\Box}} = 1.0\mathrm{E}{-6}$$

$$L^{2,\mathrm{hcp-Zn}}_{\mathrm{Al,Zn:\Box}} = 1.0\mathrm{E}{-6}$$

$$L^{3,\mathrm{hcp-Zn}}_{\mathrm{Al,Zn:\Box}} = -702.79$$

Phase AlCu–η

$$G^{\circ}(T) - H^{\mathrm{o,fcc}-A1}_{\mathrm{Cu}}(298.15\mathrm{K}) - H^{\mathrm{o,hcp}-Zn}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \\ 15000.0 + \mathrm{GHSER}_{\mathrm{Cu}} + \mathrm{GHSER}_{\mathrm{Zn}}$$

Phase Laves–$C14$

$$G^{\circ}(T) - 3.0\ H^{\mathrm{o,fcc}-A1}_{\mathrm{Cu}}(298.15\mathrm{K}) = \mathrm{G(Al:Al)} = \\ 15000.0 + 3.0\ \mathrm{GHSER}_{\mathrm{Cu}}$$

$$G^{\circ}(T) - 2.0\ H^{\mathrm{o,fcc}-A1}_{\mathrm{Cu}}(298.15\mathrm{K}) - H^{\mathrm{o,hcp}-Zn}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Al:Zn)} = \\ 15000.0 + 2.0\ \mathrm{GHSER}_{\mathrm{Cu}} + \mathrm{GHSER}_{\mathrm{Zn}}$$

$$G^{\circ}(T) - H^{\mathrm{o,fcc}-A1}_{\mathrm{Cu}}(298.15\mathrm{K}) - 2.0\ H^{\mathrm{o,hcp}-Zn}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Zn:Al)} = \\ 15000.0 + \mathrm{GHSER}_{\mathrm{Cu}} + 2.0\ \mathrm{GHSER}_{\mathrm{Zn}}$$

$$G^{\circ}(T) - 3.0\ H^{\mathrm{o,hcp}-Zn}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Zn:Zn)} = \\ 15000.0 + 3.0\ \mathrm{GHSER}_{\mathrm{Zn}}$$

$$L^{0,\mathrm{Laves}-C14}_{\mathrm{Al:Al,Zn:\Box}} = L^{0,\mathrm{Laves}-C14}_{\mathrm{Zn:Al,Zn:\Box}} = -7500 - 18\ T$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Al,Zn}} = 10465.55 - 3.39259\ T$$

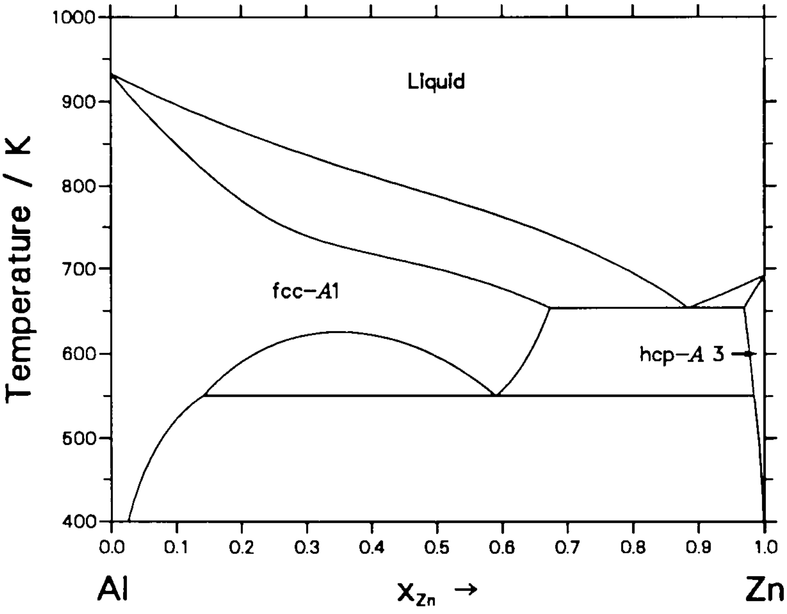


Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Zn}			T / K
Liquid ⇌ fcc-*A*1 + hcp-*A*3	Eutectic	.884	.673	.969	654.0
fcc-*A*1' ⇌ fcc-*A*1" + hcp-*A*3	Monotectic	.590	.141	.984	550.4

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group
Al-Zn	(Al)	Cu	*cF4* $Fm\bar{3}m$
	(Zn)	Mg	*hP2* $P6_3/mmc$

System Al–Zr

Solution Phases:

Liquid, bcc–$A2$, fcc–$A1$, hcp–$A3$

Compounds:

Al_2Zr, Al_2Zr_3, Al_3Zr, Al_3Zr_2, Al_3Zr_5,
Al_4Zr_5, $AlZr$, $AlZr_2$, $AlZr_3$

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc–$A2$: Substitutional, Redlich-Kister
fcc–$A1$: Substitutional, Redlich-Kister
hcp–$A3$: Substitutional, Redlich-Kister
Al_2Zr : Stoichiometric, $(Al)_2(Zr)$
Al_2Zr_3 : Stoichiometric, $(Al)_2(Zr)_3$
Al_3Zr : Stoichiometric, $(Al)_3(Zr)$
Al_3Zr_2 : Stoichiometric, $(Al)_3(Zr)_2$
Al_3Zr_5 : Stoichiometric, $(Al)_3(Zr)_5$
Al_4Zr_5 : Stoichiometric, $(Al)_4(Zr)_5$
$AlZr$: Stoichiometric, $(Al)(Zr)$
$AlZr_2$: Stoichiometric, $(Al)(Zr)_2$
$AlZr_3$: Stoichiometric, $(Al)(Zr)_3$

Assessor and Date:

N. Saunders (1991)

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase Al_2Zr

$$G°T - 2.0\ H_{Al}^{o,fcc-A1}(298.15\ K) - H_{Zr}^{o,hcp-A3}(298.15\ K) =$$
$$-\ 137430.0 + 25.44\ T + 2.0\ GHSER_{Al} + GHSER_{Zr}$$

Phase Al_2Zr_3

$$G°T - 2.0\ H_{Al}^{o,fcc-A1}(298.15\ K) - 3.0\ H_{Zr}^{o,hcp-A3}(298.15\ K) =$$
$$-\ 192135.0 + 33.0\ T + 2.0\ GHSER_{Al} + 3.0\ GHSER_{Zr}$$

Phase $\mathrm{Al_3Zr}$

$$G^{\circ}T - 3.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc-}\mathit{A}1}(298.15\ \mathrm{K}) - H_{\mathrm{Zr}}^{\mathrm{o,hcp-}\mathit{A}3}(298.15\ \mathrm{K}) = \\ -162500.0 + 28.92\ T + 3.0\ \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Zr}}$$

Phase $\mathrm{Al_3Zr_2}$

$$G^{\circ}T - 3.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc-}\mathit{A}1}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Zr}}^{\mathrm{o,hcp-}\mathit{A}3}(298.15\ \mathrm{K}) = \\ -234700.0 + 44.1\ T + 3.0\ \mathrm{GHSER_{Al}} + 2.0\ \mathrm{GHSER_{Zr}}$$

Phase $\mathrm{Al_3Zr_5}$

$$G^{\circ}T - 3.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc-}\mathit{A}1}(298.15\ \mathrm{K}) - 5.0\ H_{\mathrm{Zr}}^{\mathrm{o,hcp-}\mathit{A}3}(298.15\ \mathrm{K}) = \\ -217488.0 + 48.72\ T + 3.0\ \mathrm{GHSER_{Al}} + 5.0\ \mathrm{GHSER_{Zr}}$$

Phase $\mathrm{Al_4Zr_5}$

$$G^{\circ}T - 4.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc-}\mathit{A}1}(298.15\ \mathrm{K}) - 5.0\ H_{\mathrm{Zr}}^{\mathrm{o,hcp-}\mathit{A}3}(298.15\ \mathrm{K}) = \\ -369000.0 + 62.55\ T + 4.0\ \mathrm{GHSER_{Al}} + 5.0\ \mathrm{GHSER_{Zr}}$$

Phase AlZr

$$G^{\circ}T - H_{\mathrm{Al}}^{\mathrm{o,fcc-}\mathit{A}1}\ (298.15\ \mathrm{K}) - H_{\mathrm{Zr}}^{\mathrm{o,hcp-}\mathit{A}3}(298.15\ \mathrm{K}) = \\ -89000.0 + 17.0384\ T + \mathrm{GHSER_{Al}} + \mathrm{GHSER_{Zr}}$$

Phase $\mathrm{AlZr_2}$

$$G^{\circ}T - H_{\mathrm{Al}}^{\mathrm{o,fcc-}\mathit{A}1}\ (298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Zr}}^{\mathrm{o,hcp-}\mathit{A}3}(298.15\ \mathrm{K}) = \\ -100125.0 + 17.553\ T + \mathrm{GHSER_{Al}} + 2.0\ \mathrm{GHSER_{Zr}}$$

Phase $\mathrm{AlZr_3}$

$$G^{\circ}T - H_{\mathrm{Al}}^{\mathrm{o,fcc-}\mathit{A}1}\ (298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Zr}}^{\mathrm{o,hcp-}\mathit{A}3}(298.15\ \mathrm{K}) = \\ -108000.0 + 22.38\ T + \mathrm{GHSER_{Al}} + 3.0\ \mathrm{GHSER_{Zr}}$$

Phase bcc-$A2$

$$L_{\mathrm{Al,Zr:\square}}^{0,\mathrm{bcc-}\mathit{A}2} = -122300 + 32\ T$$

$$L_{\mathrm{Al,Zr:\square}}^{1,\mathrm{bcc-}\mathit{A}2} = -11000$$

$$L_{\mathrm{Al,Zr:\square}}^{2,\mathrm{bcc-}\mathit{A}2} = 15000$$

Phase fcc–$A1$

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Al,Zr}:\square} = -120000 + 30\ T$$

$$L^{1,\mathrm{fcc}-A1}_{\mathrm{Al,Zr}:\square} = -10000$$

$$L^{2,\mathrm{fcc}-A1}_{\mathrm{Al,Zr}:\square} = 15000$$

Phase hcp–$A3$

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Al,Zr}:\square} = -122300 + 32\ T$$

$$L^{1,\mathrm{hcp}-A3}_{\mathrm{Al,Zr}:\square} = -8000$$

$$L^{2,\mathrm{hcp}-A3}_{\mathrm{Al,Zr}:\square} = 17000$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Al,Zr}} = -125000 + 35\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Al,Zr}} = -10000 + 5.57\ T$$

$$L^{2,\mathrm{liquid}}_{\mathrm{Al,Zr}} = 15750$$

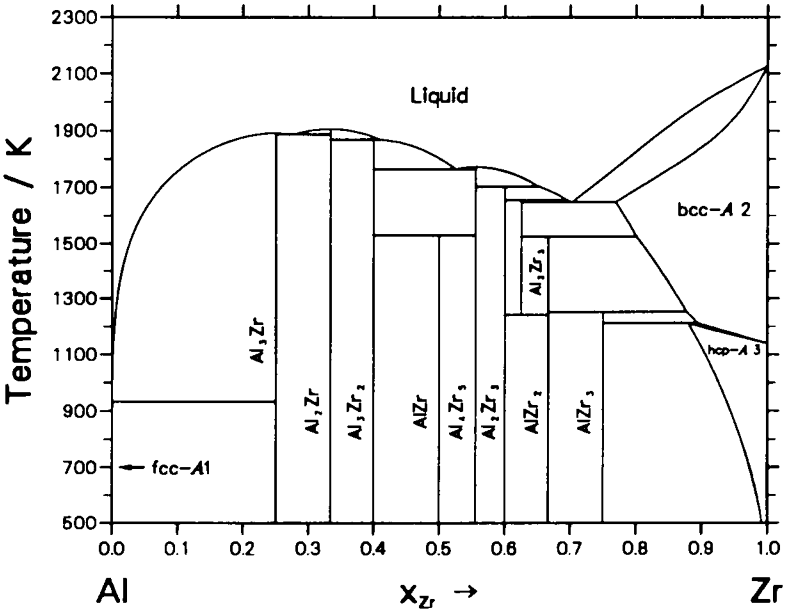


Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Zr}			T / K
Liquid $\rightleftharpoons$ fcc-$A1$ + Al_3Zr	Peritectic	.0002	.0008	.250	933.8
Al_3Zr $\rightleftharpoons$ Liquid	Congruent	.250	.250	...	1893.0
Liquid $\rightleftharpoons$ Al_3Zr + Al_2Zr	Eutectic	.277	.250	.333	1888.0
Al_2Zr $\rightleftharpoons$ Liquid	Congruent	.333	.333	...	1907.0
Liquid + Al_2Zr $\rightleftharpoons$ Al_3Zr_2	Peritectic	.410	.333	.400	1869.1
Liquid $\rightleftharpoons$ Al_3Zr_2 + Al_4Zr_5	Eutectic	.525	.400	.556	1765.3
Al_4Zr_5 $\rightleftharpoons$ Liquid	Congruent	.555	.555	...	1773.0
Liquid + Al_4Zr_5 $\rightleftharpoons$ Al_2Zr_3	Peritectic	.653	.556	.600	1701.8
Liquid + Al_2Zr_3 $\rightleftharpoons$ Al_3Zr_5	Peritectic	.696	.600	.625	1655.8
Liquid $\rightleftharpoons$ Al_3Zr_5 + bcc-$A2$	Eutectic	.702	.625	.768	1648.7
Al_2Zr_3 + bcc-$A2$ $\rightleftharpoons$ $AlZr_2$	Peritectoid	.600	.801	.666	1524.2
Al_3Zr_5 $\rightleftharpoons$ Al_2Zr_3 + $AlZr_2$	Eutectoid	.625	.600	.666	1241.7
$AlZr_2$ + bcc-$A2$ $\rightleftharpoons$ $AlZr_3$	Peritectoid	.667	.877	.750	1252.3
$AlZr_3$ + bcc-$A2$ $\rightleftharpoons$ hcp-$A3$	Peritectoid	.750	.894	.879	1212.2
Al_3Zr_2 + Al_4Zr_5 $\rightleftharpoons$ AlZr	Peritectoid	.400	.556	.500	1529.5

Table II:a - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-Zr	(Al)	Cu	$cF4$ $Fm\bar{3}m$	M 4	
	(Zr)	Mg	$hP2$ $P6_3/mmc$	M 2	
	(Zr)	W	$cI2$ $Im\bar{3}m$	M 4	
	AlZr	BCr	$oC8$ $Cmcm$	Al 4 Zr 4	
	$AlZr_2$	$InNi_2$	$hP6$ $P6_3/mmc$	Al 2 Zr_1 2 Zr_2 4	

Table II:b - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
	$AlZr_3$	$AuCu_3$	$cP4$ $Pm\bar{3}m$	Al 1 Zr 3	
	Al_2Zr	$MgZn_2$	$hP12$ $P6_3/mmc$		
	Al_2Zr_3	Al_2Zr_3	$tP20$ $P4_2/mnm$	Al 8 Zr_1 4 Zr_2 4 Zr_3 4	
	Al_3Zr	Al_3r	$tI16$ $I4/mmm$	Al_1 4 Al_2 4 Al_3 4 Zr 4	
	Al_3Zr_2	Al_3Zr_2	$oF40$ $Fdd2$	Al_1 8 Al_2 16 Al_3 16	
	Al_3Zr_4	Al_3Zr_4	$hP7$ $P\bar{6}$	Al 3 Zr_1 1 Zr_2 1 Zr_3 2	
	Al_3Zr_5	Mn_5Si_3	$hP16$ $P6_3/mcm$	Al 6 Zr_1 4 Zr_2 6	not in Masl
	Al_3Zr_5	Si_3W_5	$tI32$ $I4/mcm$	Al_1 4 Al_1 8 Zr_1 4 Zr_2 16	
	Al_4Zr_5	Ga_4Ti_5	$hP18$ $P6_3/mcm$	Al_1 2 Al_2 6 Zr_1 4 Zr_2 6	not in Masl

System B–C

Solution Phases:

Liquid, graphite, β-rhombo-B, B_4C

Modelling:

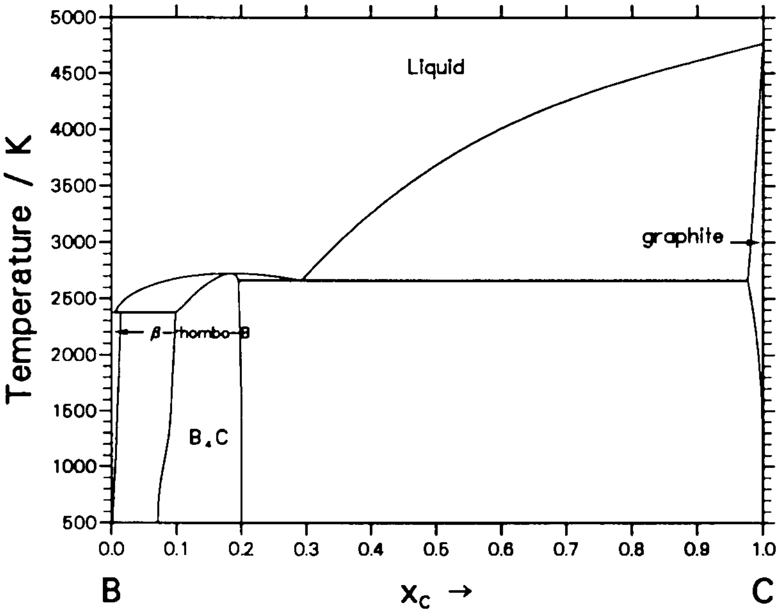
Liquid : Substitutional, Redlich-Kister
graphite : Substitutional, Redlich-Kister
β-rhombo-B : Sublattice model $(B)_{93}(B,C)_{12}$
B_4C : Sublattice model $(B_{11},B_{12})(B_2,C_2B,CB_2)$

Assessor and Date:

B. Kasper, H.L. Lukas, (1992).

Publication:

B. Kasper, Thesis, Univ. Stuttgart (Germany).



Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase B$_4$C

$$G^\circ(T) - 13.0\ H_{\mathrm{B}}^{\mathrm{o},\beta\text{-rhombo-B}}(298.15\ \mathrm{K}) - H_{\mathrm{C}}^{\mathrm{o,graphite}}(298.15\ \mathrm{K}) = \mathrm{G}(\mathrm{B}_{11}{:}\mathrm{B}_2) = -170978.12 + 22.909095\ T + 16.0\ \mathrm{GHSER_B} + \mathrm{GHSER_C}$$

$$G^\circ(T) - 14.0\ H_{\mathrm{B}}^{\mathrm{o},\beta\text{-rhombo-B}}(298.15\ \mathrm{K}) = = \mathrm{G}(\mathrm{B}_{12}{:}\mathrm{B}_2) = 10000 + 22.909095\ T + 14.0\ \mathrm{GHSER_B}$$

$$G^\circ(T) - 12.0\ H_{\mathrm{B}}^{\mathrm{o},\beta\text{-rhombo-B}}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{C}}^{\mathrm{o,graphite}}(298.15\ \mathrm{K}) = \mathrm{G}(\mathrm{B}_{11}{:}\mathrm{C}_2\mathrm{B}) = -347121.82 + 22.909095\ T + 12.0\ \mathrm{GHSER_B} + 3.0\ \mathrm{GHSER_C}$$

$$G^\circ(T) - 13.0\ H_{\mathrm{B}}^{\mathrm{o},\beta\text{-rhombo-B}}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{C}}^{\mathrm{o,graphite}}(298.15\ \mathrm{K}) = \mathrm{G}(\mathrm{B}_{12}{:}\mathrm{C}_2\mathrm{B}) = -294040.52 + 22.909095\ T + 13.0\ \mathrm{GHSER_B} + 2.0\ \mathrm{GHSER_C}$$

$$G^\circ(T) - 13.0\ H_{\mathrm{B}}^{\mathrm{o},\beta\text{-rhombo-B}}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{C}}^{\mathrm{o,graphite}}(298.15\ \mathrm{K}) = \mathrm{G}(\mathrm{B}_{11}{:}\mathrm{CB}_2) = -304040.52 + 22.909095\ T + 13.0\ \mathrm{GHSER_B} + 2.0\ \mathrm{GHSER_C}$$

$$G^\circ(T) - 14.0\ H_{\mathrm{B}}^{\mathrm{o},\beta\text{-rhombo-B}}(298.15\ \mathrm{K}) - H_{\mathrm{C}}^{\mathrm{o,graphite}}(298.15\ \mathrm{K}) = \mathrm{G}(\mathrm{B}_{12}{:}\mathrm{CB}_2) = -169978.12 + 22.909095\ T + 14.0\ \mathrm{GHSER_B} + \mathrm{GHSER_C}$$

$$L_{\mathrm{B_{11}C,B_{12}:B_2}}^{0,\mathrm{B_4C}} = 1.0\mathrm{E}{-4}$$

Phase β-rhombo-B

$$G^\circ(T) - 105.0\ H_{\mathrm{B}}^{\mathrm{o},\beta\text{-rhombo-B}}(298.15\ \mathrm{K}) = \mathrm{G}(\mathrm{B}{:}\mathrm{B}) = 105\ \mathrm{GHSER_B}$$

$$G^\circ(T) - 93.0\ H_{\mathrm{B}}^{\mathrm{o},\beta\text{-rhombo-B}}(298.15\ \mathrm{K}) - 12.0\ H_{\mathrm{C}}^{\mathrm{o,graphite}}(298.15\ \mathrm{K}) = \mathrm{G}(\mathrm{B}{:}\mathrm{C}) = 1000000 + 93.0\ \mathrm{GHSER_B} + 12.0\ \mathrm{GHSER_C}$$

$$L_{\mathrm{B:B,C}}^{0,\beta\text{-rhombo-B}} = -2769690.3$$

Phase graphite

$$L_{\mathrm{B,C}}^{0,\mathrm{graphite}} = 34385.95 + 8.6792\ T$$

Phase liquid

$$L_{\mathrm{B,C}}^{0,\mathrm{liquid}} = -67045.16 + 4.46969\ T$$

$$L_{\mathrm{B,C}}^{1,\mathrm{liquid}} = -36682.57 + 2.44551\ T$$

Table I - Invariant Reactions.

Reaction	Type	Compositions x_C			T / K
Liquid $\rightleftharpoons$ B_4C + graphite	Eutectic	.292	.195	.977	2663.4
Liquid + B_4C $\rightleftharpoons$ β-rhombo-B	Peritectic	.0056	.099	.010	2375.9
B_4C $\rightleftharpoons$ Liquid	Congruent	.184	.184	....	2725.3

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
B-C	(B)	β-rhombo-B			
	(C)	graphite			
	B_4C	B_4C	*hR15* $R\bar{3}m$	B_1 3 B_2 18 B_3 18 C 6	$B_{13}C_2$ in [91Vil]

System B–Hf

Solution Phases:

Liquid, bcc–$A2$, hcp–$A3$

Compounds:

(stable)	BHf, B_2Hf
(metastable)	B_4Hf_3

Modelling:

Liquid : Substitutional, Redlich–Kister
bcc–$A2$: Substitutional, Redlich–Kister
hcp–$A3$: Substitutional, Redlich–Kister
BHf : Stoichiometric, (B)(Hf)
B_2Hf : Stoichiometric, $(B)_2(Hf)$
B_4Hf_3 : Stoichiometric, $(B)_4(Hf)_3$

Assessor and Date:

H. Bitterman, Univ. Vienna, Austria

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase BHf

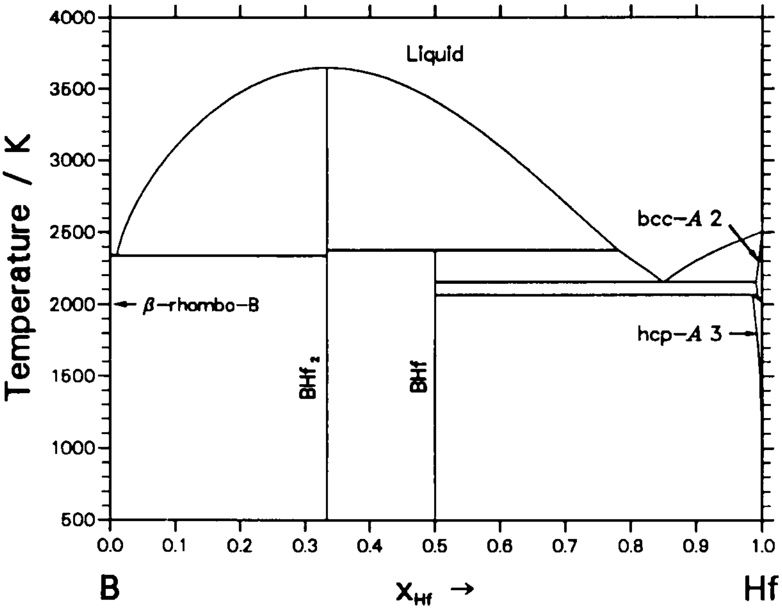
$$G°(T) - H_{B}^{o,\beta-rhombo-B}(298.15K) - H_{Hf}^{o,hcp-A3}(298.15K) = -159810 + 4.98602\ T + GHSER_{B} + GHSER_{Hf}$$

Phase B_4Hf_3

$$G°(T) - 4.0\ H_{B}^{o,\beta-rhombo-B}(298.15K) - 3.0\ H_{Hf}^{o,hcp-A3}(298.15K) = -535000 - 14.5754\ T + 4.0\ GHSER_{B} + 3.0\ GHSER_{Hf}$$

Phase B_2Hf

$$G°(T) - 2.0\ H_{B}^{o,\beta-rhombo-B}(298.15K) - H_{Hf}^{o,hcp-A3}(298.15K) = -351445 + 469.146\ T - 73.868\ T \cdot \ln T - 0.0036789\ T^{2} + 1517800\ T^{-1} - 5.2E{+}09T^{-3}$$



Phase bcc-A2

$$G^\circ(T) - 3.0\ H_B^{\circ,\beta-\text{rhombo}-B}(298.15K) - H_{Hf}^{\circ,\text{hcp}-A3}(298.15K) = -137926 + 3.0\ \text{GHSER}_B + \text{GHSER}_{Hf}$$

$$L_{Hf:B,\square}^{0,\text{bcc}-A2} = 1.0E\text{-}4$$

Phase hcp-A3

$$G^\circ(T) - 0.5\ H_B^{\circ,\beta-\text{rhombo}-B}(298.15K) - H_{Hf}^{\circ,\text{hcp}-A3}(298.15K) = -44765.7 + 0.5\ \text{GHSER}_B + \text{GHSER}_{Hf}$$

$$L_{Hf:B,\square}^{0,\text{hcp}-A3} = 1.0E\text{-}4$$

Phase liquid

$$L_{B,Hf}^{0,\text{liquid}} = -170625 - 4.85541\ T$$

$$L_{B,Hf}^{1,\text{liquid}} = -39128$$

$$L_{B,Hf}^{2,\text{liquid}} = 16331.1$$

Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Hf}			T / K
Liquid $\rightleftharpoons$ β-rhombo-B + B_2Hf	Eutectic	.010	.000	.333	2337.9
Liquid + B_2Hf $\rightleftharpoons$ + BHf	Peritectic	.780	.333	.500	2377.1
Liquid $\rightleftharpoons$ BHf + bcc-$A2$	Eutectic	.850	.500	.990	2153.6
bcc-$A2$ + BHf $\rightleftharpoons$ hcp-$A3$	Peritectic	.993	.500	.985	2063.8
B_2Hf $\rightleftharpoons$ Liquid	Congruent	.333	.333	.....	3650.0

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
B-Hf	(B)	β-rhombo-B			
	(Hf)	Mg	*hP2* $P6_3/mmc$	M 2	
	(Hf)	W	*cI2* $Im\bar{3}m$	M 2	
	BHf	BFe	*oP8* *Pnma*	B 4 Hf 4	
	B_2Hf	AlB_2	*hP3* *P6/mmm*	B 2 Hf 1	
	B_4Hf_3	B_4Ta_3	*oI14* *Immm*		(metastable)

System B–N

Solution Phases:

Liquid, gas

Compound:

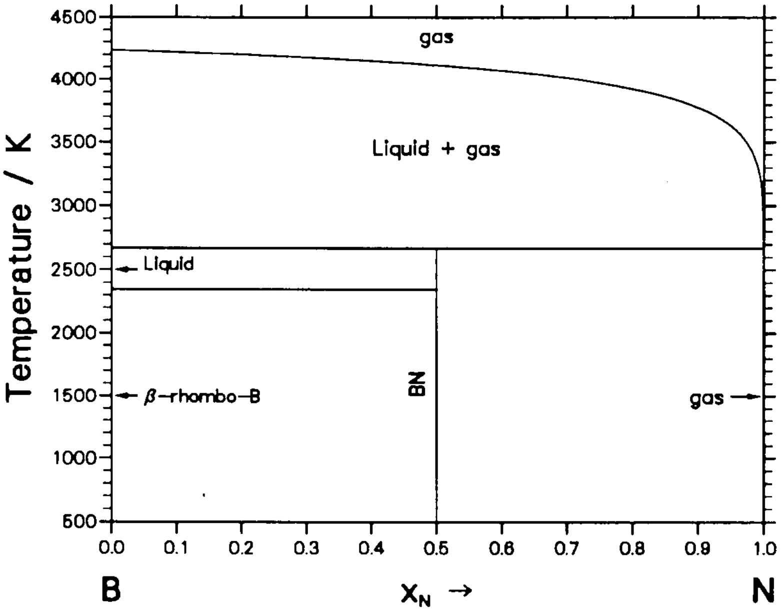
BN

Modelling:

Liquid : Substitutional, Redlich–Kister
gas : ideal (B,B_2,N,N_2,N_3,BN)
BN : Stoichiometric (B)(N)

Assessor and Date:

H. Wen, and H.L. Lukas 1992



Thermodynamic properties of the solution and compound phases ($J.mol^{-1}$)

Phase BN

$G^{\circ}(T) - H_{B}^{\circ,\beta-\mathrm{rhombo}-B}(298.15\ K) - H_{0.5N_2}^{\circ,\mathrm{gas}}(298.15\ K) =$
$- 250600 + 91.281942\ T + GHSER_B + GHSER_N$

Phase liquid

$L_{B,N}^{0,\mathrm{liquid}} = 30000.0 - 4.0\ T$

Phase gas(B,B₂,N,N₂,N₃,BN) ($P = 0.1 MPa$)

$G_{B}^{\circ,\mathrm{gas}}(T) - H_{B}^{\circ,\beta-\mathrm{rhombo}-B} = R\ T\ \ln P +$
$298.15 < T < 700.00$: $564913.402 - 13.9693124\ T + 1.6646044E\text{-}05\ T^2 - 20.80858\ T \cdot \ln T$
$700.00 < T < 2800.00$: $564920.973 - 14.1156663\ T - 20.786112\ T \cdot \ln T$
$2800.00 < T < 4075.00$: $565086.023 - 15.0515115\ T - 20.6682069\ T \cdot \ln T - 2.10566E\text{-}05\ T^2$

$G_{B_2}^{\circ,\mathrm{gas}}(T) - 2.0\ H_{B}^{\circ,\beta-\mathrm{rhombo}-B} = R\ T\ \ln P +$
$298.15 < T < 550.00$: $824867.604 - 125.766398\ T - 8.168\ T \cdot \ln T - 0.0430888612\ T^2 + 1.00098016E\text{-}05\ T^3 - 136465.972\ T^{-1}$
$550.00 < T < 2150.00$: $809306.765 + 132.643168\ T - 48.851589\ T \cdot \ln T + 0.00423205742\ T^2 - 3.22751598E\text{-}07\ T^3 + 980387.558\ T^{-1}$
$2150.00 < T < 6000.00$: $826793.716 + 32.6504991\ T - 35.6295549\ T \cdot \ln T - 4.58209505E\text{-}04\ T^2 + 1.70149264E\text{-}10\ T^3 - 3665441.32\ T^{-1}$

$G_{N}^{\circ,\mathrm{gas}}(T) - 2.0\ H_{0.5N_2}^{\circ,\mathrm{gas}}(298.15\ K) = R\ T\ \ln P +$
$298.15 < T < 2950.00$: $466446.153 + 2788.78662\ T^{-1} - 13.2660528\ T - 20.8939295\ T \cdot \ln T + 8.4552092E\text{-}05\ T^2 - 1.00186856E\text{-}08\ T^3$
$2950.00 < T < 6000.00$: $481259.023 - 7559107.28\ T^{-1} - 52.4348889\ T - 16.3761342\ T \cdot \ln T - 2.28373808E\text{-}04\ T^2 - 2.78997209E\text{-}08\ T^3$

$G_{N_2}^{\circ,\mathrm{gas}}(T) - 2.0\ H_{0.5N_2}^{\circ,\mathrm{gas}}(298.15\ K) = 2.0\ GHSER_N + R\ T\ \ln P$

$$G^{o,gas}_{N_3}(T) - 3.0\ H^{o,gas}_{0.5N_2}(298.15\ K) = R\,T\ \ln P +$$

$$\begin{array}{rcrcl}
298.15 & < T < & 800.00 & : & 403075.636 - 14.3245228\ \mathrm{T} - 29.5595416\ T\cdot\ln T \\
 & & & & - 0.02413122\ T^2 + 3.6156036\mathrm{E}{-}06\ T^3 \\
 & & & & + 55714.144\ T^{-1} \\
800.00 & < T < & 2000.00 & : & 388937.207 + 158.809275\ \mathrm{T} - 55.404528\ T\cdot\ln T \\
 & & & & - 0.0026570492\ T^2 + 1.9365644\mathrm{E}{-}07\ T^3 \\
 & & & & + 1536448.48\ T^{-1} \\
2000.00 & < T < & 6000.00 & : & 380898.006 + 210.207464\ \mathrm{T} - 62.295576\ T\cdot\ln T \\
 & & & & + 6.5726456\mathrm{E}{-}06\ T^2 - 7.868012\mathrm{E}{-}10\ T^3 \\
 & & & & + 3336949.2\ T^{-1}
\end{array}$$

$$G^{o,gas}_{BN}(T) - H^{o,\beta-\mathrm{rhombo}-B}_{B}(298.15\ K) - H^{o,gas}_{0.5N_2}(298.15\ K) = R\,T\ \ln P +$$

$$\begin{array}{rcrcl}
298.15 & < T < & 1000.00 & : & 469920.773 - 57.4937871\ \mathrm{T} - 22.339422\ T\cdot\ln T \\
 & & & & - 0.0105569014\ T^2 + 1.41488236\mathrm{E}{-}06\ T^3 \\
 & & & & - 69873.2184\ T^{-1} \\
1000.00 & < T < & 3500.00 & : & 462619.822 + 28.1899597\ \mathrm{T} - 35.0100802\ T\cdot\ln T \\
 & & & & - 7.99851096\mathrm{E}{-}04\ T^2 + 1.10267925\mathrm{E}{-}08\ T^3 \\
 & & & & + 719942.972\ T^{-1} \\
3500.00 & < T < & 6000.00 & : & 449529.29 + 65.7741362\ \mathrm{T} - 39.4662494\ T\cdot\ln T \\
 & & & & - 1.95814338\mathrm{E}{-}04\ T^2 - 9.14385307\mathrm{E}{-}10\ T^3 \\
 & & & & + 7491452\ T^{-1}
\end{array}$$

Table I - Invariant Reactions.

Reaction	Type	Compositions x_N			T / K
Liquid + gas $\rightleftharpoons$ BN	Peritectic-like	.000	1.000	.500	2670.0
Liquid $\rightleftharpoons$ BN + gas	Degenerate	.000	.000	.500	2670.0

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Comments
B-N	β-rhombo-B	β-rhombo-B	*hR108* $R\bar{3}m$	*hR105* in [91Vil]
	BN	.....	*hP4* $P6_3mc$	

System B–Si

Solution Phases:

Liquid, diamond, β-rhombo-B, B_nSi, B_3Si, B_6Si

Modelling:

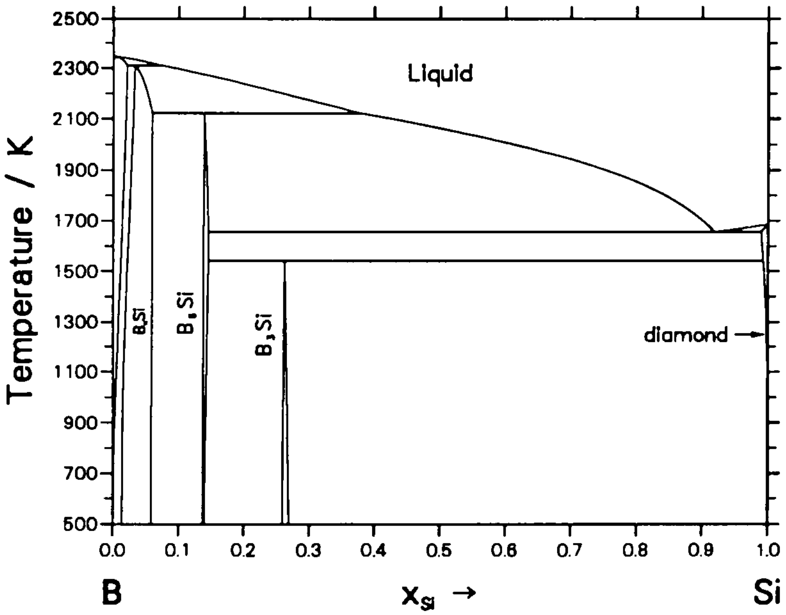
Liquid : Substitutional, Redlich-Kister
diamond : Substitutional, Redlich-Kister
β rhombo-B : Sublattice model $(B)_{93}(B,Si)_{12}$
B_nSi : Sublattice model $(B)_{61}(Si)(B,Si)_8$
B_3Si : Sublattice model $(B)_6(Si)_2(B,Si)_6$
B_6Si : Sublattice model $(B)_{210}(Si)_{23}(B,Si)_{48}$

Assessor and Date:

S. Fries, and H.L. Lukas,

Publication:

"Cost507 New Light Alloys", Leuven Proceedings, Ed. G. Effenberg (1991)



Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase B$_3$Si

$$G^\circ(T) - 12.0\ H_{\mathrm{B}}^{\mathrm{o},\beta-\mathrm{rhombo-B}}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = \mathrm{G(B{:}Si{:}B)} = 112000 + 12.0\ \mathrm{GHSER_B} + 2.0\ \mathrm{GHSER_{Si}}$$

$$G^\circ(T) - 6.0\ H_{\mathrm{B}}^{\mathrm{o},\beta-\mathrm{rhombo-B}}(298.15\ \mathrm{K}) - 8.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = \mathrm{G(B{:}Si{:}Si)} = 112000 + 6.0\ \mathrm{GHSER_B} + 8.0\ \mathrm{GHSER_{Si}}$$

$$L_{\mathrm{B:Si:B,Si}}^{0,\mathrm{B_3Si}} = -\,2400475 + 240.0475\ T$$

Phase B$_6$Si

$$G^\circ(T) - 258.0\ H_{\mathrm{B}}^{\mathrm{o},\beta-\mathrm{rhombo-B}}(298.15\ \mathrm{K}) - 23.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = \mathrm{G(B{:}Si{:}B)} = 729824.4 - 72.98244\ T + 258.0\ \mathrm{GHSER_B} + 23.0\ \mathrm{GHSER_{Si}}$$

$$G^\circ(T) - 210.0\ H_{\mathrm{B}}^{\mathrm{o},\beta-\mathrm{rhombo-B}}(298.15\ \mathrm{K}) - 71.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = \mathrm{G(B{:}Si{:}Si)} = 5454560 - 545.456\ T + 210.0\ \mathrm{GHSER_B} + 71.0\ \mathrm{GHSER_{Si}}$$

$$L_{\mathrm{B:Si:B,Si}}^{0,\mathrm{B_6Si}} = -\,15715630 + 1571.563\ T$$

Phase B$_n$Si

$$G^\circ(T) - 69.0\ H_{\mathrm{B}}^{\mathrm{o},\beta-\mathrm{rhombo-B}}(298.15\ \mathrm{K}) - H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = \mathrm{G(B{:}Si{:}B)} = -\,89819.86 + 8.981986\ T + 69.0\ \mathrm{GHSER_B} + \mathrm{GHSER_{Si}}$$

$$G^\circ(T) - 61.0\ H_{\mathrm{B}}^{\mathrm{o},\beta-\mathrm{rhombo-B}}(298.15\ \mathrm{K}) - 9.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = \mathrm{G(B{:}Si{:}Si)} = -\,176659.7 + 17.66597\ T + 61.0\ \mathrm{GHSER_B} + 9.0\ \mathrm{GHSER_{Si}}$$

$$L_{\mathrm{B:Si:B,Si}}^{0,\mathrm{B_nSi}} = -\,281573.6 + 28.15736\ T$$

Phase β–rhombo–B

$$G^\circ(T) - 93.0\ H_{\mathrm{B}}^{\mathrm{o},\beta-\mathrm{rhombo-B}}(298.15\ \mathrm{K}) - 12.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = \mathrm{G(B{:}Si)} = -\,6160.245 + 0.6160245\ T + 93.0\ \mathrm{GHSER_B} + 12.0\ \mathrm{GHSER_{Si}}$$

$$L_{\mathrm{B:B,Si}}^{0,\beta-\mathrm{rhombo-B}} = -\,725614.0 + 72.5614\ T$$

Phase diamond

$$L_{\mathrm{B,Si:\square}}^{0,\mathrm{diamond}} = 57978.16$$

Phase liquid

$$L_{\mathrm{B,Si}}^{0,\mathrm{liquid}} = 17631.92 - 1.76321\ T$$

$$L_{\mathrm{B,Si}}^{1,\mathrm{liquid}} = -\,3526.99 + 0.3527\ T$$

Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Si}			T / K
B_6Si + diamond ⇌ B_3Si	Peritectoid	.145	.993	.262	1543.0
Liquid ⇌ B_6Si + diamond	Eutectic	.919	.146	.989	1657.6
Liquid + B_nSi ⇌ B_6Si	Peritectic	.379	.059	.138	2123.0
Liquid + β-rhombo-B ⇌ B_nSi	Peritectic	.074	.021	.033	2310.0

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices		Comments
B-Si	(B)	β-rhombo-B				
	(Si)	diamond	*cF8* $Fd\bar{3}m$	M	8	
	B_nSi	B	*hR12* $P\bar{3}m$			
	B_3Si	B_4C	*hR15* $R\bar{3}m$	B M Si_1 Si_2	18 18 6 3	*hR14* in [91Vil]
	B_6Si	B_6Si	*oP280* *Pnnm*			*oP340* in [Vil91]

System B–Ti

Solution Phases:

Liquid, bcc-$A2$, hcp-$A3$

Compounds:

BTi, B_4Ti_3, B_2Ti

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-$A2$: Substitutional, Redlich-Kister
hcp-$A3$: Substitutional, Redlich-Kister
BTi : Stoichiometric, (B)(Ti)
B_4Ti_3 : Stoichiometric, $(B)_4(Ti)_3$
B_2Ti : Stoichiometric, $(B)_2(Ti)$

Assessor and Date:

C. Bätzner, June 1994

Publication:

Thesis, Univ. Stuttgart, Germany (1994)

Thermodynamic properties of the solution and compound phases ($J.mol^{-1}$)

Phase BTi

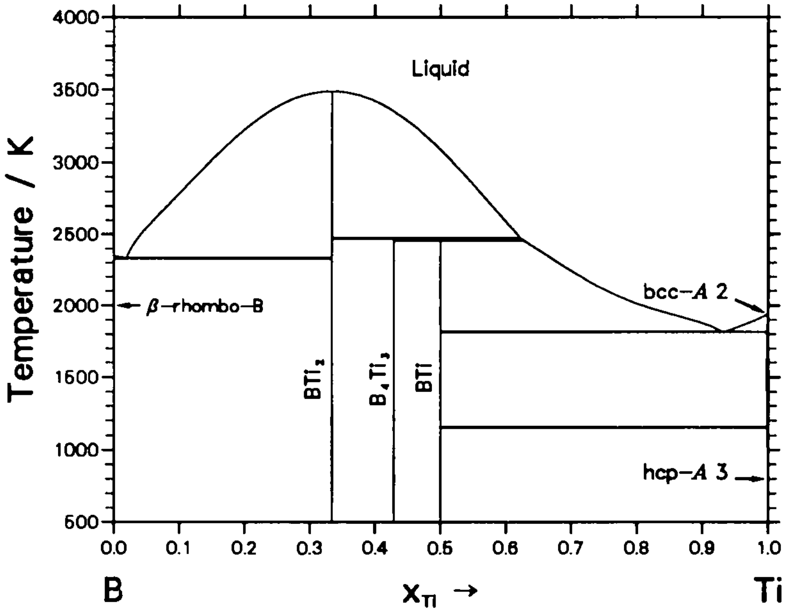
$$G^\circ(T) - H_B^{\circ,\beta-\mathrm{rhombo-B}}(298.15K) - H_{Ti}^{\circ,\mathrm{hcp}-A3}(298.15K) = \\ -166196.8 + 3.2968\ T + GHSER_B + GHSER_{Ti}$$

Phase B_4Ti_3

$$G^\circ(T) - 4.0\ H_B^{\circ,\beta-\mathrm{rhombo-B}}(298.15K) - 3.0\ H_{Ti}^{\circ,\mathrm{hcp}-A3}(298.15K) = \\ -660745.8 + 4.3472923\ T + 2.162216\ T\cdot \ln T \\ + 4.0\ GHSER_B + 3.0\ GHSER_{Ti}$$

Phase B_2Ti

$$G^\circ(T) - 2.0\ H_B^{\circ,\beta-\mathrm{rhombo-B}}(298.15K) - H_{Ti}^{\circ,\mathrm{hcp}-A3}(298.15K) = \\ -318253.47 - 2.5557\ T + 0.799221\ T\cdot \ln T \\ + 0.002843367\ T^2 + 2.0\ GHSER_B + GHSER_{Ti}$$



Phase bcc-A2

$$G^{\circ}(T) - 3.0\ H_{\mathrm{B}}^{\mathrm{o},\beta\text{-rhombo-B}}(298.15\mathrm{K}) - H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\mathrm{K}) =$$
$$- 200000 + 14.0\ T + 3.0\ \mathrm{GHSER_B} + \mathrm{GHSER_{Ti}}$$
$$L_{\mathrm{Ti:B,\square}}^{0,\mathrm{bcc-}A2} = - 260162.96 + 156.48207\ T$$

Phase hcp-*A*3

$$G^{\circ}(T) - 0.5\ H_{\mathrm{B}}^{\mathrm{o},\beta\text{-rhombo-B}}(298.15\mathrm{K}) - H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\mathrm{K}) =$$
$$- 50000 + 15.0\ T + 0.5\ \mathrm{GHSER_B} + \mathrm{GHSER_{Ti}}$$
$$L_{\mathrm{Ti:B,\square}}^{0,\mathrm{hcp-}A3} = - 21213.442$$

Phase liquid

$$L_{\mathrm{B,Ti}}^{0,\mathrm{liquid}} = - 265414.4 + 15.543418\ T$$

$$L_{\mathrm{B,Ti}}^{1,\mathrm{liquid}} = - 134303.03 + 17.709482\ T$$

$$L_{\mathrm{B,Ti}}^{2,\mathrm{liquid}} = 61691.479$$

$$L_{\mathrm{B,Ti}}^{3,\mathrm{liquid}} = 52656.13$$

Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Ti}			T / K
Liquid $\rightleftharpoons$ β-rhombo-B + B_2Ti	Eutectic	.019	.000	.333	2332.5
Liquid + B_2Ti $\rightleftharpoons$ B_4Ti_3	Peritectic	.578	.333	.428	2474.0
Liquid + B_4Ti_3 $\rightleftharpoons$ BTi	Peritectic	.627	.428	.500	2456.0
Liquid $\rightleftharpoons$ BTi + bcc-$A2$	Eutectic	.931	.500	.997	1814.1
bcc-$A2$ $\rightleftharpoons$ BTi + hcp-$A3$	Transformation	.998	.500	1.000	1156.1
B_2Ti $\rightleftharpoons$ Liquid	Congruent	.333	.333	.....	3490.0

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices
B-Ti	(B)	β-rhombo-B		
	(Ti)	Mg	$hP2$ $P6_3/mmc$	M 2
	(Ti)	W	$cI2$ $Im\bar{3}m$	M 2
	BTi	BFe	$oP8$ $Pnma$	B 4 Ti 4
	B_2Ti	AlB_2	$hP3$ $P6/mmm$	B 2 Ti 1
	B_4Ti_3	B_4Ta_3	$oI14$ $Immm$	

System C–Si

Solution Phases:

Liquid, diamond

Compounds:

SiC, Si_4C_3 (metastable)

Modelling:

Liquid : Substitutional, Redlich-Kister
diamond : Substitutional, Redlich-Kister
SiC : Stoichiometric, (Si)(C)
Si_4C_3 : Stoichiometric, $(Si)_4(C)_3$

Assessor and Date:

J. Gröbner, H. L. Lukas, and F. Aldinger.

Publication:

Calphad **20**, 2 (1996) 247-254.

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase SiC

$$G^{\circ}(T) - H_{\mathrm{C}}^{\mathrm{o,graphite}}(298.15\ \mathrm{K}) - H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = - 88583.96 + 271.1462\ T - 41.27945\ T \cdot \ln T - 0.00436266\ T^2 + 2\mathrm{E}{-}07\ T^3 + 800000\ T^{-1}$$

Phase Al_4C_3 (metastable)

$$G^{\circ}(T) - 3.0\ H_{\mathrm{C}}^{\mathrm{o,graphite}}(298.15\ \mathrm{K}) - 4.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = - 135043.86 + 949.01177\ T - 144.478096\ T \cdot \ln T - 0.01527\ T^2 + 7\mathrm{E}{-}07\ T^3 + 2800000\ T^{-1}$$

Phase liquid

$$L_{\mathrm{C,Si}}^{0,\mathrm{liquid}} = 25644.97 - 6.381115\ T$$

Phase diamond

$$L_{\mathrm{C,Si}}^{0,\mathrm{diamond}} = 93386.78$$

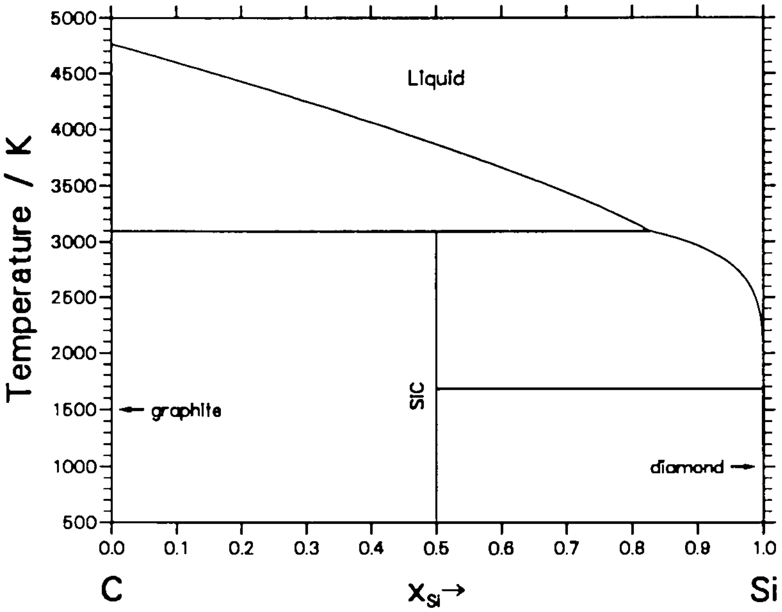


Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Si}			T / K
Liquid ⇌ diamond + SiC	Degenerate	1.000	1.000	.500	1687.0
Liquid + graphite ⇌ SiC	Peritectic	.826	.000	.500	3096.4

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices
C–Si	(C)	graphite		
	(Si)	diamond	$cF8$ $Fd\bar{3}m$	M 8
	SiC-β	ZnS (sphalerite)	$cF8$ $F\bar{4}3m$	C 4 Si 4

System C–Ti

Solution Phases:

Liquid, bcc–$A2$, fcc–$A1$, hcp–$A3$

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc–$A2$: Sub-lattice, (Ti)(C,$\square$)
fcc–$A1$: Sub-lattice, (Ti)(C,$\square$)
hcp–$A3$: Sub-lattice, (Ti)(C,$\square$)

Assessor and Date:

S. Jonsson

Publication:

Thesis, Royal Institute of Technology, Stockholm, Sweden (1993)

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase fcc–$A1$

$$\begin{aligned} G^{\circ}(T) - H_{\mathrm{C}}^{\mathrm{o,graphite}}(298.15\ \mathrm{K}) - H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}C)} = \\ -\,207709.0 + 307.438\ T - 48.0195\ T\cdot \ln T - 0.00272\ T^{2} \\ -\,2.03\mathrm{E}{+}09\ T^{-3} + 819000\ T^{-1} \end{aligned}$$

$$L_{\mathrm{Ti:C}\square}^{0,\mathrm{fcc-}A1} = -\,85115 + 6.756\ T$$

$$L_{\mathrm{Ti:C}\square}^{1,\mathrm{fcc-}A1} = -\,129429 + 31.79\ T$$

Phase bcc–$A2$

$$\begin{aligned} G^{\circ}(T) - 3.0\ H_{\mathrm{C}}^{\mathrm{o,graphite}}(298.15\ \mathrm{K}) - H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}C)} \\ 2295533 + \mathrm{GHSER}_{\mathrm{TiC}} + 2.0\ \mathrm{GHSER}_{\mathrm{C}} \end{aligned}$$

$$L_{\mathrm{Ti:C}\square}^{0,\mathrm{bcc-}A2} = -\,2590609$$

Phase hcp–$A3$

$$\begin{aligned} G^{\circ}(T) - 0.5\ H_{\mathrm{C}}^{\mathrm{o,graphite}}(298.15\ \mathrm{K}) - H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}C)} \\ -\,1432 - 4.1241\ T + 0.5\ \mathrm{GHSER}_{\mathrm{TiC}} + 0.5\ \mathrm{GHSER}_{\mathrm{C}} \end{aligned}$$

Phase liquid

$$L_{\mathrm{C,Ti}}^{0,\mathrm{liquid}} = -\,214678 - 14.314\ T$$

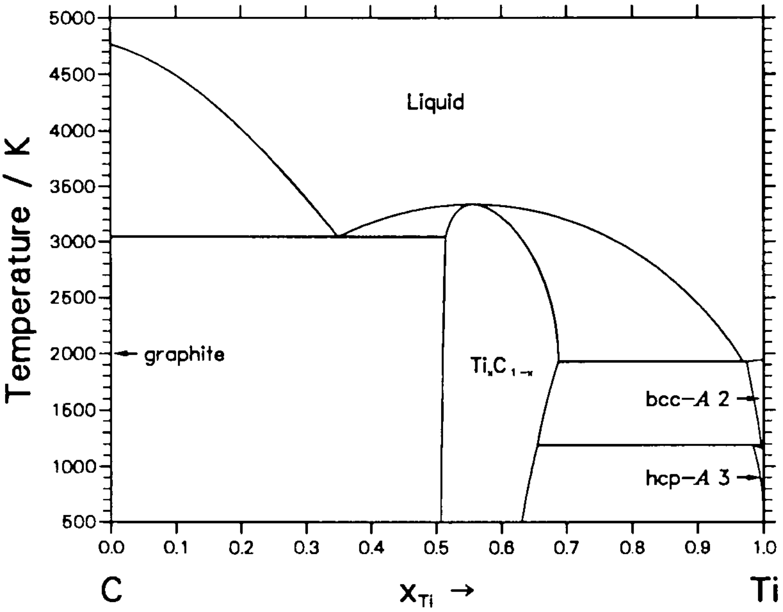


Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Ti}			T / K
Liquid ⇌ fcc–$A1^*$ + bcc–$A2$	Eutectic	.968	.687	.974	1925.2
fcc–$A1^*$ + bcc–$A2$ ⇌ hcp–$A3$	Peritectoid	.655	.996	.984	1190.0
Liquid ⇌ graphite + fcc–$A1$	Eutectic	.349	.000	.515	3044.0
fcc–$A1$ ⇌ Liquid	Congruent	.554	.554	...	3338.0

* fcc–$A1 \equiv Ti_xC_{1-x}$

Table II:a - Crystal Structure and Phase Description.

System	Phase	Structural Type	Pearson Symbol Space Group	Sub-lattices	Comments
C-Ti	(C)	graphite			
	(Ti)	Mg	$hP2$ $P6_3/mmc$	M 2	
	(Ti)	W	$I2$ $Im\bar{3}m$	M 2	

Table II:b - Crystal Structure and Phase Description.

System	Phase	Structural Type	Pearson Symbol Space Group	Sub-lattices	Comments
	CTi	ClNa	*cF*8 $Fm\bar{3}m$	M_1 4 M_2 4	
	CTi_2	$Ca_{33}Ge$	*cF*48 $Fd\bar{3}m$	C 16 Ti 32	$Ca_{33}Ge$ in [91Vil] ord. TiC_{1-x} phase not considered

System Ce–Mg

Solution Phases:

Liquid, bcc-*A*2, fcc-*A*1, hcp-*A*3

Compounds:

$CeMg$, $CeMg_2$, $CeMg_3$, Ce_5Mg_{41}, Ce_2Mg_{17}, $CeMg_{12}$

Modelling:

Liquid : Substitutional, Redlich-Kister
fcc-*A*1 : Substitutional, Redlich-Kister
hcp-*A*3 : Substitutional, Redlich-Kister
$CeMg$: Stoichiometric, $(Ce)(Mg)$
$CeMg_2$: Stoichiometric, $(Ce)(Mg)_2$
$CeMg_3$: Stoichiometric, $(Ce)(Mg)_3$
Ce_5Mg_{41} : Stoichiometric, $(Ce)_5(Mg)_{41}$
Ce_2Mg_{17} : Stoichiometric, $(Ce)_2(Mg)_{17}$
$CeMg_{12}$: Stoichiometric, $(Ce)(Mg)_{12}$

Assessor and Date:

G. Cacciamani, A. Saccone, and R. Ferro,
Calphad XXII - Salou, Spain (1993).

Thermodynamic properties of the solution and compound phases ($J.mol^{-1}$)

Phase Ce_2Mg_{17}

$$G^{\circ}(T) - 2.0\ H_{Ce}^{o,fcc-A1}(298.15\ K) - 17.0\ H_{Mg}^{o,hcp-A3}(298.15\ K) =$$
$$-\ 217170.0 + 104.5\ T + 2.0\ GHSER_{Ce} + 17.0\ GHSER_{Mg}$$

Phase Ce_5Mg_{41}

$$G^{\circ}(T) - 5.0\ H_{Ce}^{o,fcc-A1}(298.15\ K) - 41.0\ H_{Mg}^{o,hcp-A3}(298.15\ K) =$$
$$-\ 575000.0 + 299.0\ T + 5.0\ GHSER_{Ce} + 41.0\ GHSER_{Mg}$$

Phase CeMg

$$G^{\circ}(T) - H_{Ce}^{o,fcc-A1}(298.15\ K) - H_{Mg}^{o,hcp-A3}(298.15\ K) =$$
$$-\ 46000.0 + 23.32\ T + GHSER_{Ce} + GHSER_{Mg}$$

Phase $CeMg_{12}$

$$G^\circ(T) - H^{\circ,fcc-A1}_{Ce}(298.15\ \mathrm{K}) - 12.0\ H^{\circ,hcp-A3}_{Mg}(298.15\ \mathrm{K}) = \\ - 139880.0 + 84.5\ T + \mathrm{GHSER}_{Ce} + 12.0\ \mathrm{GHSER}_{Mg}$$

Phase $CeMg_2$

$$G^\circ(T) - H^{\circ,fcc-A1}_{Ce}(298.15\ \mathrm{K}) - 2.0\ H^{\circ,hcp-A3}_{Mg}(298.15\ \mathrm{K}) = \\ - 52744.6 + 15.163\ T + \mathrm{GHSER}_{Ce} + 2.0\ \mathrm{GHSER}_{Mg}$$

Phase $CeMg_3$

$$G^\circ(T) - H^{\circ,fcc-A1}_{Ce}(298.15\ \mathrm{K}) - 3.0\ H^{\circ,hcp-A3}_{Mg}(298.15\ \mathrm{K}) = \\ - 76800.0 + 26.5\ T + \mathrm{GHSER}_{Ce} + 3.0\ \mathrm{GHSER}_{Mg}$$

Phase bcc–$A2$

$$L^{0,bcc-A2}_{Ce,Mg:\square} = - 27000 + 3.3\ T$$

$$L^{1,bcc-A2}_{Ce,Mg:\square} = 25338.56 - 11.86885\ T$$

$$L^{2,bcc-A2}_{Ce,Mg:\square} = - 15106.9$$

Phase fcc–$A1$

$$L^{0,fccA1}_{Ce,Mg:\square} = - 15000 + 0.5\ T$$

Phase hcp–$A3$

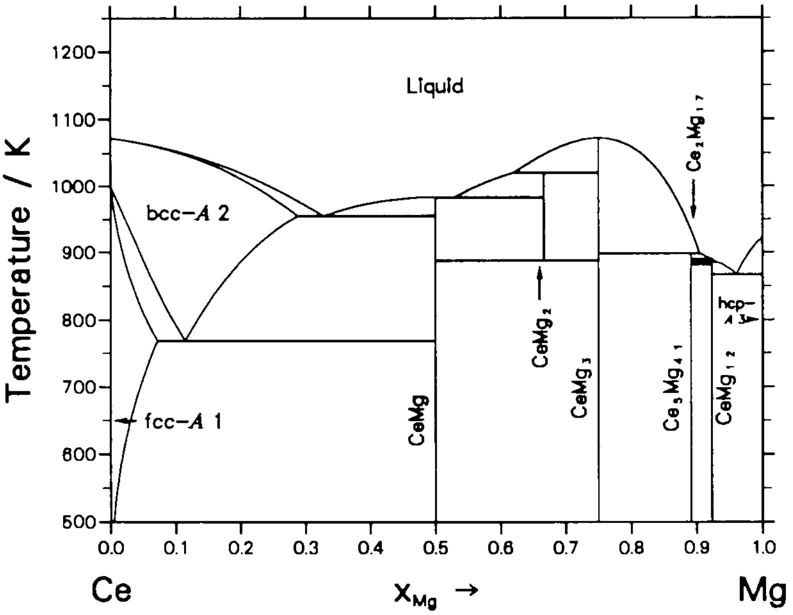
$$L^{0,hcp-A3}_{Ce,Mg:\square} = - 94337.51 + 79.95155\ T$$

Phase Liquid

$$L^{0,liquid}_{Ce,Mg} = - 39381.19 + 16.34052\ T$$

$$L^{1,liquid}_{Ce,Mg} = 25338.56 - 11.86885\ T$$

$$L^{2,liquid}_{Ce,Mg} = - 15106.9$$


Temperature / K
1200
1100
1000
900
800
700
600
500
Liquid
bcc-A 2
fcc-A 1
CeMg
CeMg₂
CeMg₃
Ce₂Mg₁₇
Ce₅Mg₄₁
CeMg₁₂
hcp-A 3
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
Ce
x_Mg →
Mg

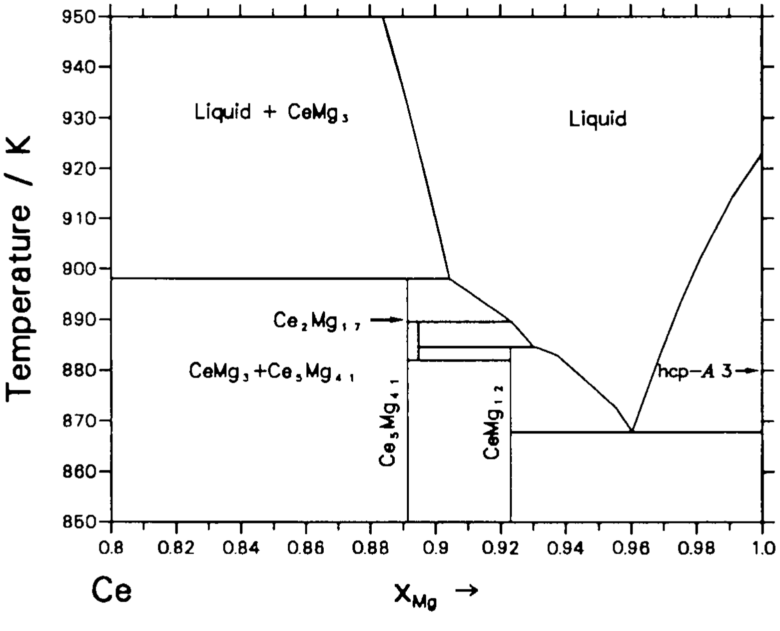

Temperature / K
950
940
930
920
910
900
890
880
870
860
850
Liquid + CeMg₃
Liquid
Ce₂Mg₁₇
CeMg₃+Ce₅Mg₄₁
Ce₅Mg₄₁
CeMg₁₂
hcp-A 3
0.8
0.82
0.84
0.86
0.88
0.9
0.92
0.94
0.96
0.98
1.0
Ce
x_Mg →

Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Mg}			T / K
Liquid ⇌ bcc-*A2* + CeMg	Eutectic	.328	.288	.500	955.1
Liquid ⇌ CeMg + $CeMg_2$	Eutectic	.528	.500	.667	982.9
Liquid + $CeMg_3$ ⇌ $CeMg_2$	Peritectic	.620	.750	.667	1020.1
Liquid + $CeMg_3$ ⇌ Ce_5Mg_{41}	Peritectic	.904	.750	.891	898.1
Liquid + Ce_5Mg_{41} ⇌ Ce_2Mg_{17}	Peritectic	.923	.891	.895	889.6
Liquid + Ce_2Mg_{17} ⇌ $CeMg_{12}$	Peritectic	.930	.895	.923	884.7
Liquid ⇌ $CeMg_{12}$ + hcp-*A3*	Eutectic	.960	.923	1.000	867.9
Ce_2Mg_{17} ⇌ Ce_5Mg_{41} + $CeMg_{12}$	Eutectoid	.895	.891	.923	882.0
$CeMg_2$ ⇌ CeMg + $CeMg_3$	Eutectoid	.667	.500	.750	888.0
bcc-*A2* ⇌ fcc-*A1* + CeMg	Eutectoid	.114	.072	.500	768.7
CeMg ⇌ Liquid	Congruent	.500	.500	....	983.8
$CeMg_3$ ⇌ Liquid	Congruent	.750	.750	....	1073.0

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Ce-Mg	(Ce)	Cu	*cF4* $Fm\bar{3}m$		
	(Ce)	W	*cI2* $Im\bar{3}m$		
	(Mg)	Mg	*hP2* $P6_3/mmc$		
	CeMg	CsCl	*cP2* $Pm\bar{3}m$	Ce 1 Mg 1	
	$CeMg_2$	Cu_2Mg	*cF24* $Fd\bar{3}m$	Ce 8 Mg 16	
	$CeMg_3$	BiF_3	*cF16* $Fm\bar{3}m$	Ce 4 Mg_1 4 Mg_2 8	
	Ce_5Mg_{41}	Ce_5Mg_{41}	*tI92* $I4/m$		10 sublattices [91Vil]
	$CeMg_{10.3}$	Th_2Ni_{17}	*hP38* $P6_3/mmc$		6 sublattices [91Vil] Ce_2Mg_{17}
	$CeMg_{12}$(I)	$ThMg_{12}$	*tI26* $I4/mmm$		$ThMn_{12}$ in [91Vil]
	$CeMg_{12}$(II)	$CeMg_{12}$(II)	*oI338* ($Immm$)		not considered

System Cr–Cu

Solution Phases:

(stable) Liquid, bcc-$A2$, fcc-$A1$
(metastable) hcp-$A3$

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-$A2$: Substitutional, Redlich-Kister
fcc-$A1$: Substitutional, Redlich-Kister
hcp-$A3$: Substitutional, Redlich-Kister

Assessor and Date:

K. Zeng and M. Hämälainen

Thermodynamic properties of the solution phases (J.mol^{-1})

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Cr,Cu}:\square} = 200000$$

Phase fcc–$A1$

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Cr,Cu}:\square} = 88112 - 30.38315\ T$$

Phase hcp–$A3$

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Cr,Cu}:\square} = 60000$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Cr,Cu}} = 35495.913 - 2.958\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Cr,Cu}} = -1001.1765$$

$$L^{2,\mathrm{liquid}}_{\mathrm{Cr,Cu}} = 5704.648$$

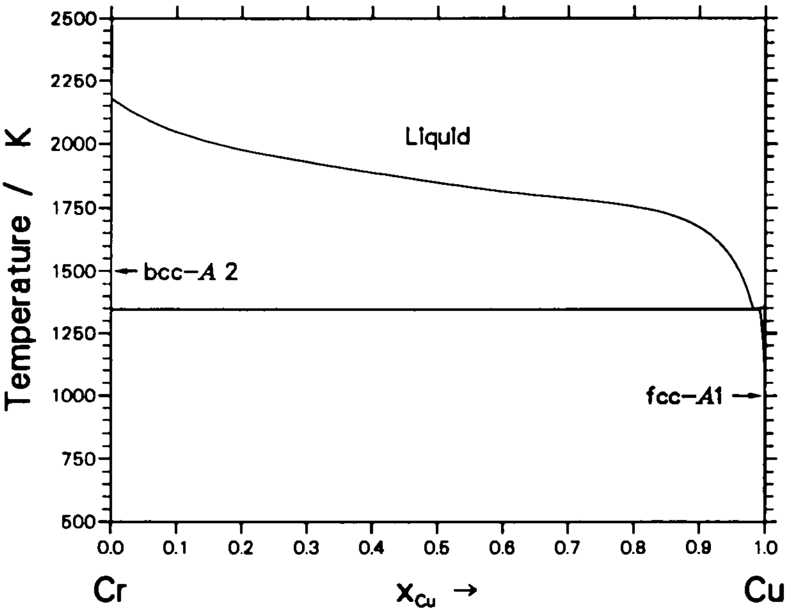


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Cu}			T / K
Liquid ⇌ bcc–$A2$ + fcc–$A1$	Eutectic	.982	.000	.992	1347.9

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group
Cr–Cu	(Cr)	W	$cI2$ $Im\bar{3}m$
	(Cu)	Cu	$cF4$ $Fm\bar{3}m$

System Cr–Mg

Solution Phases:

(stable) Liquid, bcc–A2, hcp–A3
(metastable) cbcc–A12, fcc–*A*1, hcp–Zn

Modelling:

Liquid : Substitutional, Redlich–Kister
bcc–A2 : Substitutional, Redlich–Kister
cbcc–A12 : Substitutional, Redlich–Kister
fcc–A1 : Substitutional, Redlich–Kister
hcp–A3 : Substitutional, Redlich–Kister
hcp–Zn : Substitutional, Redlich–Kister

Assessor and Date:

I. Ansara, 1991

Thermodynamic properties of the solution phases (J.mol^{-1})

Phase bcc–A2

$$L^{0,bcc-A2}_{Cr,Mg:\square} = 80\ T$$

Phase cbcc–*A*12

$$L^{0,cbcc-A12}_{Cr,Mg:\square} = 80\ T$$

Phase fcc–*A*1

$$L^{0,fcc-A1}_{Cr,Mg:\square} = 80\ T$$

Phase hcp–*A*3

$$L^{0,hcp-A3}_{Cr,Mg:\square} = 80\ T$$

Phase hcp–Zn

$$L^{0,hcp-Zn}_{Cr,Mg:\square} = 80\ T$$

Phase liquid

$$L^{0,liquid}_{Cr,Mg} = 94500.0$$

$$L^{1,liquid}_{Cr,Mg} = 12500.0$$

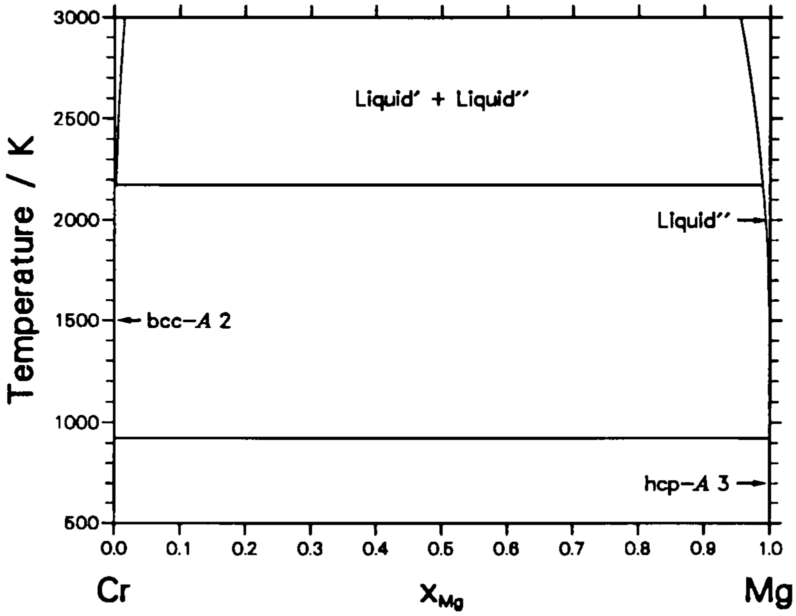


Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Mg}			T / K
Liquid' ⇌ Liquid" + bcc-$A2$	monotectic	.000	.003	.988	2174.9
Liquid" ⇌ bcc-$A2$ + hcp-$A3$	Degenerate	.000	1.000	1.000	923.0

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group
Cr-Mg	(Cr)	W	$cI2$ $Im\bar{3}m$
	(Mg)	Mg	$hP2$ $P6_3/mmc$

System Cr–Mn

Solution Phases:

Liquid, bcc–$A2$, fcc–$A1$, hcp–$A3$, cbcc–$A12$, cub–$A13$, σ–L, σ–II

Compound:

Cr_3Mn_5

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc–$A2$: Substitutional, Redlich-Kister
fcc–$A1$: Substitutional, Redlich-Kister
cbcc–$A12$: Substitutional, Redlich-Kister
cub–$A13$: Substitutional, Redlich-Kister
σ–L : Sublattice model, $(Mn)_8(Cr)_4(Cr,Mn)_{18}$
σ–II : Sublattice model, $(Mn)_8(Cr)_4(Cr,Mn)_{18}$
Cr_3Mn_5 : Stoichiometric, Cr_3Mn_5

Publication:

Scientific Group Thermodata Europe Database

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase Cr_3Mn_5

$$G^{\circ}(T) - 3.0\ H^{o,bcc-A2,para}_{Cr}(298.15\ K) - 5.0\ H^{o,cbcc-A12,para}_{Mn}(298.15\ K) = - 72550.0 + 21.1732\ T + 3.0\ GHSER_{Cr} + 5.0\ GHSER_{Mn}$$

Phase fcc–$A1$

$$L^{0,fcc-A1}_{Cr,Mn:\square} = - 19088 + 17.5423\ T$$

Phase cbcc–$A12$

$$L^{0,cbcc-A12}_{Cr,Mn:\square} = - 36796 + 20.385\ T$$

Phase liquid

$$L^{0,liquid}_{Cr,Mn} = - 15009 + 13.6587\ T$$

$$L^{1,liquid}_{Cr,Mn} = 504 + 0.9479\ T$$

Phase cub–$A13$

$$L^{0,\mathrm{cub}-A13}_{\mathrm{Cr,Mn:\square}} = -31260 + 16.4919\ T$$

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Cr,Mn:\square}} = -20328 + 18.7339\ T$$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Cr,Mn:\square}} = -9162 + 4.4183\ T$$

$$\beta^{0,\mathrm{bcc}-A2,\mathrm{mag}}_{\mathrm{Cr,Mn:\square}} = 0.48643$$

$$\beta^{2,\mathrm{bcc}-A2,\mathrm{mag}}_{\mathrm{Cr,Mn:\square}} = -0.72035$$

$$\beta^{4,\mathrm{bcc}-A2,\mathrm{mag}}_{\mathrm{Cr,Mn:\square}} = -1.93265$$

$$T^{0,\mathrm{bcc}-A2}_{\mathrm{c,Cr,Mn:\square}} = -1325$$

$$T^{2,\mathrm{bcc}-A2}_{\mathrm{c,Cr,Mn:\square}} = -1133$$

$$T^{4,\mathrm{bcc}-A2}_{\mathrm{c,Cr,Mn:\square}} = -10294$$

$$T^{6,\mathrm{bcc}-A2}_{\mathrm{c,Cr,Mn:\square}} = 26706$$

$$T^{8,\mathrm{bcc}-A2}_{\mathrm{c,Cr,Mn:\square}} = -28117$$

Phase σ-L

$$G^{\circ}(T) - 8.0\ H^{\mathrm{o,bcc-A2,para}}_{\mathrm{Cr}}(298.15\ \mathrm{K}) - 22.0\ H^{\mathrm{o,cbcc-A12,para}}_{\mathrm{Mn}}(298.15\ \mathrm{K}) =$$
$$\mathrm{G(Mn{:}Cr{:}Cr)} = 65859.5 + 8.0\ \mathrm{GFCC_{Mn}} + 22.0\ \mathrm{GHSER_{Cr}}$$

$$G^{\circ}(T) - 26.0\ H^{\mathrm{o,bcc-A2,para}}_{\mathrm{Cr}}(298.15\ \mathrm{K}) - 4.0\ H^{\mathrm{o,cbcc-A12,para}}_{\mathrm{Mn}}(298.15\ \mathrm{K}) =$$
$$\mathrm{G(Mn{:}Cr{:}Mn)} = -172946.0 + 69.0245\ T + 8.0\ \mathrm{GFCC_{Mn}} + 4.0\ \mathrm{GHSER_{Cr}} + 18.0\ \mathrm{GBCC_{Mn}}$$

$$L^{0,\sigma-\mathrm{L}}_{\mathrm{Mn:Cr:Cr,Mn}} = -1095771 + 862.0312\ T$$

Phase σ–H

$$G^{\circ}(T) - 8.0\ H^{\mathrm{o,bcc-A2,para}}_{\mathrm{Cr}}(298.15\ \mathrm{K}) - 22.0\ H^{\mathrm{o,cbcc-A12,para}}_{\mathrm{Mn}}(298.15\ \mathrm{K}) =$$
$$\mathrm{G(Mn{:}Cr{:}Cr)} = -192369.0 + 152.4742\ T + 8.0\ \mathrm{GFCC_{Mn}} + 22.0\ \mathrm{GHSER_{Cr}}$$

$$G^{\circ}(T) - 26.0\ H^{\mathrm{o,bcc-A2,para}}_{\mathrm{Cr}}(298.15\ \mathrm{K}) - 4.0\ H^{\mathrm{o,cbcc-A12,para}}_{\mathrm{Mn}}(298.15\ \mathrm{K}) =$$
$$\mathrm{G(Mn{:}Cr{:}Mn)} = -74263.0 - 10.7082\ T + 18.0\ \mathrm{GBCC_{Mn}} + 8.0\ \mathrm{GFCC_{Mn}} + 4.0\ \mathrm{GHSER_{Cr}}$$

$$L^{0,\sigma-\mathrm{H}}_{\mathrm{Mn:Cr:Cr,Mn}} = 90000$$

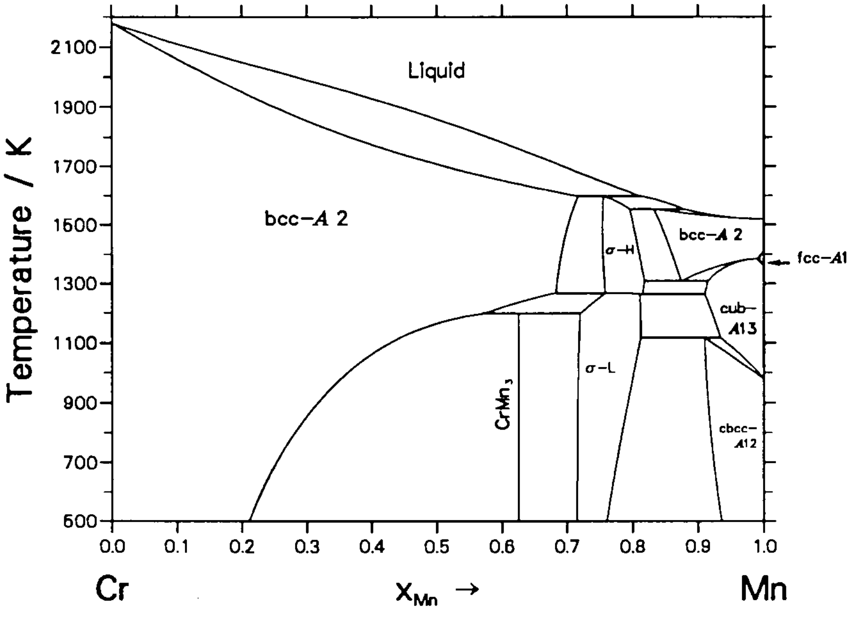


Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Mn}			T / K
bcc–$A2$ + σ–L $\rightleftharpoons$ Cr_3Mn_5	Peritectoid	.570	.719	.625	1197.8
σ–H $\rightleftharpoons$ bcc–$A2$ + σ–L	Eutectoid	.758	.683	.760	1268.1
Liquid + bcc–$A2$ $\rightleftharpoons$ σ–H	Peritectic	.813	.717	.755	1598.4
Liquid + σ–H $\rightleftharpoons$ bcc–$A2$	Peritectic	.876	.794	.831	1556.2
bcc–$A2$ $\rightleftharpoons$ cub–$A13$ + σ–H	Eutectoid	.880	.873	.894	1293.6
bcc–$A2$ + fcc–$A1$ $\rightleftharpoons$ cub–$A13$	Peritectoid	.898	.993	.913	1382.1
σ–H $\rightleftharpoons$ σ–L + cub–$A13$	Eutectoid	.815	.811	.910	1264.4
σ–L + cub–$A13$ $\rightleftharpoons$ cbcc–$A12$	Peritectoid	.812	.934	.910	1117.4

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Comments
Cr-Mn	(Cr)	W	$cI2$ $Im\bar{3}m$	
	α-Mn	α-Mn	$c58$ $I\bar{4}3m$	cbcc-$A12$
	β-Mn	β-Mn	$cP20$ $P4_1 323m$	cub-$A13$
	γ-Mn	Cu	$cF4$ $Fm3m$	fcc-$A1$
	δ—Mn	W	$cI2$ $Im\bar{3}m$	bcc-$A2$
	α' Cr_xMn_{1-x} HT	α-Mn		
	α" Cr_xMn_{1-x} LT	α-Mn		
	σ Cr_xMn_{1-x} HT	σ CrFe	$tP30$ $P4_2/mnm$	
	σ Cr_xMn_{1-x} MT	σ CrFe	$tP30$ $P4_2/mnm$	
	σ Cr_xMn_{1-x} LT	σ CrFe	$tP30$ $P4_2/mnm$	

System Cr–Si

Solution Phases:

Liquid, bcc–$A2$

Compounds:

Cr_5Si_3, CrSi,, Cr_3Si–$A15$, $CrSi_2$

Modelling:

Liquid : Substitutional, Redlich–Kister
bcc–$A2$: Substitutional, Redlich–Kister
Cr_3Si–$A15$: Sublattice model, $(Cr,Si)_3(Cr,Si)$
$CrSi_2$: Sublattice model, $(Cr,Si)(Cr,Si)_2$
Cr_5Si_3 : Stoichiometric, $(Cr)_5(Si)_3$
CrSi : Stoichiometric, (Cr)(Si)

Assessor and Date:

C.A. Coughnanowr, I. Ansara, and H.L. Lukas,

Publication:

Calphad, 18, 2, 125-140 (1994).

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Cr,Si}} = -119216.90 + 16.11445 \ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Cr,Si}} = -47614.70 + 12.17363 \ T$$

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Cr,Si}} = -104537.94 + 10.69527 \ T$$

$$L^{1,\mathrm{bcc}-A2}_{\mathrm{Cr,Si}} = -47614.70 + 12.17363 \ T$$

Phase Cr_3Si–$A15$

$$G^\circ(T) - 4.0\ H_{\mathrm{Cr}}^{\mathrm{o,bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) = \mathrm{G(Cr{:}Cr)} = \\ 20000.0 + 10.000\ T + 4.0\ \mathrm{GHSER_{Cr}}$$

$$G^\circ(T) - 3.0\ H_{\mathrm{Cr}}^{\mathrm{o,bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) - H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = \mathrm{G(Cr{:}Si)} = \\ - 126369.35 + 4.15051\ T + 3.0\ \mathrm{GHSER_{Cr}} + \mathrm{GHSER_{Si}}$$

$$G^\circ(T) - H_{\mathrm{Cr}}^{\mathrm{o,bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = \mathrm{G(Cr{:}Si)} = \\ 233507.47 - 74.15051\ T + \mathrm{GHSER_{Cr}} + 3.0\ \mathrm{GHSER_{Si}}$$

$$G^\circ(T) - 4.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = \mathrm{G(Si{:}Si)} = \\ 208000.0 - 80.000\ T + 4.0\ \mathrm{GHSER_{Si}}$$

$$L_{\mathrm{Cr,Si:Cr}}^{0,\mathrm{Cr_3Si}} = L_{\mathrm{Cr,Si:Si}}^{0,\mathrm{Cr_3Si}} = - 107840.95$$

$$L_{\mathrm{Cr:Cr,Si}}^{0,\mathrm{Cr_3Si}} = L_{\mathrm{Si:Cr,Si}}^{0,\mathrm{Cr_3Si}} = - 13020.93$$

Phase Cr_5Si_3

$$G^\circ(T) - 5.0\ H_{\mathrm{Cr}}^{\mathrm{o,bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = \\ - 316433.0 + 1065.82816\ T - 182.578184\ T\cdot \ln T \\ - 23.919688\mathrm{E{-}3}\ T^2 - 2.31728\mathrm{E{-}06}\ T^3$$

Phase CrSi

$$G^\circ(T) - H_{\mathrm{Cr}}^{\mathrm{o,bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) - H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = \\ - 78732.28 + 311.58392\ T - 51.62865\ T\cdot \ln T \\ - 4.47355\mathrm{E{-}03}\ T^2 + 391330\ T^{-1}$$

Phase $CrSi_2$

$$G^\circ(T) - 3.0\ H_{\mathrm{Cr}}^{\mathrm{o,bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) = \mathrm{G(Cr{:}Cr)} = \\ 10000.00 - 1.0\ T + 3.0\ \mathrm{GHSER_{Cr}}$$

$$G^\circ(T) - H_{\mathrm{Cr}}^{\mathrm{o,bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = \mathrm{G(Cr{:}Si)} = \\ - 96694.43 + 333.33835\ T - 57.855747\ T\cdot \ln T \\ - 13.22769\mathrm{E{-}03}\ T^2 - 0.43203\mathrm{E{-}06}\ T^3$$

$$G^\circ(T) - 2.0\ H_{\mathrm{Cr}}^{\mathrm{o,bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) - H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = \mathrm{G(Si{:}Cr)} = \\ 148569.93 - 12.65342\ T + 2.0\ \mathrm{GHSER_{Cr}} + \mathrm{GHSER_{Si}}$$

$$G^\circ(T) - 3.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = \mathrm{G(Si{:}Si)} = \\ 78860.26 - 15.77206\ T + 3.0\ \mathrm{GHSER_{Si}}$$

$$L_{\mathrm{Cr:Cr,Si}}^{0,\mathrm{CrSi_2}} = L_{\mathrm{Si:Cr,Si}}^{0,\mathrm{CrSi_2}} = - 35879.97 + 7.17599\ T$$

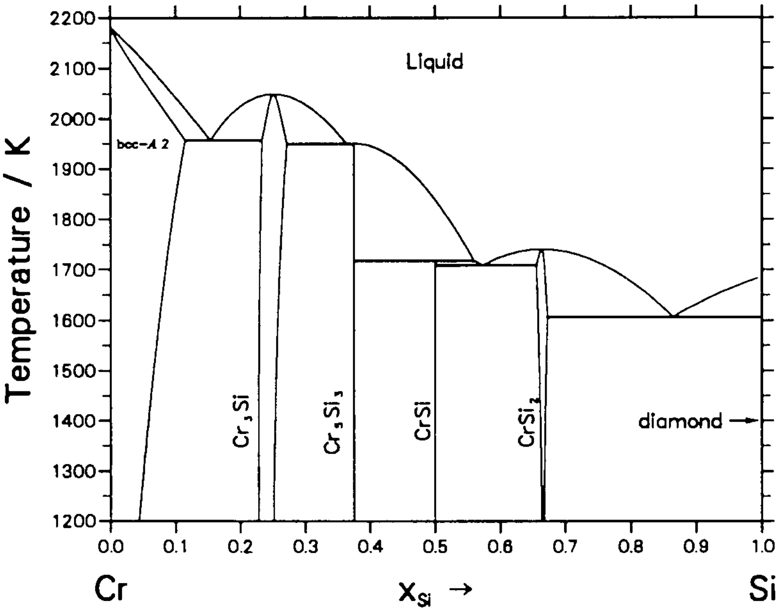


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Si}			T / K
Liquid ⇌ bcc-$A2$ + Cr_3Si-$A15$	Eutectic	.154	.115	.233	1957.4
Liquid ⇌ Cr_3Si-$A15$ + Cr_5Si_3	Eutectic	.364	.272	.375	1950.0
Liquid + Cr_5Si_3 ⇌ CrSi	Peritectic	.560	.375	.500	1718.5
Liquid ⇌ CrSi + $CrSi_2$	Eutectic	.574	.500	.656	1708.8
Liquid ⇌ $CrSi_2$ + diamond	Eutectic	.864	.673	1.000	1606.7
Cr_3Si-$A15$ ⇌ Liquid	Congruent	.025	.025	...	2049.5
Cr_5Si_3 ⇌ Liquid	Congruent	.375	.375	...	1951.0
Cr_2Si ⇌ Liquid	Congruent	.666	.666	...	1741.0

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Cr-Si	(Cr)	W	*cI2* $Im\bar{3}m$	M 2	
	(Si)	diamond-*A4*	*cF8* Fd_3m		
	CrSi	FeSi	*cP8* $P2_13$	Cr 4 Si 4	
	$CrSi_2$	$CrSi_2$	*hP9* $P6_222$	Cr 3 Si 6	
	Cr_3Si	Cr_3Si	*cP8* $Pm\bar{3}n$	Cr 6 Si 2	Cr_3Si-*A15*
	Cr_5Si_3	Si_3W_5	*tI32* $I4/mcm$	Cr_1 4 Cr_2 16 Si_1 4 Si_2 8	*tI38* in Mas1
	Cr_5Si_3	Mn_5Si_3	*hP16* $P6_3/mcm$		not considered

System Cr–Ti

Solution Phases:

Liquid, bcc–$A2$, hcp–$A3$

Compounds:

Laves–$C14$, Laves–$C15$

Modelling:

Liquid : Substitutional, Redlich–Kister
bcc–$A2$: Substitutional, Redlich–Kister
hcp–$A3$: Substitutional, Redlich–Kister
Laves–$C14$: Sublattice model, $(Cr,Ti)_2\ (Cr,Ti)$
Laves–$C15$: Sublattice model, $(Cr,Ti)_2\ (Cr,Ti)$

Assessor and Date:

N. Saunders, 1992

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase Laves–$C14$

$$G^\circ(T) - 3.0\ H_{Cr}^{o,bcc-A2,para}(298.15\ K) = G(Cr:Cr) = 15000.0 + 3.0\ \ GHSER_{Cr}$$

$$G^\circ(T) - 2.0\ H_{Cr}^{o,bcc-A2,para}(298.15\ K) - H_{Ti}^{o,hcp-A3}(298.15\ K) = G(Cr:Ti) = \\ -1440.0 - 6.75\ T + 2.0\ \ GHSER_{Cr} + GHSER_{Ti}$$

$$G^\circ(T) - H_{Cr}^{o,bcc-A2,para}(298.15\ K) - 2.0\ H_{Ti}^{o,hcp-A3}(298.15\ K) = G(Ti:Cr) = \\ 15000.0 + GHSER_{Cr} + 2.0\ \ GHSER_{Ti}$$

$$G^\circ(T) - 3.0\ H_{Ti}^{o,hcp-A3}(298.15\ K) = G(Ti:Ti) = \\ 15000.0 + 3.0\ \ GHSER_{Ti}$$

$$L_{Cr:Cr,Ti}^{0,Laves-C14} = L_{Ti:Cr,Ti}^{0,Laves-C14} = 60000.0$$

$$L_{Cr,Ti:Cr}^{0,Laves-C14} = L_{Cr,Ti:Ti}^{0,Laves-C14} = 60000.0$$

Phase Laves–$C15$

$$G^\circ(T) - 3.0\ H_{\mathrm{Cr}}^{\mathrm{o,bcc-}A2\mathrm{,para}}(298.15\ \mathrm{K}) = \mathrm{G(Cr{:}Cr)} = 15000.0 + 3.0\ \mathrm{GHSER_{Cr}}$$

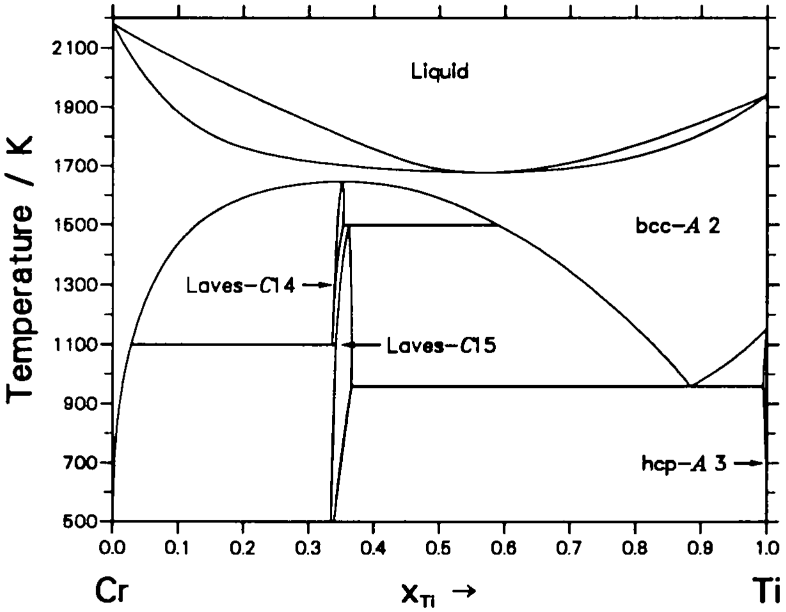
$$G^\circ(T) - 2.0\ H_{\mathrm{Cr}}^{\mathrm{o,bcc-}A2\mathrm{,para}}(298.15\ \mathrm{K}) - H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \mathrm{G(Cr{:}Ti)} = -\ 1780.0 - 6.3\ T + 2.0\ \mathrm{GHSER_{Cr}} + \mathrm{GHSER_{Ti}}$$

$$G^\circ(T) - H_{\mathrm{Cr}}^{\mathrm{o,bcc-}A2\mathrm{,para}}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Cr)} = 15000.0 + \mathrm{GHSER_{Cr}} + 2.0\ \mathrm{GHSER_{Ti}}$$

$$G^\circ(T) - 3.0\ H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A2}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Ti)} = 15000.0 + 3.0\ \mathrm{GHSER_{Ti}}$$

$$L_{\mathrm{Cr:Cr,Ti}}^{0,\mathrm{Laves-C15}} = L_{\mathrm{Ti:Cr,Ti}}^{0,\mathrm{Laves-C15}} = 50000.0$$

$$L_{\mathrm{Cr,Ti:Cr}}^{0,\mathrm{Laves-C15}} = L_{\mathrm{Cr,Ti:Ti}}^{0,\mathrm{Laves-C15}} = 10800.0 + 27\ T$$



Phase liquid

$$L_{\mathrm{Cr,Ti}}^{0,\mathrm{liquid}} = 5250$$

$$L_{\mathrm{Cr,Ti}}^{1,\mathrm{liquid}} = 1500$$

Phase hcp–$A3$

$$L_{\mathrm{Cr,Ti:\square}}^{0,\mathrm{hcp-}A3} = 32500$$

Phase bcc–$A2$

$L^{0,\mathrm{bcc}-A2}_{\mathrm{Cr,Ti:\square}} = 19100$

$L^{1,\mathrm{bcc}-A2}_{\mathrm{Cr,Ti:\square}} = 5500$

$L^{2,\mathrm{bcc}-A2}_{\mathrm{Cr,Ti:\square}} = 1750$

Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Ti}			T / K
bcc–$A2$ ⇌ Laves–$C15$ + hcp–$A3$	Eutectoid	.884	.365	.994	959.7
bcc–$A2$ + Laves–$C15$ ⇌ Laves–$C14$	Peritectoid	.593	.353	.362	1495.3
Laves–$C14$ ⇌ bcc–$A2$ + Laves–$C15$	Eutectoid	.336	.027	.342	1093.4
Laves–$C14$ ⇌ bcc–$A2$	Congruent	.333	.333	....	1645.0
bcc–$A2$ ⇌ Liquid	Congruent	.563	.563	....	1677.0

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Comments
Cr–Ti	(Cr)	W	*cI2* $Im\bar{3}m$	
	(Ti)	Mg	*hP2* $P6_3/mmc$	
	(Ti)	W	*cI2* $Im\bar{3}m$	
	α Cr_2Ti	Cu_2Mg	*cF24* $Fd\bar{3}m$	Laves–$C15$
	β Cr_2Ti	$MgZn_2$	*hP12* $P6_3/mmc$	Laves–$C14$
	γ Cr_2Ti	$MgNi_2$	*hP24* $P6_3/mmc$	Laves–$C36$

System Cr–V

Solution Phases:

Liquid, bcc–$A2$

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc–$A2$: Substitutional, Redlich-Kister

Publication:

Scientific Group Thermodata Europe Database

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Cr,V:\square}} = -9874 - 2.6964\ T$$

$$L^{1,\mathrm{bcc}-A2}_{\mathrm{Cr,V:\square}} = -1720 - 2.5237\ T$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Cr,V}} = -9874 - 2.6964\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Cr,V}} = -1720 - 2.5237\ T$$

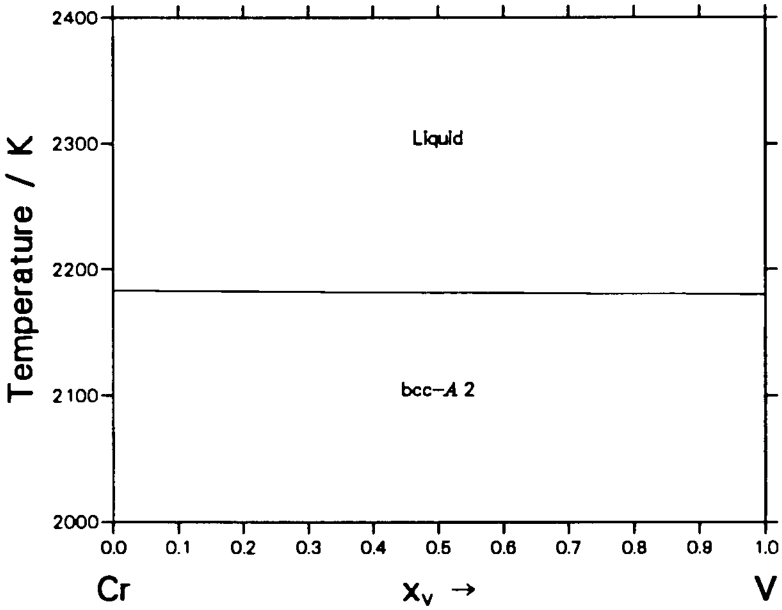


Table I - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group
Cr-V	(Cr)	W	*cI2* *Im*$\bar{3}$*m*
	(V)	W	*cI2* *Im*$\bar{3}$*m*

System Cr–Zn

Solution Phases:

(stable)	Liquid, bcc-$A2$, hcp-Zn
(metastable)	fcc-$A1$

Compounds:

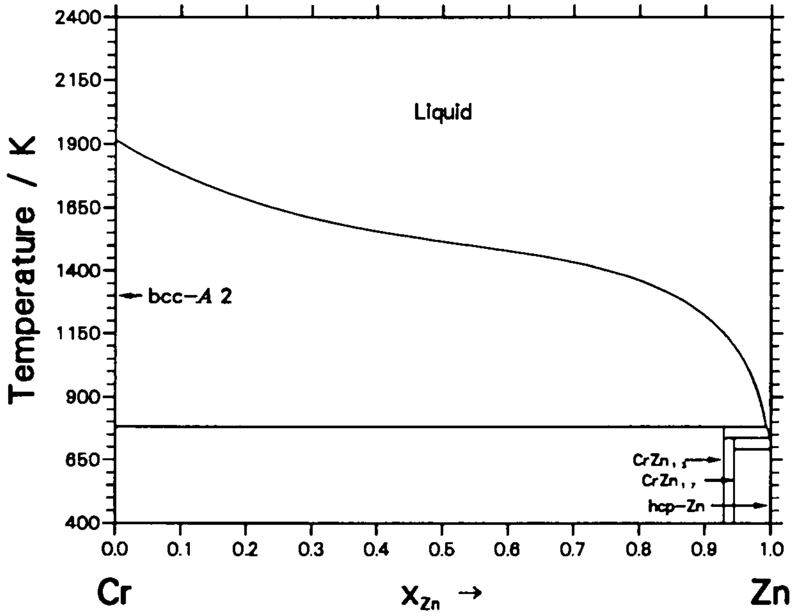
$CrZn_{13}$, $CrZn_{17}$

Modelling:

bcc-$A2$: Substitutional, Redlich-Kister
fcc-$A1$: Substitutional, Redlich-Kister
hcp-Zn : Substitutional, Redlich-Kister
Liquid : Substitutional, Redlich-Kister
$CrZn_{13}$: Stoichiometric,$(Cr)(Zn)_{13}$
$CrZn_{17}$: Stoichiometric, $(Cr)(Zn)_{17}$

Assessor and Date:

I. Ansara, 1992



Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Cr,Zn:\square}} = 80\ T$$

Phase fcc–$A1$

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Cr,Zn:\square}} = 80\ T$$

Phase hcp–Zn

$$L^{0,\mathrm{hcp-Zn}}_{\mathrm{Cr,Zn:\square}} = 80\ T$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Cr,Zn}} = 19000$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Cr,Zn}} = -1000$$

Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Zn}			T / K
Liquid + bcc–$A2$ $\rightleftharpoons$ CrZn_{13}^{*}	Peritectic	0.996	0.000	0.928	761.4
Liquid + CrZn_{13} $\rightleftharpoons$ CrZn_{17}	Peritectic	0.998	0.928	0.944	736.5
Liquid $\rightleftharpoons$ CrZn_{17} + hcp–Zn	Degenerate	0.999	0.944	0.999	692.5

* Reaction uncertain

Phase CrZn_{13}

$$G^{\circ}(T) - H^{\mathrm{o,bcc}-A2,\mathrm{para}}_{\mathrm{Cr}}(298.15\ \mathrm{K}) - 13.0\ H^{\mathrm{o,hcp-A3}}_{\mathrm{Zn}}298.15\mathrm{K})$$
$$- 9800.0 + \mathrm{GHSER_{Cr}} + 13.0\ \ \mathrm{GHSER_{Zn}}$$

Phase CrZn_{17}

$$G^{\circ}(T) - H^{\mathrm{o,bcc}-A2,\mathrm{para}}_{\mathrm{Cr}}(298.15\ \mathrm{K}) - 17.0\ H^{\mathrm{o,hcp-A3}}_{\mathrm{Zn}}(298.15\mathrm{K})$$
$$- 11700.0 + \mathrm{GHSER_{Cr}} + 17.0\ \ \mathrm{GHSER_{Zn}}$$

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group
Cr-Zn	(Cr)	W	*cI2* $Im\bar{3}m$
	(Zn)	Mg	*hP2* $P6_3/mmc$
	$CrZn_{13}$	$CoZn_{13}$	
	$CrZn_{17}$		

System Cr-Zr

Solution Phases:

(stable) Liquid, bcc–$A2$, hcp–$A3$
(metastable) fcc–$A1$

Compounds:

Laves–$C14$, Laves–$C15$, Laves–$C36$

Modelling:

bcc–$A2$: Substitutional, Redlich–Kister
fcc–$A1$: Substitutional, Redlich–Kister
hcp–$A3$: Substitutional, Redlich–Kister
Liquid : Substitutional, Redlich–Kister
Laves–$C14$: Sublattice model, $(Cr,Zr)_2(Cr,Zr)$
Laves–$C15$: Sublattice model, $(Cr,Zr)_2(Cr,Zr)$
Laves–$C36$: Sublattice model, $(Cr,Zr)_2(Cr,Zr)$

Assessor and Date:

K. Zeng, M. Hämäläinen, and I. Ansara (1993)

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase Laves–$C14$

$$G^{\circ}(T) - 3.0\ H_{\mathrm{Cr}}^{\circ,\mathrm{bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) = \mathrm{G(Cr{:}Cr)} = 15000.0 + 3.0\ \mathrm{GHSER_{Cr}}$$

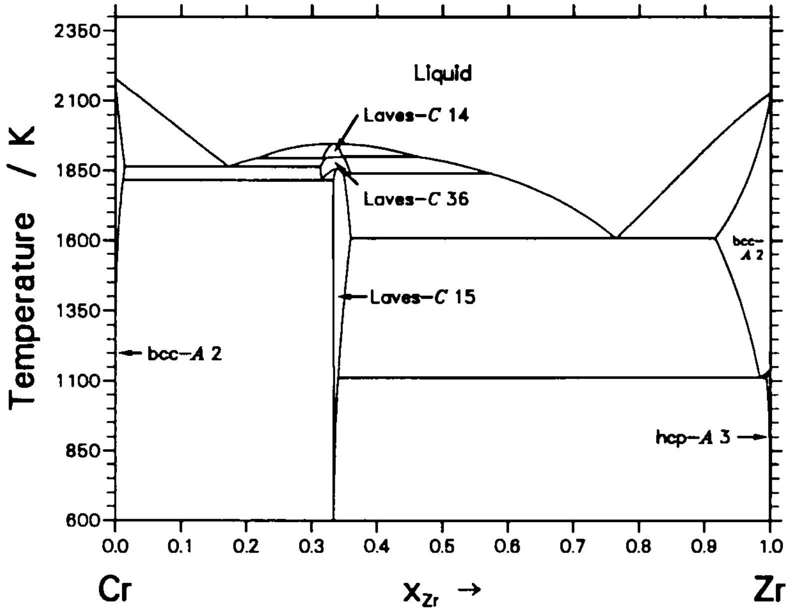
$$G^{\circ}(T) - 2.0\ H_{\mathrm{Cr}}^{\circ,\mathrm{bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) - H_{\mathrm{Zr}}^{\circ,\mathrm{hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Cr{:}Zr)} = -\,8114 - 11.652\ T + 2.0\ \mathrm{GHSER_{Cr}} + \mathrm{GHSER_{Zr}}$$

$$G^{\circ}(T) - H_{\mathrm{Cr}}^{\circ,\mathrm{bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Zr}}^{\circ,\mathrm{hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Zr{:}Cr)} = 38114 + 11.652\ T + \mathrm{GHSER_{Cr}} + 2.0\ \mathrm{GHSER_{Zr}}$$

$$G^{\circ}(T) - 3.0\ H_{\mathrm{Zr}}^{\circ,\mathrm{hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Zr{:}Zr)} = 15000.0 + 3.0\ \mathrm{GHSER_{Zr}}$$

$$L_{\mathrm{Cr,Zr:Cr}}^{0,\mathrm{Laves-C14}} = L_{\mathrm{Cr,Zr:Zr}}^{0,\mathrm{Laves-C14}} = 52300$$

$$L_{\mathrm{Cr:Cr,Zr}}^{0,\mathrm{Laves-C14}} = L_{\mathrm{Zr:Cr,Zr}}^{0,\mathrm{Laves-C14}} = 26060$$



Phase Laves–$C15$

$G^{\circ}(T) - 3.0\ H_{\mathrm{Cr}}^{\mathrm{o,bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) = \mathrm{G(Cr{:}Cr)} =$
$15000.0 + 3.0\ \mathrm{GHSER_{Cr}}$

$G^{\circ}(T) - 2.0\ H_{\mathrm{Cr}}^{\mathrm{o,bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) - H_{\mathrm{Zr}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Cr{:}Zr)} =$
$-\ 87273 + 29.915\ T + 2.0\ \mathrm{GHSER_{Cr}} + \mathrm{GHSER_{Zr}}$

$G^{\circ}(T) - H_{\mathrm{Cr}}^{\mathrm{o,bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Zr}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Zr{:}Cr)} =$
$387273 - 29.915\ T + \mathrm{GHSER_{Cr}} + 2.0\ \mathrm{GHSER_{Zr}}$

$G^{\circ}(T) - 3.0\ H_{\mathrm{Zr}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Zr{:}Zr)} =$
$15000.0 + 3.0\ \mathrm{GHSER_{Zr}}$

$L_{\mathrm{Cr,Zr:Cr}}^{0,\mathrm{Laves}-C15} = 70328$

$L_{\mathrm{Cr,Zr:Zr}}^{0,\mathrm{Laves}-C15} = 70328$

$L_{\mathrm{Cr:Cr,Zr}}^{0,\mathrm{Laves}-C15} = 62910$

$L_{\mathrm{Zr:Cr,Zr}}^{0,\mathrm{Laves}-C15} = 62910$

Phase Laves–*C*36

$$G^{\circ}(T) - 3.0\ H_{\mathrm{Cr}}^{\mathrm{o,bcc-}A2\mathrm{,para}}(298.15\ \mathrm{K}) = \mathrm{G(Cr{:}Cr)} = 15000.0 + 3.0\ \ \mathrm{GHSER_{Cr}}$$

$$G^{\circ}(T) - 2.0\ H_{\mathrm{Cr}}^{\mathrm{o,bcc-}A2\mathrm{,para}}(298.15\ \mathrm{K}) - H_{\mathrm{Zr}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \mathrm{G(Cr{:}Zr)} = -\ 70026 + 20.901\ \ T + 2.0\ \ \mathrm{GHSER_{Cr}} + \mathrm{GHSER_{Zr}}$$

$$G^{\circ}(T) - H_{\mathrm{Cr}}^{\mathrm{o,bcc-}A2\mathrm{,para}}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Zr}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \mathrm{G(Zr{:}Cr)} = 100026.08 - 20.901\ \ T + \mathrm{GHSER_{Cr}} + 2.0\ \ \mathrm{GHSER_{Zr}}$$

$$G^{\circ}(T) - 3.0\ H_{\mathrm{Zr}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \mathrm{G(Zr{:}Zr)} = 15000.0 + 3.0\ \ \mathrm{GHSER_{Zr}}$$

$$L_{\mathrm{Cr,Zr:Cr}}^{0,\mathrm{Laves-}C36} = 52614$$

$$L_{\mathrm{Cr,Zr:Zr}}^{0,\mathrm{Laves-}C36} = 52614$$

$$L_{\mathrm{Cr:Cr,Zr}}^{0,\mathrm{Laves-}C36} = 29400$$

$$L_{\mathrm{Zr:Cr,Zr}}^{0,\mathrm{Laves-}C36} = 2940$$

Phase liquid

$$L_{\mathrm{Cr,Zr}}^{0,\mathrm{liquid}} = -\ 12971.34 + 1.20015\ \ T$$

$$L_{\mathrm{Cr,Zr}}^{1,\mathrm{liquid}} = 8025.96 - 0.74259\ \ T$$

$$L_{\mathrm{Cr,Zr}}^{2,\mathrm{Liquid}} = -\ 9984.87 + 0.92383\ \ T$$

Phase bcc–*A*2

$$L_{\mathrm{Cr,Zr:}\square}^{0,\mathrm{bcc-}A2} = 16555.47 + 4.92028\ \ T$$

$$L_{\mathrm{Cr,Zr:}\square}^{1,\mathrm{bcc-}A2} = 11365.57$$

Phase fcc–*A*1

$$L_{\mathrm{Cr,Zr:}\square}^{0,\mathrm{fcc-}A1} = 20000$$

Phase hcp–*A*3

$$L_{\mathrm{Cr,Zr:}\square}^{0,\mathrm{hcp-}A3} = 15800$$

Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Zr}			T / K
Liquid ⇌ Laves-$C15$ + bcc-$A2$	Eutectic	.765	.359	.916	1607.9
Laves-$C36$ ⇌ Laves-$C15$ + Liquid	Metatectic	.359	.348	.573	1839.6
Liquid + Laves-$C14$ ⇌ Laves-$C36$	Peritectic	.461	.346	.348	1900.0
Laves-$C36$ ⇌ Liquid + Laves-$C14$	Metatectic	.316	.218	.321	1895.9
Liquid ⇌ bcc-$A2$ + Laves-$C36$	Eutectic	.173	.014	.313	1864.6
Laves-$C36$ ⇌ bcc-$A2$ + Laves-$C15$	Eutectoid	.314	.012	.333	1816.1
bcc-$A2$ ⇌ Laves-$C15$ + hcp-$A3$	Eutectoid	.984	.340	.994	1112.3
Laves-$C14$ ⇌ Liquid	Congruent	.333	.333	....	1946.5
Laves-$C15$ ⇌ Laves-$C36$	Congruent	.340	.340	....	1858.0

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Cr-Zr	(Cr)	W	$cI2$ $Im\bar{3}m$	M 2	
	(Zr)	Mg	$hP2$ $P6_3/mmc$	M 2	
	(Zr)	W	$cI2$ $Im\bar{3}m$	M 4	
	α-Cr_2Zr	Cu_2Mg	$cF24$ $Fd\bar{3}m$	M_1 8 M_2 16	Laves-$C15$
	β-Cr_2Zr	$MgNi_2$	$hP24$ $P6_3/mmc$	Cr_1 6 Cr_2 6 Zr_1 3 Zr_2 3	Laves-$C36$
	γ-Cr_2Zr	$MgZn_2$	$hP12$ $P6_3/mmc$	Cr 2 Cr 6 Zr 4	Laves-$C14$

System Cu–Fe

Solution Phases:

(stable)	:	Liquid, fcc–$A1$, bcc–$A2$
(metastable)	:	hcp–$A3$

Modelling:

Liquid	:	Substitutional, Redlich–Kister
bcc–$A2$	:	Substitutional, Redlich–Kister
fcc–$A1$	:	Substitutional, Redlich–Kister
hcp–$A3$	:	Substitutional, Redlich–Kister

Assessor and Date:

I. Ansara, and Å. Jansson

Publication:

Trita-Mac-0533, Dec. 1993, Materials Research Center, The Royal Institute of Technology, Stockholm (Sweden)

Thermodynamic properties of the solution phases (J.mol^{-1})

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Cu,Fe}:\square} = 39258.0 - 4.14983\ T$$

Phase fcc–$A1$

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Cu,Fe}:\square} = 48232.5 - 8.60954\ T$$

$$L^{1,\mathrm{fcc}-A1}_{\mathrm{Cu,Fe}:\square} = 8861.88 - 5.28975\ T$$

Phase hcp–$A3$

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Cu,Fe}:\square} = 48232.5 - 8.60954\ T$$

$$L^{1,\mathrm{hcp}-A3}_{\mathrm{Cu,Fe}:\square} = 8861.88 - 5.28975\ T$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Cu,Fe}} = 36088.0 - 2.32968\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Cu,Fe}} = 324.53 - 0.03270\ T$$

$$L^{2,\mathrm{liquid}}_{\mathrm{Cu,Fe}} = 10355.40 - 3.60297\ T$$

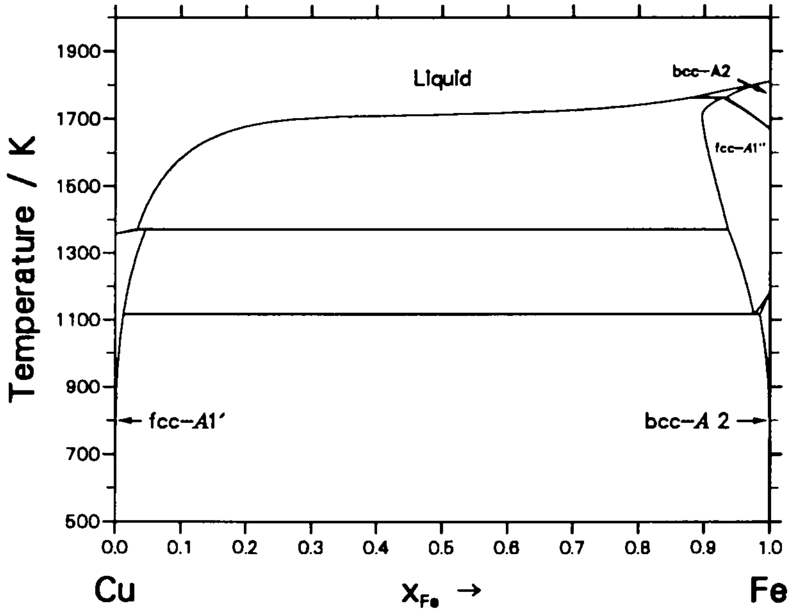


Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Fe}			T / K
Liquid + bcc-$A2$ ⇌ fcc-$A1$"	Peritectic	.880	.933	.927	1762.4
Liquid + fcc-$A1$" ⇌ fcc-$A1$'	Peritectic	.034	.936	.047	1371.4
fcc-$A1$" ⇌ fcc-$A1$' + bcc-$A2$	Eutectoid	.975	.012	.984	1115.9

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group
Cu–Fe	(Cu)	Cu	$cF4$ $Fm\bar{3}m$
	(Fe)	Cu	$cF4$ $Fm\bar{3}m$
	(Fe)	W	$cI2$ $Im\bar{3}m$

System Cu–Li

Solution Phases:
(stable) Liquid, bcc–$A2$, fcc–$A1$

Solution Phases:
(metastable) hcp–$A3$

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc–$A2$: Substitutional, Redlich-Kister
fcc–$A1$: Substitutional, Redlich-Kister
hcp–$A3$: Substitutional, Redlich-Kister

Assessor and Date:
N. Saunders, 1991

Thermodynamic properties of the solution phases (J.mol^{-1})

Phase bcc–$A2$

$$L^{0,bcc-A2}_{Cu,Li:\square} = 50000$$

Phase fcc–$A1$

$$L^{0,fcc-A1}_{Cu,Li:\square} = 2750 + 13.0\ T$$

$$L^{1,fcc-A1}_{Cu,Li:\square} = -1000$$

Phase hcp–$A3$

$$L^{0,hcp-A3}_{Cu,Li:\square} = 2042 + 10.9617\ T$$

Phase liquid

$$L^{0,liquid}_{Cu,Li} = 66000 - 44.723\ T$$

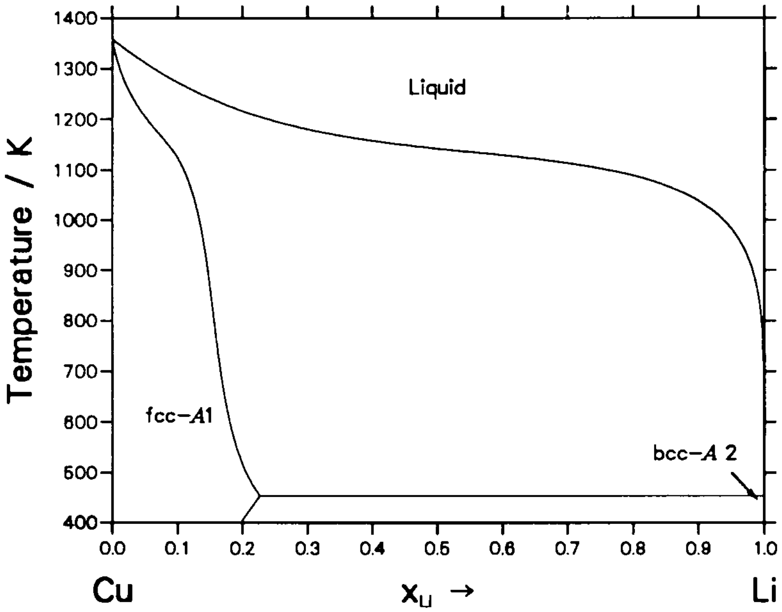


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Li}			T / K
Liquid ⇌ fcc-A1 + bcc-A2	Degenerate	1.000	0.228	1.000	453.6

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pears. Symb. Space Group
Cu-Li	(Cu)	Cu	$cF4$ $Fm\bar{3}m$
	(Li)	W	$cI2$ $Im\bar{3}m$

System Cu–Mg

Solution Phases:

(stable) : Liquid, fcc-$A1$, hcp-$A3$
(metastable) : bcc-$B2$, hcp-Zn

Compound:

(stable) Laves-$C15$, $CuMg_2$
(metastable) Laves-$C14$, Laves-$C36$, CuZn-γ
MgZn, Mg_2Zn_3, Mg_2Zn_{11}

Modelling:

Liquid : Substitutional, Redlich-Kister
fcc-$A1$: Substitutional, Redlich-Kister
hcp-$A3$: Substitutional, Redlich-Kister
Laves-$C15$: Sublattice-model, $Cu,Mg)_{0.5}(Cu,Mg)_{0.5}(\square)_3$
$CuMg_2$: Stoichiometric, $CuMg_2$
bcc-$A2$: see below
bcc-$B2$: Sublattice model, $(Cu,Mg)_{0.5}(Cu,Mg)_{0.5}$
Two descriptions of the bcc-$A2$:bcc-$B2$ order-disorder transformation are given: one which includes the parameters of the order and disordered phases in a single description (equation 21 in the thermodynamic modelling chapter), and a second one where the order and disorder contributions are expressed by equation 23. For the second case, the parameters are in a frame.
hcp-Zn : Substitutional, Redlich-Kister
CuZn-γ : Stoichiometric, $(Cu)_2(Cu)_2(Cu)_3(Mg)_6$
Mg_2Zn_{11} : Stoichiometric, $(Cu)_{11}(Mg)_2$
Mg_2Zn_3 : Stoichiometric, $(Cu)_3(Mg)_2$
MgZn : Stoichiometric, $(Cu)_{13}(Mg)_{12}$
Laves-$C14$: Sublattice-model, $(Cu,Mg)_2(Cu,Mg)$
Laves-$C36$: Sublattice-model, $(Cu,Mg)_2(Cu,Mg)$

Assessor and Date:

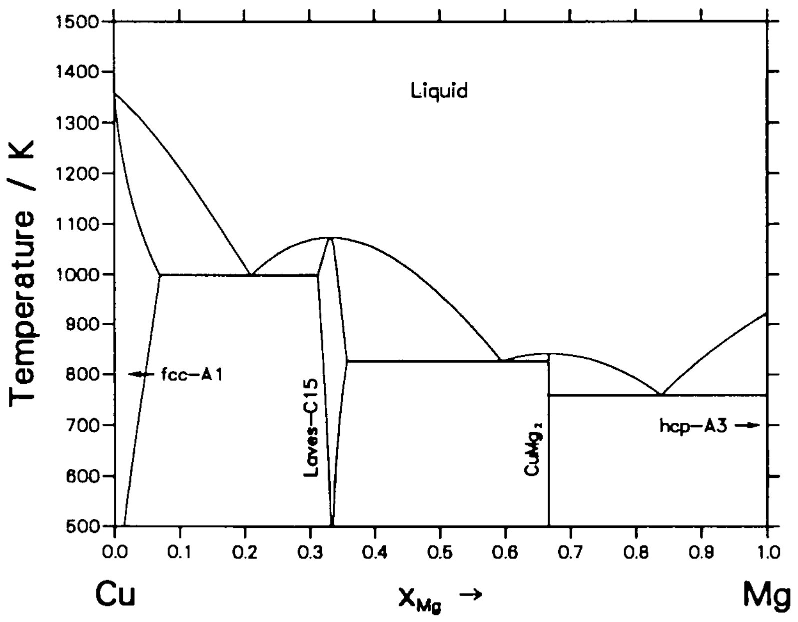
C.A. Coughnanowr, I. Ansara, R. Luoma,
M. Hämäläinen, and H.L. Lukas

Publication:

Z. für Metallkde., 82, 7, 574-581 (1991).

Comments:

A new assessment was performed where the lattice stabilities of Cu and Mg in the Laves-$C15$ structure were taken equal to 15kJ/formula unit, in order to ensure consistency in the database.



Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase liquid

$L^{0,\mathrm{liquid}}_{\mathrm{Cu,Mg}} = -36962.71 + 4.74394\ T$

$L^{1,\mathrm{liquid}}_{\mathrm{Cu,Mg}} = -8182.19$

Phase fcc–*A*1

$L^{0,\mathrm{fcc}-A1}_{\mathrm{Cu,Mg:\square}} = -22059.61 + 5.63232\ T$

Phase hcp–*A*3

$L^{0,\mathrm{hcp}-A3}_{\mathrm{Cu,Mg:\square}} = 22500.0 - 3.0\ T$

Phase hcp–Zn

$$L^{0,\mathrm{hcp-Zn}}_{\mathrm{Cu,Mg:\square}} = 22500.0 - 3.0\ T$$

Phase Laves–$C14$

$$G^{\circ}(T) - 3.0\ H^{\mathrm{o,fcc-}A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Cu)} = 15000.0 + 3.0\ \mathrm{GHSER_{Cu}}$$

$$\begin{aligned}G^{\circ}(T) - 2.0\ H^{\mathrm{o,fcc-}A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - H^{\mathrm{o,hcp-}A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Mg)} =&\\ - 24691.0 + 364.73085\ T - 69.276417\ T\cdot \ln T - 5.19246\mathrm{E\text{-}}04\ T^{2}&\\ + 143502\ T^{-1} - 5.65953\mathrm{E\text{-}}6\ T^{3}&\end{aligned}$$

$$\begin{aligned}G^{\circ}(T) - H^{\mathrm{o,fcc-}A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - 2.0\ H^{\mathrm{o,hcp-}A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Cu)} =&\\ 74970.96 - 16.46448\ T + \mathrm{GHSER_{Cu}} + 2.0\ \mathrm{GHSER_{Mg}}&\end{aligned}$$

$$G^{\circ}(T) - 3.0\ H^{\mathrm{o,fcc-}A1}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Mg)} = 15000.0 + 3.0\ \mathrm{GHSER_{Mg}}$$

$$L^{0,\mathrm{Laves-C14}}_{\mathrm{Cu,Mg:Cu}} = L^{0,\mathrm{Laves-C14}}_{\mathrm{Cu,Mg:Mg}} = 13011.35$$

$$L^{0,\mathrm{Laves-C14}}_{\mathrm{Cu:Cu,Mg}} = L^{0,\mathrm{Laves-C14}}_{\mathrm{Mg:Cu,Mg}} = 6599.45$$

Phase Laves–$C15$

$$G^{\circ}(T) - 3.0\ H^{\mathrm{o,fcc-}A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Cu)} = 15000.0 + 3.0\ \mathrm{GHSER_{Cu}}$$

$$\begin{aligned}G^{\circ}(T) - 2.0\ H^{\mathrm{o,fcc-}A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - H^{\mathrm{o,hcp-}A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Mg)} =&\\ - 54691.0 + 364.73085\ T - 69.276417\ T\cdot \ln T - 5.19246\mathrm{E\text{-}}04\ T^{2}&\\ + 143502\ T^{-1} - 5.65953\mathrm{E\text{-}}6\ T^{3}&\end{aligned}$$

$$\begin{aligned}G^{\circ}(T) - H^{\mathrm{o,fcc-}A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - 2.0\ H^{\mathrm{o,hcp-}A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Cu)} =&\\ 104970.96 - 16.46448\ T + \mathrm{GHSER_{Cu}} + 2.0\ \mathrm{GHSER_{Mg}}&\end{aligned}$$

$$G^{\circ}(T) - 3.0\ H^{\mathrm{o,fcc-}A1}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Mg)} = 15000.0 + 3.0\ \mathrm{GHSER_{Mg}}$$

$$L^{0,\mathrm{Laves-C15}}_{\mathrm{Cu,Mg:Cu}} = L^{0,\mathrm{Laves-C15}}_{\mathrm{Cu,Mg:Mg}} = 13011.35$$

$$L^{0,\mathrm{Laves-C15}}_{\mathrm{Cu:Cu,Mg}} = L^{0,\mathrm{Laves-C15}}_{\mathrm{Mg:Cu,Mg}} = 6599.45$$

Phase Laves–$C36$

$$G^{\circ}(T) - 3.0\ H^{\mathrm{o,fcc-}A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Cu)} = 15000.0 + 3.0\ \mathrm{GHSER_{Cu}}$$

$$\begin{aligned}G^{\circ}(T) - 2.0\ H^{\mathrm{o,fcc-}A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - H^{\mathrm{o,hcp-}A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Mg)} =&\\ - 34691.0 + 364.73085\ T - 69.276417\ T\cdot \ln T - 5.19246\mathrm{E\text{-}}04\ T^{2}&\\ + 143502\ T^{-1} - 5.65953\mathrm{E\text{-}}6\ T^{3}&\end{aligned}$$

$$G^{\circ}(T) - H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Cu)} =$$
$$84970.96 - 16.46448\ T + \mathrm{GHSER_{Cu}} + 2.0\ \ \mathrm{GHSER_{Mg}}$$

$$G^{\circ}(T) - 3.0\ H_{\mathrm{Mg}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Mg)} = 15000.0 + 3.0\ \ \mathrm{GHSER_{Mg}}$$

$$L^{\mathrm{0,Laves-C36}}_{\mathrm{Cu,Mg:Cu}} = L^{\mathrm{0,Laves-C36}}_{\mathrm{Cu,Mg:Mg}} = 13011.35$$

$$L^{\mathrm{0,Laves-C36}}_{\mathrm{Cu:Cu,Mg}} = L^{\mathrm{0,Laves-C36}}_{\mathrm{Mg:Cu,Mg}} = 6599.45$$

Phase CuMg$_2$

$$G^{\circ}(T) - H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) =$$
$$-\ 28620.0 + 1.86456\ T + \mathrm{GHSER_{Cu}} + 2.0\ \ \mathrm{GHSER_{Mg}}$$

Phase CuZn–γ

$\mathrm{K4} = -\ 11552.71 - 1.67824\ T$
$\mathrm{K5} = 15732.3 - 10.26575\ T$
$\mathrm{K7} = 9000.0 - 1.5\ T$

$$G^{\circ}(T) - 7.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 6.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Cu{:}Cu{:}Mg)} =$$
$$13.0\ \ \mathrm{K4} + 2.0\ \ \mathrm{K5} + 6.0\ \ \mathrm{K7} + 7.0\ \ \mathrm{GHSER_{Cu}} + 6.0\ \ \mathrm{GHSER_{Mg}}$$

Phase Mg$_2$Zn$_{11}$

$$G^{\circ}(T) - 11.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Cu)} =$$
$$0.0 + 11.0\ \ \mathrm{GHSER_{Cu}} + 2.0\ \ \mathrm{GHSER_{Mg}}$$

Phase Mg$_2$Zn$_3$

$$G^{\circ}(T) - 3.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Cu)} =$$
$$0.0 + 3.0\ \ \mathrm{GHSER_{Cu}} + 2.0\ \ \mathrm{GHSER_{Mg}}$$

Phase MgZn

$$G^{\circ}(T) - 13.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 12.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Cu)} =$$
$$0.0 + 13.0\ \ \mathrm{GHSER_{Cu}} + 12.0\ \ \mathrm{GHSER_{Mg}}$$

Phase bcc–$B2$

$G^{*}\mathrm{Cu} : \mathrm{Mg} = 0.0$
$L^{0}\mathrm{Cu}, \mathrm{Mg} = -\ 2500$

$$G^{\circ}(T) - H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Cu)} = \mathrm{GBCC_{Cu}}$$

$$G^{\circ}(T) - 0.5\ H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Mg)} =$$
$$G^{*}\mathrm{Cu} : \mathrm{Mg} + 0.5\ \ L^{0}_{\mathrm{Cu,Mg}} + 0.5\ \ \mathrm{GBCC_{Cu}} + 0.5\ \ \mathrm{GBCC_{Mg}}$$

$$G^\circ(T) - 0.5\ H^{o,fcc-A1}_{Cu}(298.15\ K) - 0.5\ H^{o,hcp-A3}_{Mg}(298.15\ K) = G(Mg{:}Cu) = G^{*}Cu : Mg + L^{0}_{Cu,Mg} + 0.5\ \ GBCC_{Cu} + 0.5\ \ GBCC_{Mg}$$

$$G^\circ(T) - H^{o,hcp-A3}_{Mg}(298.15\ K) = G(Mg{:}Mg) = \ GBCC_{Mg}$$

$$L^{0,bcc-B2}_{Cu,Mg:Cu:\square} = L^{0,bcc-B2}_{Cu,Mg:Mg:\square} = -\ G^{*}Cu : Mg + L^{0}Cu, Mg$$

$$L^{0,bcc-B2}_{Cu:Cu,Mg:\square} = L^{0,bcc-B2}_{Mg:Cu,Mg:\square} = -\ G^{*}Cu : Mg + L^{0}Cu, Mg$$

Phase bcc–$B2$

$G^{*}_{Cu:Mg} = 0.0$
$L^{0}_{Cu,Mg} = -\ 2500$

$$G^\circ(T) - H^{o,fcc-A1}_{Cu}(298.15\ K) = G(Cu{:}Cu) = 0.0$$

$$G^\circ(T) - 0.5\ H^{o,fcc-A1}_{Cu}(298.15\ K) - 0.5\ H^{o,hcp-A3}_{Mg}(298.15\ K) = G(Cu{:}Mg) = 2.0\ G^{*}Cu : Mg$$

$$G^\circ(T) - 0.5\ H^{o,fcc-A1}_{Cu}(298.15\ K) - 0.5\ H^{o,hcp-A3}_{Mg}(298.15\ K) = G(Mg{:}Cu) = 2.0\ G^{*}Cu : Mg$$

$$G^\circ(T) - H^{o,hcp-A3}_{Mg}(298.15\ K) = G(Mg{:}Mg) = 0.0$$

Phase bcc–$A2$

$L^{0,bcc-A2}_{Cu,Mg:\square} = 4.0\ \ L^{0}Cu, Mg$

Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Mg}			T / K
Liquid ⇌ fcc–$A1$ + Laves–$C15$	Eutectic	.209	.069	.313	998.6
Liquid ⇌ Laves–$C15$ + $CuMg_2$	Eutectic	.595	.356	.667	825.5
Liquid ⇌ $CuMg_2$ + hcp–$A3$	Eutectic	.839	.667	1.000	759.7
$CuMg_2$ ⇌ Liquid	Congruent	0.666	0.666	...	841.0
Laves–$C15$ ⇌ Liquid	Congruent	0.333	0.333	...	1073.5

System Cu–Ni

Solution Phases:

(stable)	Liquid, fcc–A1
(metastable)	bcc–$A2$, hcp–$A3$

Modelling:

Liquid	:	Substitutional, Redlich-Kister
bcc–$A2$	:	Substitutional, Redlich-Kister
fcc–$A1$	:	Substitutional, Redlich-Kister
hcp–$A3$	:	Substitutional, Redlich-Kister

Assessor and Date:

S. an Mey

Publication:

Calphad, **16**, (3), 255-260 (1992).

Thermodynamic properties of the solution phases (J.mol^{-1})

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Cu,Ni:\square}} = 8047.72 + 3.42217\ T$$

$$L^{1,\mathrm{bcc}-A2}_{\mathrm{Cu,Ni:\square}} = -\,2041.3 + 0.99714\ T$$

Phase fcc–$A1$

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Cu,Ni:\square}} = 8047.72 + 3.42217\ T$$

$$L^{1,\mathrm{fcc}-A1}_{\mathrm{Cu,Ni:\square}} = -\,2041.3 + 0.99714\ T$$

$$T^{0,\mathrm{fcc}-A1}_{\mathrm{c,Cu,Ni:\square}} = -\,935.5$$

$$T^{1,\mathrm{fcc}-A1}_{\mathrm{c,Cu,Ni:\square}} = -\,594.9$$

$$\beta^{0,\mathrm{mag,fcc}-A1}_{\mathrm{Cu,Ni:\square}} = -\,0.7316$$

$$\beta^{1,\mathrm{mag,fcc}-A1}_{\mathrm{Cu,Ni:\square}} = -\,0.3174$$

Phase hcp-$A3$

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Cu,Ni:\square}} = 8047.72 + 3.42217\ T$$

$$L^{1,\mathrm{hcp}-A3}_{\mathrm{Cu,Ni:\square}} = -2041.3 + 0.99714\ T$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Cu,Ni}} = 12048.61 + 1.29893\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Cu,Ni}} = -1861.61 + 0.94201\ T$$

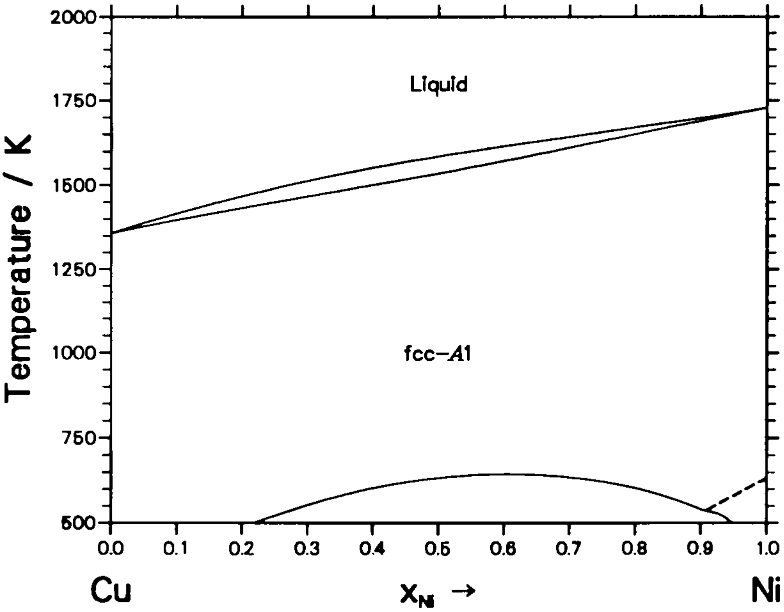


Table I – Invariant Reaction.

Reaction	Type	Compositions x_{Ni}	T / K
fcc-$A1$' ⇌ fcc-$A1$"	Critical Temp.	0.600 0.600	641.0

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group
Cu-Ni	(Cu)	Cu	$cF4$ $Fm\bar{3}m$
	(Ni)	Cu	$cF4$ $Fm\bar{3}m$

System Cu–Si

Solution Phases:

(stable)	Liquid, bcc–$A2$, fcc–$A1$
(metastable)	hcp–$A3$

Compounds:

(stable)	$Cu_{56}Si_{11}$–γ, Cu_4Si–ϵ, $Cu_{19}Si_6$–η, $Cu_{33}Si_7$–δ
(metastable)	Laves–$C15$

Modelling:

Liquid : Substitutional, Redlich–Kister
bcc–$A2$: Substitutional, Redlich–Kister
fcc–$A1$: Substitutional, Redlich–Kister
hcp–$A3$: Substitutional, Redlich–Kister
$Cu_{56}Si_{11}$–γ : Stoichiometric, $(Cu)_{56}(Si)$
Cu_4Si–ϵ : Stoichiometric, $(Cu)_4(Si)$
$Cu_{19}Si_6$–η : Stoichiometric, $(Cu)_{19}(Si)_6$
$Cu_{33}Si_7$–δ : Stoichiometric, $(Cu)_{33}(Si)_7$
Laves-$C15$: Sublattice model, $(Cu,Si)_2(Cu,Si)$

Assessor and Date:

M. Jacobs, 1991. Revised by T. Bühler et al. 1997

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase bcc–$A2$

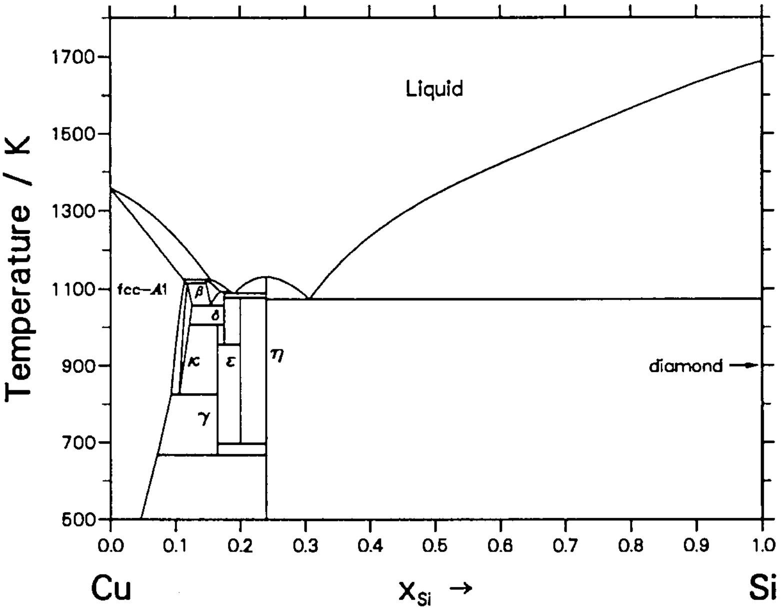
$$L^{0,bcc-A2}_{Cu,Si:\Box} = -21740 + 3.9\ T$$

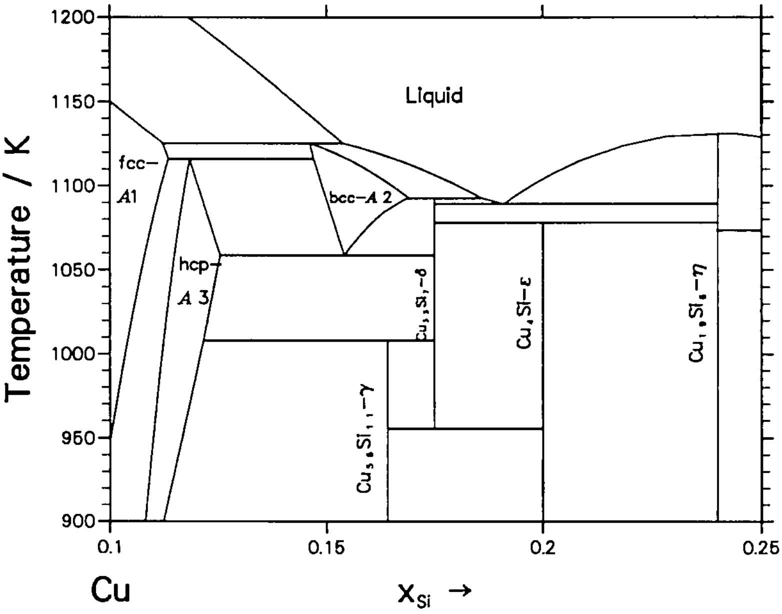
$$L^{1,bcc-A2}_{Cu,Si:\Box} = -40000 - 4.39\ T$$

$$L^{2,bcc-A2}_{Cu,Si:\Box} = -100$$

Phase fcc–$A1$

$$L^{0,fcc-A1}_{Cu,Si:\Box} = -34105.96 - 1.908\ T$$


Temperature / K
1700
1500
1300
1100
900
700
500
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
Cu
x_Si →
Si
Liquid
fcc–A1
β
δ
κ
ε
η
γ
diamond →


Temperature / K
1200
1150
1100
1050
1000
950
900
0.1
0.15
0.2
0.25
Cu
x_Si →
Liquid
fcc–A1
hcp–A 3
bcc–A 2
Cu56Si11–γ
Cu33Si7–δ
Cu4Si–ε
Cu19Si6–η

Phase hcp-A3

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Cu,Si:\square}} = -19948 - 2.356\ T$$

$$L^{1,\mathrm{hcp}-A3}_{\mathrm{Cu,Si:\square}} = -23800 - 1.97\ T$$

$$L^{2,\mathrm{hcp}-A3}_{\mathrm{Cu,Si:\square}} = -20$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Cu,Si}} = -39688.86 + 14.27467\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Cu,Si}} = -49937.13 + 29.78960\ T$$

$$L^{2,\mathrm{liquid}}_{\mathrm{Cu,Si}} = -31810.16 + 18.00804\ T$$

Phase $\mathrm{Cu_{33}Si_7}$–δ

$$G^\circ(T) - 33.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - 7.0\ H^{\circ,\mathrm{diamond}}_{\mathrm{Si}}(298.15\ \mathrm{K}) = -200372.4 + 4985.675\ T - 955.5312\ T\cdot \ln T - 0.101066\ T^2 + 4.2396\mathrm{E}\text{-}06\ T^3 + 2968440\ T^{-1}$$

Phase $\mathrm{Cu_{56}Si_{11}}$–γ

$$G^\circ(T) - 56.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - 11.0\ H^{\circ,\mathrm{diamond}}_{\mathrm{Si}}(298.15\ \mathrm{K}) = 69000 + 405\ T - 107.73\ T\cdot \ln T + 46.0\ \mathrm{GHSER_{Cu}} + 11.0\ \mathrm{GHSER_{Si}}$$

Phase $\mathrm{Cu_4Si}$–ϵ

$$G^\circ(T) - 4.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{diamond}}_{\mathrm{Si}}(298.15\ \mathrm{K}) = -39974.35 + 858.5047\ T - 154.6764\ T\cdot \ln T + 0.01074864\ T^2 + 5.1335\mathrm{E}\text{-}07\ T^3 + 386580\ T^{-1}$$

Phase $\mathrm{Cu_{19}Si_6}$–η

$$G^\circ(T) - 19.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - 6.0\ H^{\circ,\mathrm{diamond}}_{\mathrm{Si}}(298.15\ \mathrm{K}) = -137488.5 + 3119.537\ T - 595.1259\ T\cdot \ln T - 0.0619575\ T^2 + 2.434\mathrm{E}\text{-}06\ T^3 + 2057075\ T^{-1}$$

Phase Laves-$C15$

$$G^\circ(T) - 3.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) = G(\mathrm{Cu{:}Cu}) = 15000.0 + 3.0\ \mathrm{GHSER_{Cu}}$$

$$G^\circ(T) - 2.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{diamond}}_{\mathrm{Si}}(298.15\ \mathrm{K}) = G(\mathrm{Cu{:}Si})\ 15000.0 + 2.0\ \mathrm{GHSER_{Cu}} + \mathrm{GHSER_{Si}}$$

$$G^\circ(T) - H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - 2.0\ H^{\circ,\mathrm{diamond}}_{\mathrm{Si}}(298.15\ \mathrm{K}) = G(\mathrm{Si{:}Cu})\ 15000.0 + \mathrm{GHSER_{Cu}} + 2.0\ \mathrm{GHSER_{Si}}$$

$$G^\circ(T) - 3.0\ H^{\circ,\mathrm{diamond}}_{\mathrm{Si}}(298.15\ \mathrm{K}) = G(\mathrm{Si{:}Si})\ 15000.0 + 3.0\ \mathrm{GHSER_{Si}}$$

$$L^{0,\mathrm{Laves}-C15}_{\mathrm{Cu,Si:Cu}} = L^{0,\mathrm{Laves}-C15}_{\mathrm{Cu,Si:Si}} = 15305 + 20.69\ T$$

Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Si}			T / K
Liquid + fcc-$A1$ $\rightleftharpoons$ β^{*}	Peritectic	.154	.112	.146	1125.4
fcc-$A1$ + β^{*} $\rightleftharpoons$ β^{**}	Peritectoid	.113	.147	.118	1115.9
$\beta^{*} \rightleftharpoons \beta^{**} + \delta$	Eutectoid	.154	.125	.175	1058.6
Liquid + $\beta^{*} \rightleftharpoons \delta$	Peritectic	.186	.169	.175	1092.7
Liquid $\rightleftharpoons \delta + \eta$	Eutectic	.191	.175	.240	1089.2
$\eta + \delta \rightleftharpoons \epsilon$	Peritectoid	.175	.240	.200	1077.9
$\delta \rightleftharpoons \beta^{***} + \epsilon$	Eutectoid	.175	.164	.200	955.6
$\beta^{**} + \delta \rightleftharpoons \beta^{***}$	Peritectoid	.121	.175	.164	1008.3
$\epsilon \rightleftharpoons \beta^{***} + \eta$	Eutectoid	.200	.164	.240	696.5
$\beta^{**} \rightleftharpoons$ fcc-$A1$ + β^{***}	Eutectoid	.105	.093	.164	825.5
$\beta^{***} \rightleftharpoons$ fcc-$A1$ + η	Eutectoid	.164	.072	.240	667.8
Liquid $\rightleftharpoons \eta$ + diamond	Eutectic	.306	.240	1.000	1073.7
$\eta \rightleftharpoons$ Liquid	Congruent	.240	.240	....	1132.0

* $\beta \equiv$ bcc-$A2$, ** $\kappa \equiv$ hcp-$A3$, ** $\gamma \equiv$ cub-$A13$

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Cu-Si	(Cu)	Cu	$cF4$ $Fm\bar{3}m$	M 4	
	(Si)	diamond	$cF8$ $Fd\bar{3}m$	M 8	
	κ	Mg	$hP2$ $P6_3/mmc$	M 2	hcp-$A3$ Cu_7Si in [91Vil]
	Cu_3Si		t^{**}		η, η', η'' in Mas2 denoted Cu_4Si-ϵ
	δ		$hP72$		
	γ	β-Mn	$cP20$ $P4_132$	M_1 8 M_2 12	
	β	W	$cI2$ $Im\bar{3}m$	M 2	bcc-$A2$

System Cu–Y

Solution Phases:

Liquid, bcc–$A2$, hcp–$A3$, Cu_6Y

Compound:

Cu_4Y, Cu_6Y, Cu_7Y_2, Cu_2Y-R, Cu_2Y-H, CuY

Modelling:

Liquid : Substitutional, Redlich–Kister
bcc–$A2$: Substitutional, Redlich–Kister
hcp–$A3$: Substitutional, Redlich–Kister
Cu_6Y : Sublattice model, $(Cu)_5(Cu_2,Y)$
Cu_4Y : Stoichiometric, $(Cu)_4(Y)$
Cu_7Y_2 : Stoichiometric, $(Cu)_7(Y)_2$
Cu_2Y-R : Stoichiometric, $(Cu)_2(Y)$
Cu_2Y-H : Stoichiometric, $(Cu)_2(Y)$
CuY : Stoichiometric, $(Cu)(Y)$

Assessor and Date:

T. Jantzen, 1997.

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase bcc–$A2$

$$L^{0,\text{bcc}-A2}_{\text{Cu,Y}:\square} = 80.0\ T$$

Phase hcp–$A3$

$$L^{0,\text{hcp}-A3}_{\text{Cu,Y}:\square} = 80.0\ T$$

Phase liquid

$$L^{0,\text{liquid}}_{\text{Cu,Y}} = -\,88958.06 + 21.5667\ T$$

$$L^{1,\text{liquid}}_{\text{Cu,Y}} = -\,33607.31 + 3.10462\ T$$

$$L^{2,\text{liquid}}_{\text{Cu,Y}} = 8083.16 - 0.74669\ T$$

Phase fcc-$A1$

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Cu,Y}} = 80.0\ T$$

Phase $\mathrm{Cu_2Y}$-R

$$G^\circ(T) - 2.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Y}}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Y)} = -\ 65324.22 + 6.03462\ T + 2.0\ \mathrm{GHSER_{Cu}} + \mathrm{GHSER_{Y}}$$

Phase $\mathrm{Cu_2Y}$-H

$$G^\circ(T) - 2.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Y}}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Y)} = -\ 51788.22 - 5.96538\ T + 2.0\ \mathrm{GHSER_{Cu}} + \mathrm{GHSER_{Y}}$$

Phase $\mathrm{Cu_4Y}$

$$G^\circ(T) - 4.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Y}}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Y)} = -89328.5 + 8.25205\ T + 4.0\ \mathrm{GHSER_{Cu}} + \mathrm{GHSER_{Y}}$$

Phase $\mathrm{Cu_6Y}$

$$G^\circ(T) - 7.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Cu_2)} = 35000.0 + 7.0\ \mathrm{GHSER_{Cu}}$$

$$G^\circ(T) - 5.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Y}}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Y)} = -\ 89797.58 + 8.2954\ T + 5.0\ \mathrm{GHSER_{Cu}} + \mathrm{GHSER_{Y}}$$

$$L^{0,\mathrm{Cu_6Y}}_{\mathrm{Cu{:}Cu_2,Y}} = -\ 34386.27 + 3.17656\ T$$

Phase $\mathrm{Cu_7Y_2}$

$$G^\circ(T) - 7.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - 2.0\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Y}}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Y)} = -\ 168519.6 + 15.56757\ T + 7.0\ \mathrm{GHSER_{Cu}} + 2.0\ \mathrm{GHSER_{Y}}$$

Phase CuY

$$G^\circ(T) - H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Y}}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Y)} = -\ 44616.68 + 4.12162\ T + \mathrm{GHSER_{Cu}} + \mathrm{GHSER_{Y}}$$

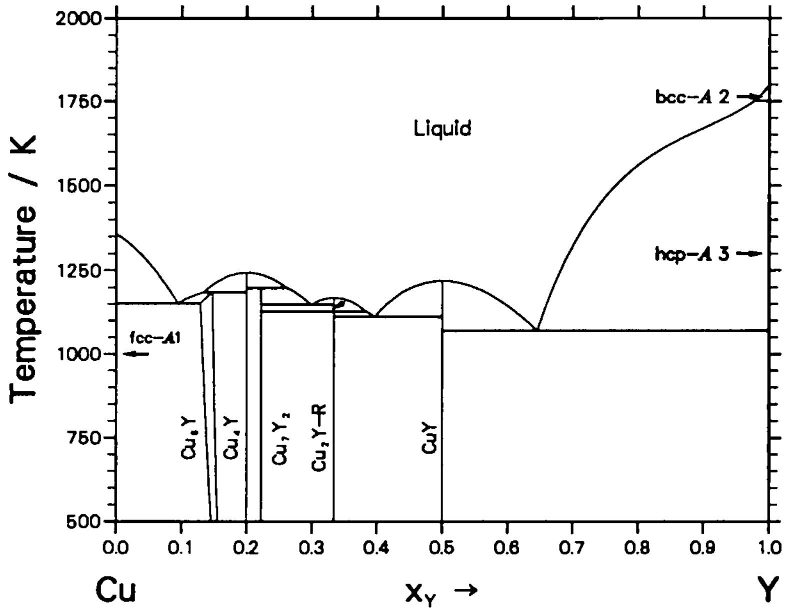


Table I - Invariant Reactions.

Reaction	Type	Compositions x_Y			T / K
Liquid $\rightleftharpoons$ CuY + hcp-$A3$	Eutectic	.646	.646	1.000	1070.0
Liquid $\rightleftharpoons$ Cu_2Y-R + CuY	Eutectic	.396	.333	.500	1113.0
Liquid $\rightleftharpoons$ Cu_2Y-H + Cu_7Y_2	Eutectic	.299	.222	.333	1148.6
Liquid $\rightleftharpoons$ Cu_4Y + Cu_7Y_2	Peritectic	.262	.200	.222	1198.0
Liquid + Cu_4Y $\rightleftharpoons$ Cu_6Y	Peritectic	.133	.200	.147	1184.0
Liquid $\rightleftharpoons$ fcc-$A1$ + Cu_6Y	Eutectic	.094	.000	.129	1153.0
hcp-$A3$ $\rightleftharpoons$ bcc-$A2$	Polymorphic	1.000	1.000	....	1752.0
Cu_2Y-R $\rightleftharpoons$ Cu_2Y-H	Polymorphic	.333	.333	....	1128.0
Liquid $\rightleftharpoons$ Cu_4Y	Congruent	.200	.200	....	1224.0
Liquid $\rightleftharpoons$ Cu_2Y-H	Congruent	.333	.333	....	1149.0
Liquid $\rightleftharpoons$ CuY	Congruent	.500	.500	....	1220.0

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Cu-Y	(Cu)	Cu	$cF4$ $Fm\bar{3}m$	M 4	
	(Y)	W	$cI2$ $Im\bar{3}m$	M 4	
	(Y)	Mg	$hP2$ $P6_3/mmc$	M 2	
	Cu_6Y				not in [91Vil]
	Cu_5Y	$CaCu_5$	$hP6$ $P6/mmm$	Y 1 Cu_1 2 Cu_2 3	quoted as metastable in 90Mas]
	Cu_4Y	$CaCu_5$?	$hP6$ $P6/mmm$		not quoted in [91Vil]
	Cu_7Y_2				not in [91Vil]
	Cu_2Y	$CeCu_2$	$oI12$ $Imma$	Y 4 Cu 8	
	CuY	CsCl	$cP2$ $Pm\bar{3}m$	Cu 1 Y 1	bcc-$B2$

System Cu–Zn

Solution Phases:

(stable) : Liquid, bcc–$A2$, bcc–$B2$, fcc–$A1$, hcp–$A3$(CuZn–ϵ), hcp–Zn

:

Solution Phases:

(stable) : CuZn–γ
(metastable) : Laves–$C14$, Laves–$C15$, Laves–$C36$

Modelling:

Liquid : Substitutional, Redlich–Kister
fcc–$A1$: Substitutional, Redlich–Kister
hcp–$A3$(CuZn–ϵ) : Substitutional, Redlich–Kister
hcp–Zn : Substitutional, Redlich–Kister
CuZn–γ : Sublattice, $(Cu,Zn)_2(Cu,Zn)_2(Cu)_3(Zn)_6$
bcc–$A2$: see below
bcc–$B2$: Sublattice model, $(Cu,Zn)_{0.5}(Cu,Zn)_{0.5}(\square)_3$
Two descriptions of the bcc–$A2$:bcc–$B2$ order-disorder transformation are given: one which includes the parameters of the order and disordered phases in a single description (equation 21 in the thermodynamic modelling chapter), and a second one where the order and disorder contributions are expressed by equation 23. For the second case, the parameters are in a frame.
Two descriptions of the bcc–$A2$:bcc–$B2$ order-disorder
Laves–$C14$: Sublattice model, $(Cu,Zn)_2(Cu,Zn)$
Laves–$C15$: Sublattice model, $(Cu,Zn)_2(Cu,Zn)$
Laves–$C36$: Sublattice model, $(Cu,Zn)_2(Cu,Zn)$

Assessor and Date:

M. Kowalski, and P.J. Spencer,

Publication:

J. Phase Equil., **14**, 4, 432-438 (1993).

Comments:

Based on Kowalski's data, a new assessment was performed to differentiate the two hexagonal forms of Zn.

Thermodynamic properties of the solution and compound phases(J.mol^{-1})

Phase fcc–$A1$

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Cu,Zn:}\square} = -\,42803.75 + 10.02258\ T$$

$$L^{1,\mathrm{fcc}-A1}_{\mathrm{Cu,Zn:}\square} = 2936.39 - 3.05323\ T$$

$$L^{2,\mathrm{fcc}-A1}_{\mathrm{Cu,Zn:}\square} = 9034.2 - 5.39314\ T$$

Phase hcp–$A3$

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Cu,Zn:}\square} = -\,36475 + 4.896\ T$$

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Cu,Zn:}\square} = 24790.0 - 10.135\ T$$

Phase hcp–Zn

$$L^{0,\mathrm{hcp-Zn}}_{\mathrm{Cu,Zn}} = -\,14432.17 - 10.7814\ T$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Cu,Zn}} = -\,40695.54 + 12.65269\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Cu,Zn}} = 4402.72 - 6.55425\ T$$

$$L^{2,\mathrm{liquid}}_{\mathrm{Cu,Zn}} = 7818.1 - 3.25416\ T$$

Phase bcc–$B2$

$$\begin{aligned}
G^{*}_{\mathrm{Cu:Zn:}\square} &= -\,3085.0\\
L^{0}_{\mathrm{Cu,Zn}} &= -\,12898.97 + 3.26598\ T\\
L^{1}_{\mathrm{Cu,Zn}} &= 945.265 - 0.80679\ T\\
L^{2}_{\mathrm{Cu,Zn}} &= 1921.485 - 1.86969\ T
\end{aligned}$$

$$G^{\circ}(T) - H^{\mathrm{o,fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) = \mathrm{G}\ (\mathrm{Cu:Cu:}\square) = \mathrm{GBCC_{Cu}}$$

$$G^{\circ}(T) - 0.5\ \ H^{\mathrm{o,fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - 0.5\ \ H^{\mathrm{o,hcp-Zn}}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \mathrm{G}\ (\mathrm{Cu:Zn:}\square) = G^{*}_{\mathrm{Cu:Zn}} + L^{0}_{\mathrm{Cu,Zn}} + 0.5\ \ \mathrm{GBCC_{Cu}} + 0.5\ \ \mathrm{GBCC_{Zn}}$$

$$G^{\circ}(T) - 0.5\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - 0.5\ H^{\circ,\mathrm{hcp-Zn}}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \mathrm{G}\ (\mathrm{Zn:Cu:\square}) =$$

$$G^{*}_{\mathrm{Cu:Zn:\square}} + L^{0}_{\mathrm{Cu,Zn}} + 0.5\ \mathrm{GBCC}_{\mathrm{Cu}} + 0.5\ \mathrm{GBCC}_{\mathrm{Zn}}$$

$$G^{\circ}(T) - 0.5\ H^{\circ,\mathrm{hcp-Zn}}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \mathrm{G}\ (\mathrm{Zn:Zn:\square}) = \mathrm{GBCC}_{\mathrm{Zn}}$$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Cu,Zn:Cu:\square}} = L^{0,\mathrm{bcc}-B2}_{\mathrm{Cu:Cu,Zn:\square}} = -\ G^{*}_{\mathrm{Cu:Zn:\square}} + L^{0}_{\mathrm{Cu,Zn}} + 3.0\ L^{1}_{\mathrm{Cu,Zn}} + 3.0\ L^{2}_{\mathrm{Cu,Zn}}$$

$$L^{1,\mathrm{bcc}-B2}_{\mathrm{Cu,Zn:Cu:\square}} = L^{1,\mathrm{bcc}-B2}_{\mathrm{Cu:Cu,Zn:\square}} = L^{1}_{\mathrm{Cu,Zn}} + 4.0\ L^{2}_{\mathrm{Cu,Zn}}$$

$$L^{2,\mathrm{bcc}-B2}_{\mathrm{Cu,Zn:Cu:\square}} = L^{2,\mathrm{bcc}-B2}_{\mathrm{Cu:Cu,Zn:\square}} = L^{2}_{\mathrm{Cu,Zn}}$$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Cu,Zn:Zn:\square}} = L^{0,\mathrm{bcc}-B2}_{\mathrm{Zn:Cu,Zn:\square}} = -\ G^{*}_{\mathrm{Cu:Zn:\square}} + L^{0}_{\mathrm{Cu,Zn}} - 3.0\ L^{1}_{\mathrm{Cu,Zn}} + 3.0\ L^{2}_{\mathrm{Cu,Zn}}$$

$$L^{1,\mathrm{bcc}-B2}_{\mathrm{Cu,Zn:Zn:\square}} = L^{1,\mathrm{bcc}-B2}_{\mathrm{Zn:Cu,Zn:\square}} = L^{1}_{\mathrm{Cu,Zn}} - 4.0\ L^{2}_{\mathrm{Cu,Zn}}$$

$$L^{2,\mathrm{bcc}-B2}_{\mathrm{Cu,Zn:Zn:\square}} = L^{2,\mathrm{bcc}-B2}_{\mathrm{Zn:Cu,Zn:\square}} = L^{2}_{\mathrm{Cu,Zn}}$$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Cu,Zn:Cu,Zn:\square}} = -\ 24.0\ L^{2}_{\mathrm{Cu,Zn}}$$

Phase bcc–$B2$

$G^{*}_{\mathrm{Cu:Zn:\square}} = -\ 3085.0$
$L^{0}_{\mathrm{Cu,Zn}} = -\ 12898.97 + 3.26598\ T$
$L^{1}_{\mathrm{Cu,Zn}} = 945.265 - 0.80679\ T$
$L^{2}_{\mathrm{Cu,Zn}} = 1921.485 - 1.86969\ T$

$$G^{\circ}(T) - H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) = \mathrm{G}(\mathrm{Cu:Cu:\square}) = 0.0$$

$$G^{\circ}(T) - 0.5\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - 0.5\ H^{\circ,\mathrm{hcp-Zn}}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \mathrm{G}(\mathrm{Cu:Zn:\square}) = 2.0\ G^{*}_{\mathrm{Cu:Zn:\square}}$$

$$G^{\circ}(T) - 0.5\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - 0.5\ H^{\circ,\mathrm{hcp-Zn}}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \mathrm{G}(\mathrm{Zn:Cu:\square}) = 2.0\ G^{*}_{\mathrm{Cu:Zn:\square}}$$

$$G^{\circ}(T) - H^{\circ,\mathrm{hcp-Zn}}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \mathrm{G}(\mathrm{Zn:Zn:\square}) = 0.0$$

Phase bcc–$A2$

$L^{0,\mathrm{bcc-A2}}_{\mathrm{Cu,Zn:\square}} = 4.0\ L^{0}_{\mathrm{Cu,Zn}}$
$L^{1,\mathrm{bcc-A2}}_{\mathrm{Cu,Zn:\square}} = 8.0\ L^{1}_{\mathrm{Cu,Zn}}$
$L^{2,\mathrm{bcc-A2}}_{\mathrm{Cu,Zn:\square}} = 16.0\ L^{2}_{\mathrm{Cu,Zn}}$

Phase CuZn–γ

$K4 = -\ 11552.71 - 1.67824\ T$

$K5 = \ 15732.3 - 10.26575\ T$

$K6 = \ 37289.2 - 13.05259\ T$

$$G^{\circ}(T) - 7.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 6.0\ H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Cu{:}Cu{:}Zn)} = 13.0\ \mathrm{K4} + 2.0\ \mathrm{K5} + 7.0\ \mathrm{GHSER_{Cu}} + 6.0\ \mathrm{GHSER_{Zn}}$$

$$G^{\circ}(T) - 5.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 8.0\ H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Zn{:}Cu{:}Cu{:}Zn)} = 13.0\ \mathrm{K4} + 2.0\ \mathrm{K5} + 2.0\ \mathrm{K6} + 5.0\ \mathrm{GHSER_{Cu}} + 8.0\ \mathrm{GHSER_{Zn}}$$

$$G^{\circ}(T) - 5.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 8.0\ H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Zn{:}Cu{:}Zn)} = 13.0\ \mathrm{K4} + 5.0\ \mathrm{GHSER_{Cu}} + 8.0\ \mathrm{GHSER_{Zn}}$$

$$G^{\circ}(T) - 3.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 10.0\ H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Zn{:}Zn{:}Cu{:}Zn)} = 13.0\ \mathrm{K4} + 2.0\ \mathrm{K6} + 3.0\ \mathrm{GHSER_{Cu}} + 10.0\ \mathrm{GHSER_{Zn}}$$

Phase Laves–$C14$

$$G^{\circ}(T) - 3.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Cu)} = 15000.0 + 3.0\ \mathrm{GHSER_{Cu}}$$

$$G^{\circ}(T) - 2.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Zn)} = 15000.0 + 2.0\ \mathrm{GHSER_{Cu}} + \mathrm{GHSER_{Zn}}$$

$$G^{\circ}(T) - H_{\mathrm{Cu}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Zn{:}Cu)} = 15000.0 + \mathrm{GHSER_{Cu}} + 2.0\ \mathrm{GHSER_{Zn}}$$

$$G^{\circ}(T) - 3.0\ H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Zn{:}Zn)} = 15000.0 + 3.0\ \mathrm{GHSER_{Zn}}$$

$$L_{\mathrm{Cu,Zn:Cu}}^{\mathrm{0,Laves-C14}} = L_{\mathrm{Cu,Zn:Zn}}^{\mathrm{0,Laves-C14}} = -\ 75305.48$$

Phase Laves–$C15$

$$G^{\circ}(T) - 3.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Cu)} = 15000.0 + 3.0\ \mathrm{GHSER_{Cu}}$$

$$G^{\circ}(T) - 2.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Zn)} = 15000.0 + 2.0\ \mathrm{GHSER_{Cu}} + \mathrm{GHSER_{Zn}}$$

$$G^{\circ}(T) - H_{\mathrm{Cu}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Zn{:}Cu)} = 15000.0 + \mathrm{GHSER_{Cu}} + 2.0\ \mathrm{GHSER_{Zn}}$$

$$G^{\circ}(T) - 3.0\ H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Zn{:}Zn)} = 15000.0 + 3.0\ \mathrm{GHSER_{Zn}}$$

$$L_{\mathrm{Cu,Zn:Cu}}^{\mathrm{0,Laves-C15}} = L_{\mathrm{Cu,Zn:Zn}}^{\mathrm{0,Laves-C15}} = -\ 78824.62$$

$$L_{\mathrm{Cu,Zn:Cu}}^{\mathrm{1,Laves-C15}} = L_{\mathrm{Cu,Zn:Zn}}^{\mathrm{0,Laves-C15}} = 25529.06$$

Phase Laves–$C36$

$$G^{\circ}(T) - 3.0\ H^{\mathrm{o,fcc-}A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Cu)} = 15000.0 + 3.0\ \ \mathrm{GHSER_{Cu}}$$

$$G^{\circ}(T) - 2.0\ H^{\mathrm{o,fcc-}A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - H^{\mathrm{o,hcp-Zn}}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Zn)} = 15000.0 + 2.0\ \ \mathrm{GHSER_{Cu}} + \mathrm{GHSER_{Zn}}$$

$$G^{\circ}(T) - H^{\mathrm{o,fcc-}A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - 2.0\ H^{\mathrm{o,hcp-Zn}}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Zn{:}Cu)} = 15000.0 + \mathrm{GHSER_{Cu}} + 2.0\ \ \mathrm{GHSER_{Zn}}$$

$$G^{\circ}(T) - 3.0\ H^{\mathrm{o,hcp-Zn}}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Zn{:}Zn)} = 15000.0 + 3.0\ \ \mathrm{GHSER_{Zn}}$$

$$L^{0,\mathrm{Laves-C36}}_{\mathrm{Cu,Zn:Cu}} = L^{0,\mathrm{Laves-C36}}_{\mathrm{Cu,Zn:Zn}} = -90226.26$$

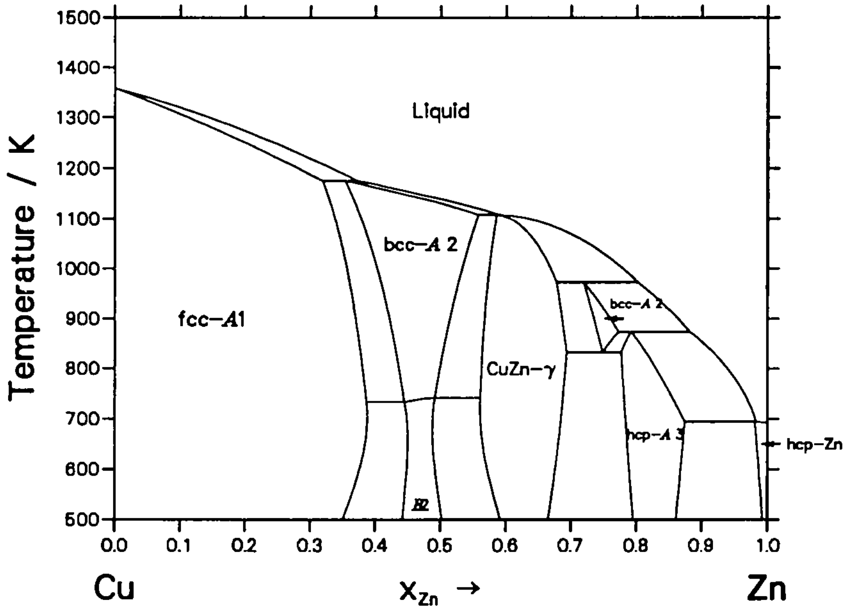


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Zn}			T / K
Liquid + fcc–$A1$ ⇌ bcc–$A2$	Peritectic	.373	.319	.353	1175.3
Liquid + bcc–$A2$ ⇌ CuZn–γ	Peritectic	.592	.558	.586	1108.3
Liquid + CuZn–γ ⇌ bcc–$A2$	Peritectic	.802	.678	.719	972.5
Liquid + bcc–$A2$ ⇌ hcp–$A3$	Peritectic	.882	.773	.792	873.4
bcc–$A2$ ⇌ CuZn–γ + hcp–$A3$	Eutectoid	.748	.693	.777	831.9
Liquid + hcp–$A3$ ⇌ hcp–Zn	Peritectic	.983	.874	.981	694.4

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Cu-Zn	(Cu)	Cu	*cF4* $Pm\bar{3}m$	M 4	
	(Zn)	Mg	*hP2* $P6_3/mmc$	M 2	
	β	W	*cI2* $Im\bar{3}m$	M 2	bcc–*A2*
	β'	CsCl	*cP2* $Pm\bar{3}m$	Cu 1 Zn 1	bcc-*B2*
	δ	$CuZn_2$	*hP3* $P\bar{6}$	Cu 1 Zn_1 1 Zn_2 1	assumed as bcc–*A2*
	ϵ	Mg	*hP2* $P6_3mmc$	M 2	 CuZn–*A3*
	γ	Cu_5Zn_8	*cI52* $I\bar{4}3m$	Cu_1 8 Cu_2 12 Zn_1 8 Zn_2 24	Cu_5Zn

System Cu–Zr

Solution Phases:

Liquid, bcc-*A*2, hcp-*A*3

Compounds:

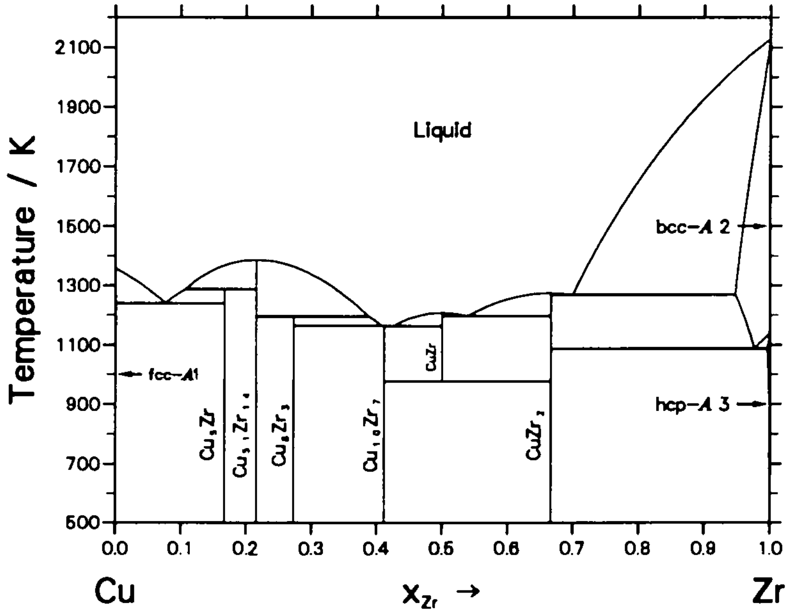
Cu_5Zr, $Cu_{51}Zr_{14}$, $Cu_{10}Zr_7$, CuZr, $CuZr_2$, Cu_8Zr_3

Modelling:

Liquid : Substitutional, Redlich-Kister
Cu_5Zr : Stoichiometric, $(Cu)_5(Zr)$
$Cu_{51}Zr_{14}$: Stoichiometric, $(Cu)_{51}(Zr)_{14}$
$Cu_{10}Zr_7$: Stoichiometric, $(Cu)_{10}(Zr)_7$
Cu_8Zr_3 : Stoichiometric, $(Cu)_8(Zr)_3$
CuZr : Stoichiometric, (Cu)(Zr)
$CuZr_2$: Stoichiometric, $(Cu)(Zr)_2$

Assessor and Date:

K. Zeng, and M. Hämäläinen 1993



Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase bcc–$A2$

$$L^{0,\text{bcc}-A2}_{\text{Cu,Zr:}\square} = -7381.13$$

Phase fcc–$A1$

$$L^{0,\text{fcc}-A1}_{\text{Cu,Zr:}\square} = 2233$$

Phase hcp–$A3$

$$L^{0,\text{hcp}-A3}_{\text{Cu,Zr:}\square} = 11336.85$$

Phase liquid

$$L^{0,\text{liquid}}_{\text{Cu,Zr}} = -61685.53 + 11.29235\ T$$

$$L^{1,\text{liquid}}_{\text{Cu,Zr}} = -8830.66 + 5.04565\ T$$

Phase $Cu_{10}Zr_7$

$$G^\circ(T) - 10.0\ H^{\text{o,fcc}-A1}_{\text{Cu}}(298.15\ \text{K}) - 7.0\ H^{\text{o,hcp}-A1}_{\text{Zr}}(298.15\ \text{K}) = \\ -241750.0 + 10.0\ \text{GHSER}_{\text{Cu}} + 7.0\ \text{GHSER}_{\text{Zr}}$$

Phase $Cu_{51}Zr_{14}$

$$G^\circ(T) - 51.0\ H^{\text{o,fcc}-A1}_{\text{Cu}}(298.15\ \text{K}) - 14.0\ H^{\text{o,hcp}-A1}_{\text{Zr}}(298.15\ \text{K}) = \\ -843412.7 + 51.0\ \text{GHSER}_{\text{Cu}} + 14.0\ \text{GHSER}_{\text{Zr}}$$

Phase Cu_5Zr

$$G^\circ(T) - 5.0\ H^{\text{o,fcc}-A1}_{\text{Cu}}(298.15\ \text{K}) - H^{\text{o,hcp}-A1}_{\text{Zr}}(298.15\ \text{K}) = \\ -61794 + 5.0\ \text{GHSER}_{\text{Cu}} + \text{GHSER}_{\text{Zr}}$$

Phase Cu_8Zr_3

$$G^\circ(T) - 8.0\ H^{\text{o,fcc}-A1}_{\text{Cu}}(298.15\ \text{K}) - 3.0\ H^{\text{o,hcp}-A1}_{\text{Zr}}(298.15\ \text{K}) = \\ -148063.1 + 8.0\ \text{GHSER}_{\text{Cu}} + 3.0\ \text{GHSER}_{\text{Zr}}$$

Phase CuZr

$$G^\circ(T) - H^{\text{o,fcc}-A1}_{\text{Cu}}(298.15\ \text{K}) - H^{\text{o,hcp}-A1}_{\text{Zr}}(298.15\ \text{K}) = \\ -20104.24 - 7.63196\ T + \text{GHSER}_{\text{Cu}} + \text{GHSER}_{\text{Zr}}$$

Phase $CuZr_2$

$$G^\circ(T) - H^{\text{o,fcc}-A1}_{\text{Cu}}(298.15\ \text{K}) - 2.0\ H^{\text{o,hcp}-A1}_{\text{Zr}}(298.15\ \text{K}) = \\ -43904.01 + 5.19051\ T + \text{GHSER}_{\text{Cu}} + 2.0\ \text{GHSER}_{\text{Zr}}$$

Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Zr}			T / K
Liquid $\rightleftharpoons$ fcc-$A1$ + Cu_5Zr	Eutectic	.078	.001	.167	1240.8
Liquid + $Cu_{51}Zr_{14}$ $\rightleftharpoons$ Cu_5Zr	Peritectic	.107	.215	.167	1287.5
$Cu_{51}Zr_{14}$ $\rightleftharpoons$ Liquid	Congruent	.215	.215	....	1386.0
Liquid + $Cu_{51}Zr_{14}$ $\rightleftharpoons$ Cu_8Zr_3	Peritectic	.388	.273	.215	1195.3
Liquid $\rightleftharpoons$ Cu_8Zr_3 + $Cu_{10}Zr_7$	Eutectic	.408	.273	.412	1164.2
$Cu_{10}Zr_7$ $\rightleftharpoons$ Liquid	Congruent	.412	.412	....	1164.2
Liquid $\rightleftharpoons$ $Cu_{10}Zr_7$ + CuZr	Eutectic	.425	.412	.500	1163.2
CuZr $\rightleftharpoons$ $Cu_{10}Zr_7$ + $CuZr_2$	Eutectoid	.500	.412	.667	976.7
Liquid $\rightleftharpoons$ CuZr + $CuZr_2$	Eutectic	.538	.500	.667	1196.7
CuZr $\rightleftharpoons$ Liquid	Congruent	.500	.500	....	1208.5
Liquid $\rightleftharpoons$ $CuZr_2$ + bcc-$A2$	Eutectic	.700	.666	.947	1269.5
$CuZr_2$ $\rightleftharpoons$ Liquid	Congruent	.666	.666	....	1275.0
bcc-$A2$ $\rightleftharpoons$ $CuZr_2$ + hcp-$A3$	Eutectoid	.975	.667	.992	1095.2

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Cu-Zr	(Cu)	Cu	*cF4* $Fm\bar{3}m$	M 4	
	(Zr)	Mg	*hP2* $P6_3/mmc$	M 2	
	(Zr)	W	*cI2* $Im\bar{3}m$	M 4	
	CuZr	ClCs	*cP2* $Pm\bar{3}m$	M_1 1 M_2 1	bcc-B2
	$CuZr_2$	$MoSi_2$	*tI6* $I4/mmm$	Cu 2 Zr 4	
	$Cu_{10}Zr_7$	$Ni_{10}Zr_7$	*oC68* $Aba2$		
	Cu_9Zr_2		*tP24* $P4/m$		o^{**} in [91Vil]
	Cu_5Zr	$AuBe_5$	*Cf24* $F\bar{4}3m$	Cu_1 4 Cu_2 16 Zr 4	
	$Cu_{51}Zr_{14}$	$Ag_{51}Gd_{14}$	*hP65* $P6/m$		*hP68* in [91Vil]
	Cu_8Zr_3	Cu_8Hf_3	*oP44* $Pnma$		

System Fe–Mg

Solution Phases:

Liquid, fcc–$A1$, bcc–$A2$, hcp–$A3$

Modelling:

Liquid : Substitutional, Redlich–Kister
fcc–$A1$: Substitutional, Redlich–Kister
bcc–$A2$: Substitutional, Redlich–Kister
hcp–$A3$: Substitutional, Redlich–Kister

Assessor and Date:

J. Tibballs (1991)

Thermodynamic properties of the solution phases (J.mol^{-1})

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Fe,Mg:}\square} = 65700.0$$

Phase fcc–$A1$

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Fe,Mg:}\square} = 65200.0$$

Phase hcp–$A3$

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Fe,Mg:}\square} = 92400.0$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Fe,Mg}} = 61343.0 + 1.5\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Fe,Mg}} = -2700.0$$

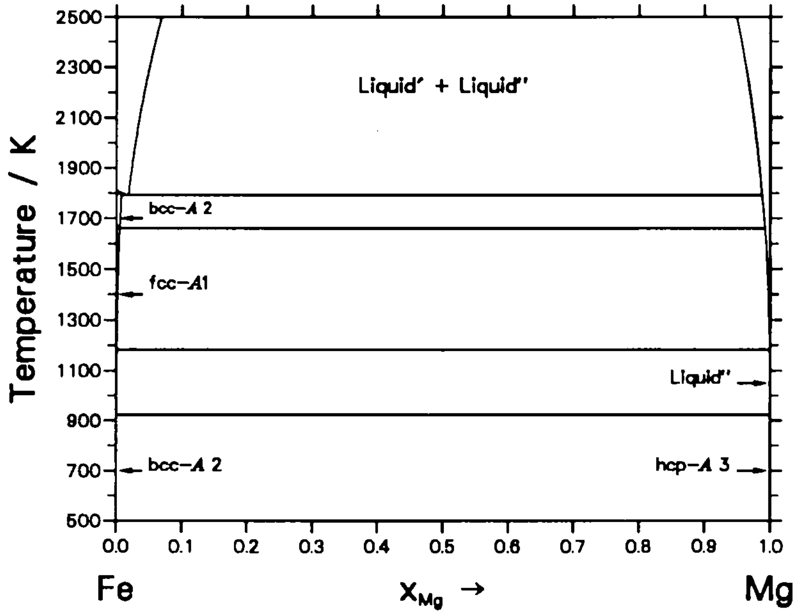


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Mg}			T / K
Liquid' ⇌ bcc-*A*2 + Liquid"	Monotectic	.018	.008	.987	1791.4
Liquid" + bcc-*A*2 ⇌ fcc-*A*1	Degenerate	.992	.005	.005	1661.6
Liquid" + bcc-*A*2 ⇌ fcc-*A*1	Degenerate	.999	.001	.001	1183.4
Liquid" +bcc-*A*2 ⇌ hcp–*A*3	Degenerate	1.000	.000	1.000	922.9

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol] Space Group
Fe–Mg	(Fe)	Cu	*cF4* $Pm\bar{3}m$
	(Fe)	W	*cI2* $Im\bar{3}m$
	(Mg)	Mg	*hP2* $P6_3/mmc$

System Fe–Mn

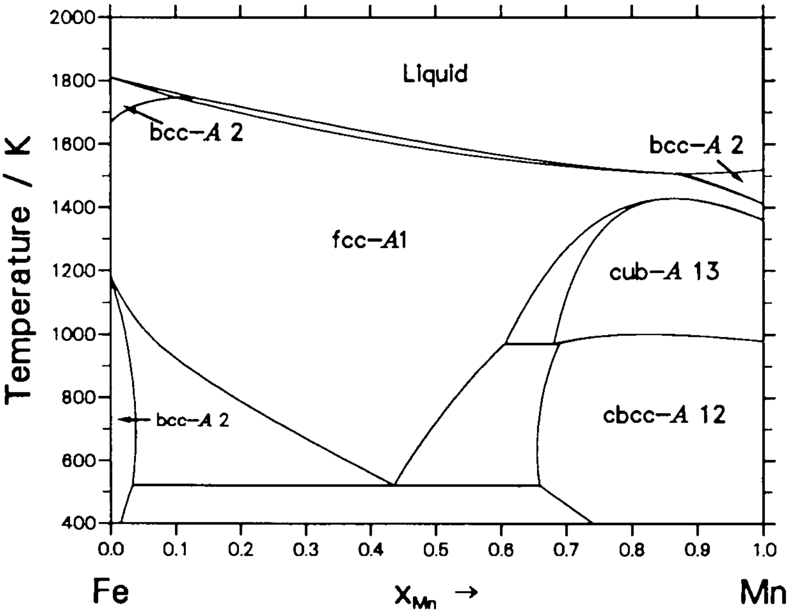
Solution Phases:
(stable) Liquid, bcc–*A*2, cbcc–*A*12, cub–*A*13, fcc–*A*1

Solution Phases:
(metastable) hcp–*A*3

Modelling:

Liquid : Substitutional, Redlich–Kister
bcc–*A*2 : Substitutional, Redlich–Kister
bcc–*A*12 : Substitutional, Redlich–Kister
cub–*A*13 : Substitutional, Redlich–Kister
fcc–*A*1 : Substitutional, Redlich–Kister
hcp–*A*3 : Substitutional, Redlich–Kister

Assessor and Date:
Scientific Group Thermodata Europe Database



Thermodynamic properties of the solution phases (J.mol^{-1})

Phase bcc–*A2*

$L^{0,\mathrm{bcc}-A2}_{\mathrm{Fe,Mn:\Box}} = -2759 + 1.237\ \mathrm{T}$

$T^{0,\mathrm{bcc}-A2}_{c,\mathrm{Fe,Mn:\Box}} = 123$

$\beta^{0,\mathrm{mag,bcc}-A2}_{\mathrm{Fe,Mn:\Box}} = 0$

Phase cbcc–*A12*

$L^{0,\mathrm{cbcc}-A12}_{\mathrm{Fe,Mn:\Box}} = -10184$

Phase cub–*A13*

$L^{0,\mathrm{cub}-A13}_{\mathrm{Fe,Mn:\Box}} = -11518 + 2.819\ \mathrm{T}$

Phase fcc-A1

$L^{0,\mathrm{fcc}-A1}_{\mathrm{Fe,Mn:\Box}} = -7762 + 3.865\ \mathrm{T}$

$L^{1,\mathrm{fcc}-A1}_{\mathrm{Fe,Mn:\Box}} = -259$

$T^{0,\mathrm{fcc}-A1}_{c,\mathrm{Fe,Mn:\Box}} = -2282$

$T^{1,\mathrm{fcc}-A1}_{c,\mathrm{Fe,Mn:\Box}} = -2068$

$\beta^{0,\mathrm{mag,fcc}-A1}_{\mathrm{Fe,Mn:\Box}} = 0$

Phase liquid

$L^{0,\mathrm{liquid}}_{\mathrm{Fe,Mn}} = -3950 + 0.489\ \mathrm{T}$

$L^{1,\mathrm{liquid}}_{\mathrm{Fe,Mn}} = 1145$

Phase hcp–*A3*

$L^{0,\mathrm{hcp}-A3}_{\mathrm{Fe,Mn}} = -5582 + 3.865\ \mathrm{T}$

$L^{1,\mathrm{hcp}-A3}_{\mathrm{Fe,Mn}} = 273$

Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Mn}			T / K
cub–$A13$ $\rightleftharpoons$ fcc–$A1$ + cbcc–$A12$	Eutectoid	.681	.606	.690	973.2
fcc–$A1$ $\rightleftharpoons$ bcc–$A2$ + cbcc–$A12$	Eutectoid	.436	.033	.659	521.3
Liquid + bcc–$A2$ $\rightleftharpoons$ fcc–$A1$	Peritectic	.100	.129	.129	1746.8
Liquid + bcc–$A2$ $\rightleftharpoons$ fcc–$A1$	Peritectic	.867	.877	.875	1507.2

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Comments
Fe–Mn	(Fe)	Cu	$cF4$ $Pm\bar{3}m$	
	(Fe)	W	$cI2$ $Im\bar{3}m$	
	α–Mn	α–Mn	c58 $I\bar{4}3m$	cbcc–$A12$
	β–Mn	β–Mn	$cP20$ $P4_132$	cub–$A13$
	γ–Mn	Cu	$cF4$ $Fm3$m	
	δ–Mn	W	$cI2$ $Im\bar{3}m$	

System Fe–Si

Solution Phases:

Liquid, bcc–$A2$, bcc–$B2$, fcc–$A1$

Compounds:

Fe_5Si_3, FeSi, Fe_2Si, $FeSi_2$–L, $FeSi_2$–H

Modelling:

Liquid : Substitutional, Redlich–Kister
fcc–$A1$: Substitutional, Redlich–Kister
bcc–$B2$: Sublattice model , $(Fe,Si)_{0.5}(Fe,Si)_{0.5}(\square)_3$
Two descriptions of the bcc–$A2$:bcc–$B2$ order-disorder transformation are given: one which includes the parameters of the order and disordered phases in a single description (equation 21 in the thermodynamic modelling chapter), and a second one where the order and disorder contributions are expressed by equation 23. For the second case, the parameters are in a frame.
bcc–$A2$: see bcc–$B2$
Fe_2Si : Stoichiometric, $(Fe)_2(Si)$
Fe_5Si_3 : Stoichiometric, $(Fe)_5(Si)_3$
$FeSi_2$–L : Stoichiometric, $(Fe)(Si)_2$
$FeSi_2$–H : Stoichiometric, $(Fe)_3(Si)_7$
FeSi : Stoichiometric, $(Fe)(Si)$

Assessor and Date:

J. Lacaze, and B. Sundman

Publication:

Met. Trans., **22A**, (10), 2211-2223 (1991).

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase Fe_2Si

$$G^{\circ}(T) - 2.0\ H_{Fe}^{o,bcc-A2,para}(298.15\ K) - H_{Si}^{o,diamond}(298.15\ K) =$$
$$-\ 71256.6 - 10.62\ T + 2.0\ GHSER_{Fe} + GHSER_{Si}$$

Phase $\mathrm{Fe_5Si_3}$

$$G^\circ(T) - 5.0\ H_{\mathrm{Fe}}^{\mathrm{o,bcc-}A2\mathrm{,para}}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) =$$
$$-\ 241144 + 2.16\ T + 5.0\ \mathrm{GHSER_{Fe}} + 3.0\ \mathrm{GHSER_{Si}}$$

Phase $\mathrm{FeSi_2}$-L

$$G^\circ(T) - H_{\mathrm{Fe}}^{\mathrm{o,bcc-}A2\mathrm{,para}}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) =$$
$$-\ 82149.0 + 10.44\ T + \mathrm{GHSER_{Fe}} + 2.0\ \mathrm{GHSER_{Si}}$$

Phase $\mathrm{FeSi_2}$-H

$$G^\circ(T) - 3.0\ H_{\mathrm{Fe}}^{\mathrm{o,bcc-}A2\mathrm{,para}}(298.15\ \mathrm{K}) - 7.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) =$$
$$-\ 196490 - 9.2\ T + 3.0\ \mathrm{GHSER_{Fe}} + 7.0\ \mathrm{GHSER_{Si}}$$

Phase FeSi

$$G^\circ(T) - H_{\mathrm{Fe}}^{\mathrm{o,bcc-}A2\mathrm{,para}}(298.15\ \mathrm{K}) - H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) =$$
$$-\ 72761.2 + 4.44\ T + \mathrm{GHSER_{Fe}} + \mathrm{GHSER_{Si}}$$

Phase liquid

$$L_{\mathrm{Fe,Si}}^{0,\mathrm{liquid}} = -\ 164434.6 + 41.9773\ T$$

$$L_{\mathrm{Fe,Si}}^{1,\mathrm{liquid}} = -\ 21.523\ T$$

$$L_{\mathrm{Fe,Si}}^{2,\mathrm{liquid}} = -\ 18821.542 + 22.07\ T$$

$$L_{\mathrm{Fe,Si}}^{3,\mathrm{liquid}} = 9695.8$$

Phase fcc–$A1$

$$L_{\mathrm{Fe,Si:\square}}^{0,\mathrm{fcc-A1}} = -\ 125247.7 + 41.166\ T$$

$$L_{\mathrm{Fe,Si:\square}}^{1,\mathrm{fcc-A1}} = -\ 142707.6$$

$$L_{\mathrm{Fe,Si:\square}}^{2,\mathrm{fcc-A1}} = 89907.3$$

Phase bcc–$B2$

$$G^\circ(T) - H_{\mathrm{Fe}}^{\mathrm{o,bcc-}A2\mathrm{,para}}(298.15\ \mathrm{K}) = \mathrm{G(Fe{:}Fe{:}\square)} = \mathrm{GHSER_{Fe}}$$

$$T_{\mathrm{c,Fe:Fe\square}}^{\mathrm{bcc-}B2} = 1043 \qquad \beta_{\mathrm{c,Fe:Fe\square}}^{\mathrm{bcc-}B2} = 2.22$$

$$G^\circ(T) - 0.5\ H_{\mathrm{Fe}}^{\mathrm{o,bcc-}A2\mathrm{,para}}(298.15\ \mathrm{K}) - 0.5\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = \mathrm{G(Fe{:}Si{:}\square)} =$$
$$-\ 48761.565 + 11.62\ T + 0.5\ \mathrm{GHSER_{Fe}} + 0.5\ \mathrm{GBCC_{Si}}$$

$$T_{\mathrm{c,Fe:Si\square}}^{0,\mathrm{bcc-}B2} = 521.5 \qquad \beta_{\mathrm{c,Si:Fe\square}}^{0,\mathrm{bcc-}B2} = 1.11$$

$$G^{\circ}(T) - 0.5\ H_{\mathrm{Fe}}^{\circ,\mathrm{bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) - 0.5\ H_{\mathrm{Si}}^{\circ,\mathrm{diamond}}(298.15\ \mathrm{K}) = \mathrm{G}(\mathrm{Si{:}Fe{:}}\square) = - 48761.565 + 11.62\ T + 0.5\ \mathrm{GHSER}_{\mathrm{Fe}} + 0.5\ \mathrm{GBCC}_{\mathrm{Si}}$$

$$T_{\mathrm{c,Si:Fe}\square}^{0,\mathrm{bcc}-B2} = 521.5 \qquad \beta_{\mathrm{c,Si:Fe:}\square}^{0,\mathrm{bcc}-B2} = 1.11$$

$$G^{\circ}(T) - H_{\mathrm{Si}}^{\circ,\mathrm{diamond}}(298.15\ \mathrm{K}) = \mathrm{G}(\mathrm{Si{:}Si{:}}\square) = \mathrm{GBCC}_{\mathrm{Si}}$$

$$L_{\mathrm{Fe,Si:Fe:}\square}^{0,\mathrm{bcc}-B2} = L_{\mathrm{Fe:Fe,Si:}\square}^{0,\mathrm{bcc}-B2} = - 50771 + 11.62\ T$$

$$L_{\mathrm{Fe,Si:Fe:}\square}^{1,\mathrm{bcc}-B2} = L_{\mathrm{Fe:Fe,Si:}\square}^{1,\mathrm{bcc}-B2} = 4016$$

$$L_{\mathrm{Fe,Si:Fe:}\square}^{2,\mathrm{bcc}-B2} = L_{\mathrm{Fe:Fe,Si:}\square}^{2,\mathrm{bcc}-B2} = 3890$$

$$L_{\mathrm{Fe,Si:Si}\square}^{0,\mathrm{bcc}-B2} = L_{\mathrm{Si:Fe,Si:}\square}^{0,\mathrm{bcc}-B2} = 18493 + 11.62\ T$$

$$L_{\mathrm{Fe,Si:Si:}\square}^{1,\mathrm{bcc}-B2} = L_{\mathrm{Si:Fe,Si:}\square}^{1,\mathrm{bcc}-B2} = - 27104$$

$$L_{\mathrm{Fe,Si:Si:}\square}^{2,\mathrm{bcc}-B2} = L_{\mathrm{Si:Fe,Si:}\square}^{2,\mathrm{bcc}-B2} = 3890$$

$$L_{\mathrm{Fe,Si:Fe,Si:}\square}^{0,\mathrm{bcc}-B2} = - 93360$$

$$T_{\mathrm{c,Fe,Si:Fe:}\square}^{0,\mathrm{bcc}-B2} = T_{\mathrm{c,Fe:Fe,Si:}\square}^{0,\mathrm{bcc}-B2} = 189$$

$$T_{\mathrm{c,Fe,Si:Fe:}\square}^{1,\mathrm{bcc}-B2} = T_{\mathrm{c,Fe:Fe,Si:}\square}^{1,\mathrm{bcc}-B2} = 63$$

$$T_{\mathrm{c,Fe,Si:Si:}\square}^{0,\mathrm{bcc}-B2} = T_{\mathrm{c,Si:Fe,Si:}\square}^{0,\mathrm{bcc}-B2} = - 189$$

$$T_{\mathrm{c,Fe,Si:Si:}\square}^{1,\mathrm{bcc}-B2} = T_{\mathrm{c,Si:Fe,Si:}\square}^{1,\mathrm{bcc}-B2} = 63$$

$G_{\mathrm{Fe:Si:}\square}^{*} = - 1260\ R \qquad (R = 8.31451)$
$L_{\mathrm{Fe,Si}}^{0} = - 27809 + 11.62\ T$
$L_{\mathrm{Fe,Si}}^{1} = - 11544$
$L_{\mathrm{Fe,Si}}^{2} = 3890$

Phase bcc–$B2$

$$G^{\circ}(T) - H_{\mathrm{Fe}}^{\circ,\mathrm{bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) = \mathrm{G}(\mathrm{Fe{:}Fe{:}}\square) = 0.0$$

$$G^{\circ}(T) - 0.5\ H_{\mathrm{Fe}}^{\circ,\mathrm{bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) - 0.5\ H_{\mathrm{Si}}^{\circ,\mathrm{diamond}}(298.15\ \mathrm{K}) = \mathrm{G}(\mathrm{Fe{:}Si{:}}\square) = 2.0\ G_{\mathrm{Fe:Si:}\square}^{*}$$

$$G^{\circ}(T) - 0.5\ H_{\mathrm{Fe}}^{\circ,\mathrm{bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) - 0.5\ H_{\mathrm{Si}}^{\circ,\mathrm{diamond}}(298.15\ \mathrm{K}) = \mathrm{G}(\mathrm{Si{:}Fe{:}}\square) = 2.0\ G_{\mathrm{Fe:Si:}\square}^{*}$$

$$G^{\circ}(T) - H_{\mathrm{Si}}^{\circ,\mathrm{diamond}}(298.15\ \mathrm{K}) = \mathrm{G}(\mathrm{Si{:}Si{:}}\square) = 0.0$$

Phase bcc–$A2$

$L_{\mathrm{Fe,Si:}\square}^{0,\mathrm{bcc}-A2} = 4.0\ L_{\mathrm{Fe,Si}}^{0}$
$L_{\mathrm{Fe,Si:}\square}^{1,\mathrm{bcc}-A2} = 8.0\ L_{\mathrm{Fe,Si}}^{1}$
$T_{\mathrm{C,Fe,Si:}\square}^{1,\mathrm{bcc}-A2} = 63$
$L_{\mathrm{Fe,Si:}\square}^{2,\mathrm{bcc}-A2} = 16.0\ L_{\mathrm{Fe,Si}}^{2}$

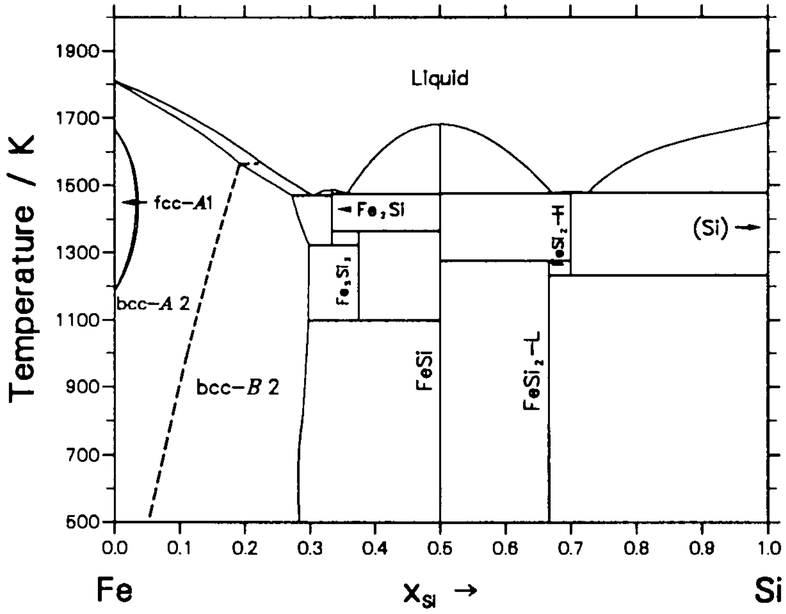


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Si}			Temp. / K
Liquid ⇌ bcc–$B2$ + Fe_2Si	Eutectic	.273	.267	.333	1470.6
Fe_2Si ⇌ bcc–$B2$ + Fe_5Si_3	Eutectoid	.333	.299	.375	1322.8
Fe_5Si_3 ⇌ bcc–$B2$ + FeSi	Eutectoid	.375	.298	.500	1097.8
Fe_2Si + FeSi ⇌ Fe_5Si_3	Peritectoid	.333	.500	.375	1364.4
Liquid ⇌ Fe_2Si + FeSi	Eutectic	.357	.333	.500	1475.8
Liquid ⇌ FeSi + $FeSi_2$–H	Eutectic	.672	.500	.700	1477.2
FeSi + $FeSi_2$–H ⇌ $FeSi_2$–L	Peritectoid	.500	.700	.666	1275.7
$FeSi_2$–H ⇌ $FeSi_2$–L + (Si)	Eutectoid	.700	.667	1.000	1232.9
Liquid ⇌ $FeSi_2$–H + (Si)	Eutectic	.725	.700	1.000	1478.3
Fe_2Si ⇌ Liquid	Congruent	.333	.333	....	1488.0
FeSi ⇌ Liquid	Congruent	.500	.500	....	1683.0
$FeSi_2$–H ⇌ Liquid	Congruent	.700	.700	....	1482.0

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Fe–Si	(Fe)	Cu	$cF4$ $Pm\bar{3}m$		
	(Fe)	W	$cI2$ $Im\bar{3}m$		
	(Si)	diamond	$cF8$ $Fd\bar{3}m$		
	$FeSi_2$-L		$tP3$ $P4/mmm$	Fe 1 Si 2	
	$FeSi_2$-H		$oC48$ $Cmca$	Fe_1 8 Fe_2 8 Si_1 8 Si_2 16	
	Fe_2Si		$hP6$ $P\bar{3}m1$	Fe_1 1 Fe_2 1 Fe_3 2 Si 2	
	FeSi		$cP8$ $P2_13$	Fe 4 Si 4	
	Fe_5Si_3		$hP16$ $P6_3/mmc$	Fe_1 4 Fe_2 6 Si 6	
	bcc-$B2$	CsCl	$cP2$ $Fm\bar{3}m$		$\alpha2$ in [90Mas]

System Fe–Ti

Solution Phases:

Liquid, bcc–$A2$, fcc–$A1$, hcp–$A3$

Compounds:

FeTi, Laves–$C14$

Modelling:

Liquid : Substitutional, Redlich–Kister
bcc–$A2$: Substitutional, Redlich–Kister
fcc–$A1$: Substitutional, Redlich–Kister
hcp–$A3$: Substitutional, Redlich–Kister
Laves–$C14$: Sublattice model, $(\mathrm{Fe,Ti})_2\,(\mathrm{Fe,Ti})$
FeTi : Sublattice model, (Fe,Ti)(Fe,Ti)

Assessor and Date:

M.H. Rand 1995

Thermodynamic properties of the solution and compound phases ($\mathrm{J.mol}^{-1}$)

Phase FeTi

$$G^{\circ}(T) - H_{\mathrm{Fe}}^{\mathrm{o,bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) - H_{\mathrm{Ti}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) =$$
$$-\ 51584.05 + 238.686\ \ T - 44.858\ \ T\cdot \ln T - 0.008493\ \ T^2 + 100500\ \ T^{-1}$$

Phase Laves–$C14$

$$G^{\circ}(T) - 3.0\ \ H_{\mathrm{Fe}}^{\mathrm{o,bcc}-A3,\mathrm{para}}(298.15\ \mathrm{K}) = \mathrm{G(Fe{:}Fe)} = 15000.0 + 3.0\ \ \mathrm{GHSER_{Fe}}$$

$$G^{\circ}(T) - 2.0\ \ H_{\mathrm{Fe}}^{\mathrm{o,bcc}-A3,\mathrm{para}}(298.15\ \mathrm{K}) - H_{\mathrm{Ti}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Fe{:}Ti)} =$$
$$-\ 1440.0 - 6.75\ \ \mathrm{T} + 2.0\ \ \mathrm{GHSER_{Fe}} + \mathrm{GHSER_{Ti}}$$

$$G^{\circ}(T) - H_{\mathrm{Fe}}^{\mathrm{o,bcc}-A3,\mathrm{para}}(298.15\ \mathrm{K}) - 2.0\ \ H_{\mathrm{Ti}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Fe)} =$$
$$15000.0 + \mathrm{GHSER_{Fe}} + 2.0\ \ \mathrm{GHSER_{Ti}}$$

$$G^{\circ}(T) - 3.0\ \ H_{\mathrm{Ti}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Ti)} =$$
$$15000 + 3.0\ \ \mathrm{GHSER_{Ti}}$$

$$L_{\mathrm{Fe:Fe,Ti}}^{0,\mathrm{Laves}-C14} = L_{\mathrm{Ti:Fe,Ti}}^{0,\mathrm{Laves}-C14} = 60000$$

$$L_{\mathrm{Fe,Ti:Fe}}^{0,\mathrm{Laves}-C14} = L_{\mathrm{Fe,Ti:Ti}}^{0,\mathrm{Laves}-C14} = 60000$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Fe,Ti}} = -62273.8 + 5.6939\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Fe,Ti}} = -5491.468$$

Phase fcc–$A1$

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Fe,Ti}:\square} = -42000$$

Phase hcp–$A3$

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Fe,Ti}:\square} = 18500 - 15\ T$$

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Fe,Ti}:\square} = -52400.65 + 10.7268\ T$$

$$L^{1,\mathrm{bcc}-A2}_{\mathrm{Fe,Ti}:\square} = -7442 + 0.41968\ T$$

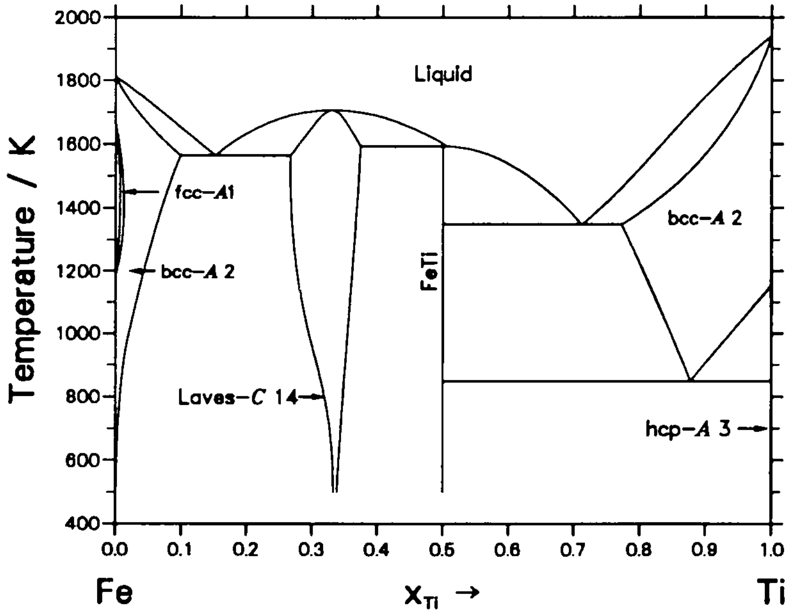


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Ti}			T / K
Liquid ⇌ FeTi* + bcc–$A2$	Eutectic	.712	.500	.772	1349.3
bcc–$A2$ ⇌ FeTi* + hcp–$A3$	Eutectoid	.877	.500	.999	849.4
Liquid + Laves–$C14$ ⇌ FeTi*	Peritectic	.506	.334	.500	1593.4
Laves–$C14$ ⇌ bcc–$A2$	Congruent	.333	.333	....	1707.0
Liquid ⇌ bcc–$A2$ + Laves–$C14$	Eutectic	.152	.099	0.267	1564.4

* FeTi ≡ bcc–$B2$

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Comments
Fe–Ti	(Fe)	Cu	$cF4$ $Pm\bar{3}m$	
	(Fe)	W	$cI2$ $Im\bar{3}m$	
	(Ti)	Mg	$hP2$ $P6_3/mmc$	
	(Ti)	W	$cI2$ $Im\bar{3}m$	
	FeTi	CsCl	$cP2$ $Pm\bar{3}m$	bcc–$B2$
	β Fe_2Ti	$MgZn_2$	$hP12$ $P6_3/mmc$	Laves–$C14$

System Hf–Ti

Solution Phases:

(stable) Liquid, bcc–$A2$, hcp–$A3$
(metastable) fcc–$A1$

Modelling:

Liquid : Substitutional, Redlich–Kister
bcc–$A2$: Substitutional, Redlich–Kister
fcc–$A1$: Substitutional, Redlich–Kister
hcp–$A3$: Substitutional, Redlich–Kister

Assessor and Date:

H. Bitterman, Univ. Wien, Austria, 1997

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase liquid

$$L^{0,\text{liquid}}_{\text{Hf,Ti}} = -4993.5 - 7.10316\ T$$

Phase fcc–$A1$

$$L^{0,\text{fcc}-A1}_{\text{Hf,Ti:}\square} = 1.0\text{E-}4$$

Phase hcp–$A3$

$$L^{0,\text{hcp}-A3}_{\text{Hf,Ti:}\square} = 13644 - 10.6383\ T$$

Phase bcc–$A2$

$$L^{0,\text{bcc}-A2}_{\text{Hf,Ti:}\square} = 3003.24 - 7.4114\ T$$

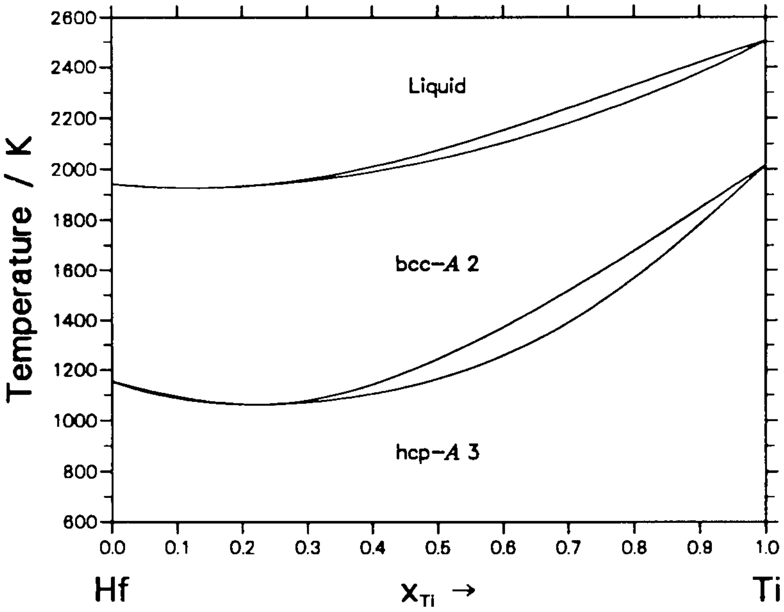


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Ti}			T / K
hcp–$A3$ ⇌ bcc–$A2$	Congruent	.224	.224	....	1063.3
bcc–$A2$ ⇌ Liquid	Congruent	.120	.120	....	1296.0

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Comments
Hf–Ti	(Hf)	Mg	$hP2$ $P6_3/mmc$	
	(Hf)	W	$cI2$ $Im\bar{3}m$	
	(Ti)	Mg	$hP2$ $P6_3/mmc$	
	(Ti)	W	$cI2$ $Im\bar{3}m$	

System Li–Mg

Solution Phases:

(stable) Liquid, bcc-$A2$, hcp-$A3$
(metastable) fcc-$A1$

Compounds:

(metastable) $Al_{12}Mg_{17}$, AlLi

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-$A2$: Substitutional, Redlich-Kister
fcc-$A1$: Substitutional, Redlich-Kister
hcp-$A3$: Substitutional, Redlich-Kister
$Al_{12}Mg_{17}$: Sublattice model, $(Li,Mg)_{24}(Li,Mg)_{10}(Mg)_{24}$
AlLi : Sublattice model,$(Li,Mg)(Li,Mg,\square)$

Assessor and Date:

N. Saunders, 1991

Comments:

The models describing the metastable phases are compatible with the ones used in the Al-Mg system(Version I).

Thermodynamic properties of the solution phases ($J.mol^{-1}$)

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Li,Mg}:\square} = -18335 + 8.49\ T$$

$$L^{1,\mathrm{bcc}-A2}_{\mathrm{Li,Mg}:\square} = 3481$$

$$L^{2,\mathrm{bcc}-A2}_{\mathrm{Li,Mg}:\square} = 2658 - 0.114\ T$$

Phase fcc-$A1$

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Li,Mg:\square}} = -6856.0$$

Phase hcp-$A3$

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Li,Mg:\square}} = -6856.0$$

$$L^{1,\mathrm{hcp}-A3}_{\mathrm{Li,Mg:\square}} = 4000.0$$

$$L^{2,\mathrm{hcp}-A3}_{\mathrm{Li,Mg:\square}} = 4000.0$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Li,Mg}} = -14935 + 10.371\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Li,Mg}} = -1789 + 1.143\ T$$

$$L^{2,\mathrm{liquid}}_{\mathrm{Li,Mg}} = 6533 - 6.6915\ T$$

Phase $\mathrm{Al_{12}Mg_{17}}$

$G^\circ(T) - 34.0\ H^{\mathrm{o,bcc}-A2}_{\mathrm{Li}}(298.15\ \mathrm{K}) - 24.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Li{:}Li{:}Mg)} =$
$290000 + 34.0\ \mathrm{GHSER_{Li}} + 24.0\ \mathrm{GHSER_{Mg}}$

$G^\circ(T) - 10.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) - 48.0\ H^{\mathrm{o,bcc}-A2}_{\mathrm{Li}}(298.15\ \mathrm{K}) = \mathrm{G(Li{:}Li{:}Mg)} =$
$290000 + 10.0\ \mathrm{GHSER_{Li}} + 48.0\ \mathrm{GHSER_{Mg}}$

$G^\circ(T) - 24.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) - 34.0\ H^{\mathrm{o,bcc}-A2}_{\mathrm{Li}}(298.15\ \mathrm{K}) = \mathrm{G(Li{:}Li{:}Mg)} =$
$290000 + 24.0\ \mathrm{GHSER_{Li}} + 34.0\ \mathrm{GHSER_{Mg}}$

$G^\circ(T) - 58.0\ H^{\mathrm{o,bcc}-A2}_{\mathrm{Li}}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Mg{:}Mg)} = 0.0$

Phase AlLi

$G^\circ(T) - 2.0\ H^{\mathrm{o,bcc}-A2}_{\mathrm{Li}}(298.15\ \mathrm{K}) = \mathrm{G(Li{:}Li)} =$
$2.0\ \mathrm{GHSER_{Li}}$

$G^\circ(T) - H^{\mathrm{o,bcc}-A2}_{\mathrm{Li}}(298.15\ \mathrm{K}) - H^{\mathrm{o,hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Li{:}Mg)} =$
$-9168 + 4.2\ T + \mathrm{GHSER_{Li}} + \mathrm{GBCC_{Mg}}$

$G^\circ(T) - H^{\mathrm{o,bcc}-A2}_{\mathrm{Li}}(298.15\ \mathrm{K}) - H^{\mathrm{o,hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Li)} =$
$-9168 + 4.2\ T + \mathrm{GHSER_{Li}} + \mathrm{GBCC_{Mg}}$

$G^\circ(T) - 2.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Mg)} = 0.0$

$G^\circ(T) - H^{\mathrm{o,bcc}-A2}_{\mathrm{Li}}(298.15\ \mathrm{K}) - H^{\mathrm{o,hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Li{:}\square)} =$
$50000 + \mathrm{GHSER}_{Li}$

$G^\circ(T) - H^{\mathrm{o,hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}\square)} = 0.0$

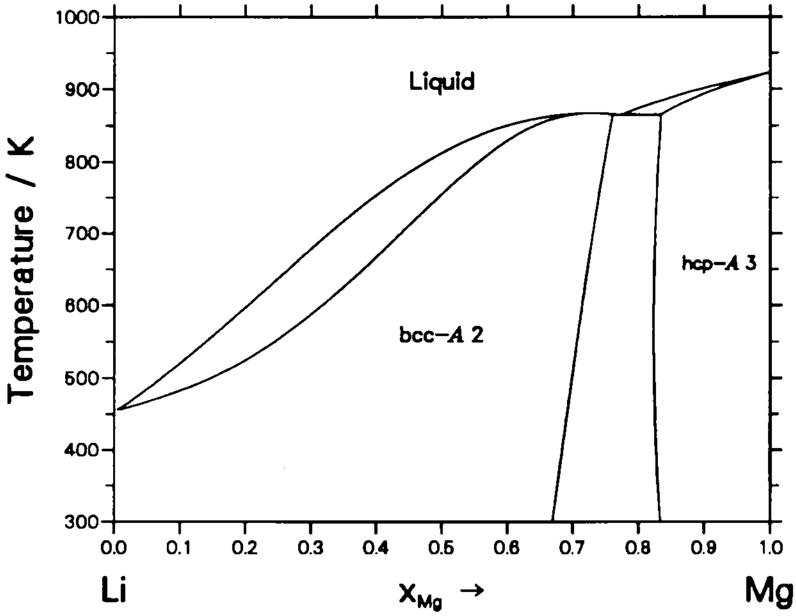


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Mg}			T / K
Liquid ⇌ bcc–$A2$ + hcp–$A3$	Eutectic	.774	.760	.834	865.2
Liquid ⇌ bcc–$A2$	Congurent	.727	.727	....	867.4

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group
Li-Mg	(Li)	W	$cI2$ $Im\bar{3}m$
	(Mg)	Mg	$hP2$ $P6_3/mmc$

System Li-Zr

Solution Phases:

(stable) Liquid, bcc-$A2$, hcp-$A3$
(metastable) fcc-$A1$

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-$A2$: Substitutional, Redlich-Kister
fcc-$A1$: Substitutional, Redlich-Kister
hcp-$A3$: Substitutional, Redlich-Kister

Assessor and Date:

N. Saunders, 1991

Thermodynamic properties of the solution phases (J.mol^{-1})

Phase bcc-$A2$

$$L^{0,\mathrm{bcc-}A2}_{\mathrm{Li,Zr:\square}} = 100000$$

Phase fcc-$A1$

$$L^{0,\mathrm{fcc-}A1}_{\mathrm{Li,Zr:\square}} = 100000$$

Phase hcp-$A3$

$$L^{0,\mathrm{hcp-}A3}_{\mathrm{Li,Zr:\square}} = 100000$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Li,Zr}} = 100000$$

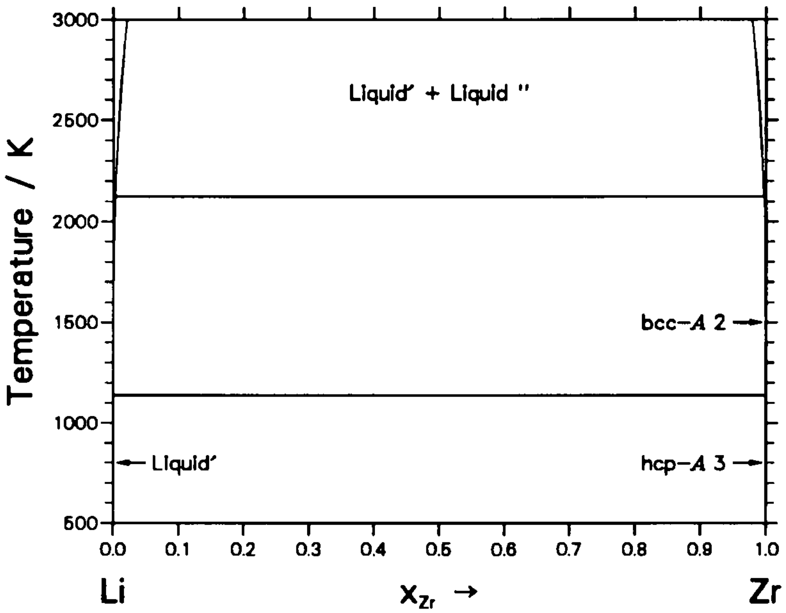


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Zr}			T / K
hcp-$A3$ ⇌ bcc-$A2$	Allotropic	1.000	1.000	....	1139.45
Liquid" ⇌ Liquid' + bcc-$A2$	Monotectic	.996	.003	.998	2124.9
Liquid' ⇌ bcc-$A2$ + hcp-$A3$	Degenerate	.000	.000	1.000	453.6

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group
Li-Zr	(Li)	W	$cI2$ $Im\bar{3}m$
	(Zr)	Mg	$hP2$ $P6_3/mmc$
	(Zr)	W	$cI2$ $Im\bar{3}m$

System Mg–Mn

Solution Phases:

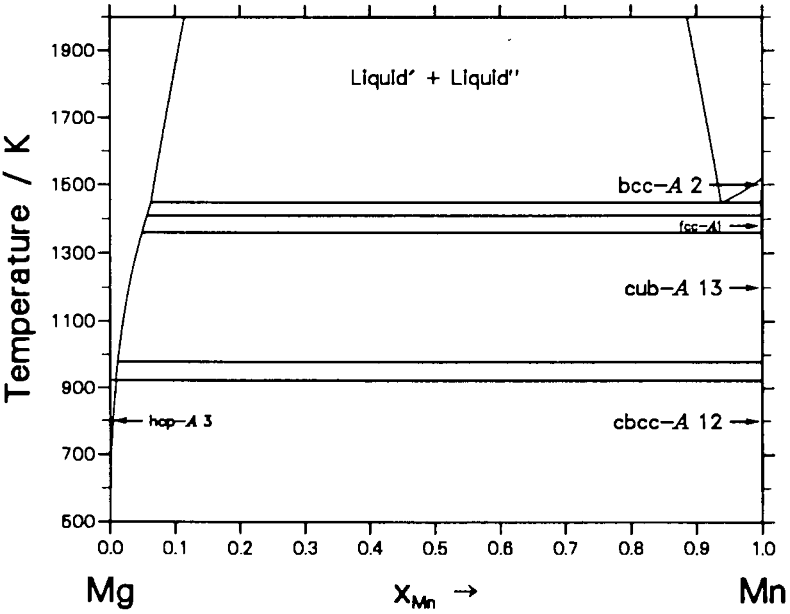
Liquid, bcc–*A*2, hcp–*A*3, cbcc–*A*12, cub-A13, fcc–*A*1

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc–*A*2 : Substitutional, Redlich-Kister
bcc–*A*12 : Substitutional, Redlich-Kister
cub-A13 : Substitutional, Redlich-Kister
hcp–*A*3 : Substitutional, Redlich-Kister
fcc–*A*1 : Substitutional, Redlich-Kister

Assessor and Date:

J. Tibballs 1991



Thermodynamic properties of the solution phases (J.mol^{-1})

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Mg,Mn}:\square} = 70000.0$$

Phase cbcc–$A12$

$$L^{0,\mathrm{cbcc}-A12}_{\mathrm{Mg,Mn:Va}} = 70000.0$$

Phase cub–$A13$

$$L^{0,\mathrm{cub}-A13}_{\mathrm{Mg,Mn:Va}} = 70000.0$$

Phase fcc–$A1$

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Mg,Mn}} = 70000.0$$

Phase hcp–$A3$

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Mg,Mn:Va}} = 32985.0 + 2.5\ T$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Mg,Mn}} = 19125.0 + 12.5\ T$$

Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Mn}			T / K
Liquid' + cbcc–$A12$ ⇌ hcp–$A3$	Peritectic	.008	1.000	.009	923.8
cub–$A13$ ⇌ Liquid' + cbcc–$A12$	Metatectic	.999	.012	1.000	980.5
fcc–$A1$ ⇌ Liquid' + cub–$A13$	Metatectic	.999	.048	1.000	1351.7
bcc–$A2$ ⇌ Liquid' + fcc–$A1$	Metatectic	.998	.057	.999	1409.6
Liquid" ⇌ Liquid' + bcc–$A2$	Monotectic	.937	.063	.998	1447.0

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Comments
Mg–Mn	(Mg)	Mg	$hP2$ $P6_3/mmc$	
	α–Mn	α–Mn	c58 $I\bar{4}3m$	cbcc–$A12$
	β-Mn	β-Mn	$cP20$ $P4_1323m$	cub–$A13$
	γ-Mn	Cu	$cF4$ $Fm3m$	
	δ-Mn	W	$cI2$ $Im\bar{3}m$	

System Mg–Ni

Solution Phases:

Liquid, fcc–*A*1

Compounds:

Mg_2Ni, Laves–*C*36

Modelling:

Liquid : Substitutional, Redlich-Kister
fcc–*A*1 : Substitutional, Redlich-Kister
Mg_2Ni : Stoichiometric, $(Mg)_2(Ni)$
Laves-*C*36 : Sublattice model, $(Mg,Ni)_2(Mg,Ni)$

Comments:

M. Jacobs assumed the Laves–*C*36 phase to be stoichiometric. The thermodynamic description of that phase was modified and is now consistent with the one in the database.

Assessor and Date:

M. Jacobs September 1991 (Laves–*C*36 modified by I. Ansara December 1997).

Thermodynamic properties of the solution and compound phases ($J.mol^{-1}$)

Phase bcc–*A*2

$$L^{0,\text{bcc}-A2}_{\text{Mg,Ni}:\square} = 80\ T$$

Phase fcc–*A*1

$$L^{0,\text{fcc}-A1}_{\text{Mg,Ni}:\square} = 80\ T$$

Phase hcp–*A*3

$$L^{0,\text{hcp}-A3}_{\text{Mg,Ni}:\square} = 80\ T$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Mg,Ni}} = -\ 42304.49 + 7.45704\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Mg,Ni}} = -\ 15611.66 + 9.11885\ T$$

Phase Laves-$C36$

$$G^{\circ}(T) - 3.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Mg)} = 15000.0 + \mathrm{GHSER}_{\mathrm{Mg}}$$

$$G^{\circ}(T) - H^{\mathrm{o,hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) - 2.0\ H^{\mathrm{o,fcc}-A1,\mathrm{para}}_{\mathrm{Ni}}(298.15\ \mathrm{K}) = -74136.0 + 293.9216\ T - 54.35385\ T\cdot \ln T - 0.03329235\ T^2 + 5.14203\mathrm{E}{-}06\ T^3 - 99.0\ T^{-1}$$

$$G^{\circ}(T) - 2.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) - H^{\mathrm{o,fcc}-A1,\mathrm{para}}_{\mathrm{Ni}}(298.15\ \mathrm{K}) = 104136.0 - 293.9216\ T + 54.35385\ T\cdot \ln T + 0.03329235\ T^2 - 5.14203\mathrm{E}{-}06\ T^3 + 99.0\ T^{-1}$$

$$G^{\circ}(T) - 3.0\ H^{\mathrm{o,fcc}-A1,\mathrm{para}}_{\mathrm{Ni}}(298.15\ \mathrm{K}) = \mathrm{G(Ni{:}Ni)} = 15000.0 + \mathrm{GHSER}_{\mathrm{Ni}}$$

$$L^{0,\mathrm{Laves}-C36}_{\mathrm{Mg,Ni:Mg}} = L^{0,\mathrm{Laves}-C36}_{\mathrm{Mg,Ni:Ni}} = 50000$$

$$L^{0,\mathrm{Laves}-C36}_{\mathrm{Mg:Mg,Ni}} = L^{0,\mathrm{Laves}-C36\mathrm{A}}_{\mathrm{Ni:Mg,Ni}} = 50000$$

Phase Mg_2Ni

$$G^{\circ}(T) - 2.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) - H^{\mathrm{o,fcc}-A1,\mathrm{para}}_{\mathrm{Ni}}(298.15\ \mathrm{K}) = -82211.0 + 571.0183\ T - 95.992\ T\cdot \ln T$$

Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Ni}			T / K
Liquid ⇌ Laves-$C36$ + fcc-$A1$	Eutectic	.802	.666	1.000	1366.6
Liquid ⇌ $MgNi_2$	Congruent	.666	.666	....	1420.0
Liquid + Mg_2Ni ⇌ Laves-$C36$	Peritectic	.278	.666	.333	1032.2
Liquid ⇌ + hcp-$A3$ Mg_2Ni	Eutectic	.101	.000	.333	780.0

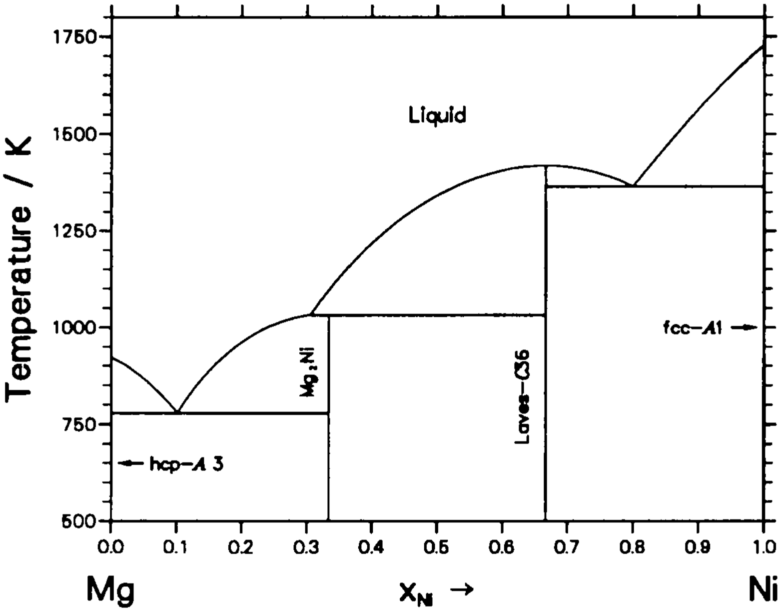


Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Mg-Ni	(Mg)	Mg	*hP2* $P6_3/mmc$	M 2	
	(Ni)	Cu	*cF4* $Fm\bar{3}m$	M 4	
	$MgNi_2$	$MgNi_2$	*hP24* $P6_3/mmc$	Mg_1 4 Mg_2 4 Ni_1 4 Ni_2 6 Ni_3 6	
	Mg_2Ni	Mg_2Ni	*hP18* $P6_222$	Mg_1 6 Mg_2 6 Ni_1 3 Ni_2 3	in Mas2, Mg_2Ni related to Al_2Cu-*C*16 type according to [90Mas]

System Mg–Si

Solution Phases:

(stable)	Liquid, hcp-*A3*
(metastable)	fcc-*A1*

Compound:

(stable)	Mg_2Si
(metastable)	Laves-*C15*

Modelling:

Liquid : Substitutional, Redlich-Kister
hcp-*A3* : Substitutional, Redlich-Kister
fcc-*A1* : Substitutional, Redlich-Kister
Mg_2Si : Stoichiometric, $(Mg)_2(Si)$
Laves-*C15* : Sublattice model, $(Mg,Si)_2(Mg,Si)$

Publication:

H. Heufel, T. Gödecke, H.-L. Lukas, and F. Sommer,
J. Alloys and Comp., **247**, (1-2), 31-42 (1997).

Thermodynamic properties of the solution and compound phases ($J.mol^{-1}$)

Phase liquid

$$L^{0,\text{liquid}}_{\text{Mg,Si}} = -83864.26 + 32.44438\ T$$

$$L^{1,\text{liquid}}_{\text{Mg,Si}} = 18027.41 - 19.61202\ T$$

$$L^{2,\text{liquid}}_{\text{Mg,Si}} = 2486.67 - 0.31084\ T$$

$$L^{3,\text{liquid}}_{\text{Mg,Si}} = 18541.17 - 2.317664\ T$$

$$L^{4,\text{liquid}}_{\text{Mg,Si}} = -12338.84 + 1.54236\ T$$

Phase hcp–*A3*

$$L^{0,\text{hcp}-A3}_{\text{Mg,Si}:\square} = -7148.79 + 0.89361\ T$$

Phase fcc−$A1$

$$L^{0,\mathrm{fcc-}A1}_{\mathrm{Mg,Si:\square}} = -7148.79 + 0.89361\ T$$

Phase Mg$_2$Si

$$G^\circ(T) - 2.0\ H^{\mathrm{o,hcp-}A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) - H^{\mathrm{o,diamond}}_{\mathrm{Si}}(298.15\ \mathrm{K}) =$$
$$-92250.0 + 440.4\ T - 75.9\ T \cdot \ln T - 0.0018\ T^2 + 630000\ T^{-1}$$

Phase Laves-C15

$$G^\circ(T) - 2.0\ H^{\mathrm{o,hcp-}A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) - H^{\mathrm{o,diamond}}_{\mathrm{Si}}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Si)} =$$
$$104970.96 - 16.46448\ T + 2.0\ \mathrm{GHSER_{Mg}} + \mathrm{GHSER_{Si}}$$
$$G^\circ(T) - H^{\mathrm{o,hcp-}A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) - 2.0\ H^{\mathrm{o,diamond}}_{\mathrm{Si}}(298.15\ \mathrm{K}) = \mathrm{G(Si{:}Mg)} =$$
$$41039.0 + 6.25\ T + \mathrm{GHSER_{Mg}} + 2.0\ \mathrm{GHSER_{Si}}$$

$L^{0,\mathrm{Laves}_C15}_{\mathrm{Mg,Si:Mg}}$ = 15000.0

=

$L^{0,\mathrm{Laves}_C15}_{\mathrm{Mg,Si:Si}}$ = 15000.0

=

$L^{0,\mathrm{Laves}_C15}_{\mathrm{Mg:Mg,Si}}$ = 8000.0

=

$L^{0,\mathrm{Laves}_C15}_{\mathrm{Si:Mg,Si}}$ = 8000.0

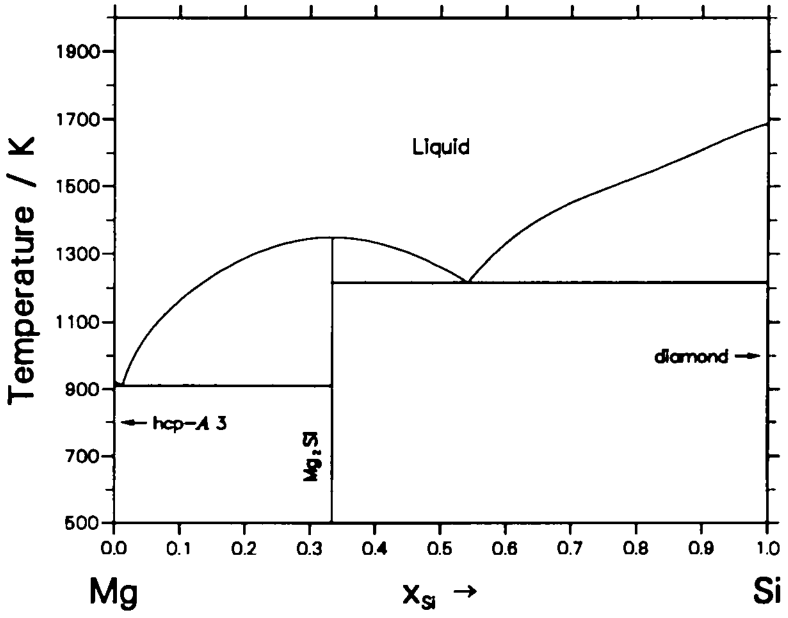


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Si}			T / K
Liquid $\rightleftharpoons$ hcp–$A3$ + Mg_2Si	Eutectic	.013	.000	.333	911.8
Liquid $\rightleftharpoons$ Mg_2Si + diamond	Eutectic	.530	.333	1.000	1214.4
Mg_2Si $\rightleftharpoons$ Liquid	Congruent	.333	.333	...	1350.0

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub–lattices
Mg–Si	(Mg)	Mg	$hP2$ $P6_3/mmc$	M 2
	(Si)	diamond	$cF8$ $Fd\bar{3}m$	M 8
	Mg_2Si	CaF_2	$cF12$ $Fm\bar{3}m$	Mg 8 Si 4

System Mg–Y

Solution Phases:

Liquid, bcc-$A2$, hcp-$A3$

Compounds:

MgY, $Mg_{24}Y_5$, Mg_2Y

Modelling:

Liquid : Substitutional, Redlich–Kister
bcc-A2 : Substitutional, Redlich–Kister
hcp-A3 : Substitutional, Redlich–Kister
MgY : Stoichiometric, (Mg)(Y)
Mg_2Y : Stoichiometric, $(Mg)_2(Y)$
$Mg_{24}Y_5$: Sublattice model, $(Mg)_{24}(Mg,Y)_5$

Assessor and Date:

H.L. Lukas, 1991

Thermodynamic properties of the solution and compound phases ($J.mol^{-1}$)

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Mg,Y:}\square} = -38570.0 + 15.0\ T$$

$$L^{1,\mathrm{bcc}-A2}_{\mathrm{Mg,Y:}\square} = -8204.21$$

Phase hcp–$A3$

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Mg,Y:}\square} = -16582.94 + 4.77482\ T$$

$$L^{1,\mathrm{hcp}-A3}_{\mathrm{Mg,Y:}\square} = -7077.87$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Mg,Y}} = -25802.51 + 4.30042\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Mg,Y}} = -19229.76 + 3.20497\ T$$

Phase fcc-A1

$$L^{0,\text{fcc}-A1}_{\text{Mg,Y}} = 0.0001$$

Phase $Mg_{24}Y_5$

$$G^{\circ}(T) - 24.0\ H^{\text{o,hcp}-A3}_{\text{Mg}}(298.15\ \text{K}) - 5.0\ H^{\text{o,hcp}-A3}_{\text{Y}}(298.15\ \text{K}) = \text{G(Mg:Y)} =$$
$$-\ 227282.28 + 36.52985\ T + 24.0\ \text{GHSER}_{\text{Mg}} + 5.0\ \text{GHSER}_{\text{Y}}$$

Phase Mg_2Y

$$G^{\circ}(T) - 2.0\ H^{\text{o,hcp}-A3}_{\text{Mg}}(298.15\ \text{K}) - H^{\text{o,hcp}-A3}_{\text{Y}}(298.15\ \text{K}) = \text{G(Mg:Y)} =$$
$$-\ 39075.78 + 6.51258\ T + 2.0\ \text{GHSER}_{\text{Mg}} + \text{GHSER}_{\text{Y}}$$

Phase MgY

$$G^{\circ}(T) - H^{\text{o,hcp}-A3}_{\text{Mg}}(298.15\ \text{K}) - H^{\text{o,hcp}-A3}_{\text{Y}}(298.15\ \text{K}) = \text{G(Mg:Y)} =$$
$$-\ 32162.76 + 8.0\ T + \text{GHSER}_{\text{Mg}} + \text{GHSER}_{\text{Y}}$$

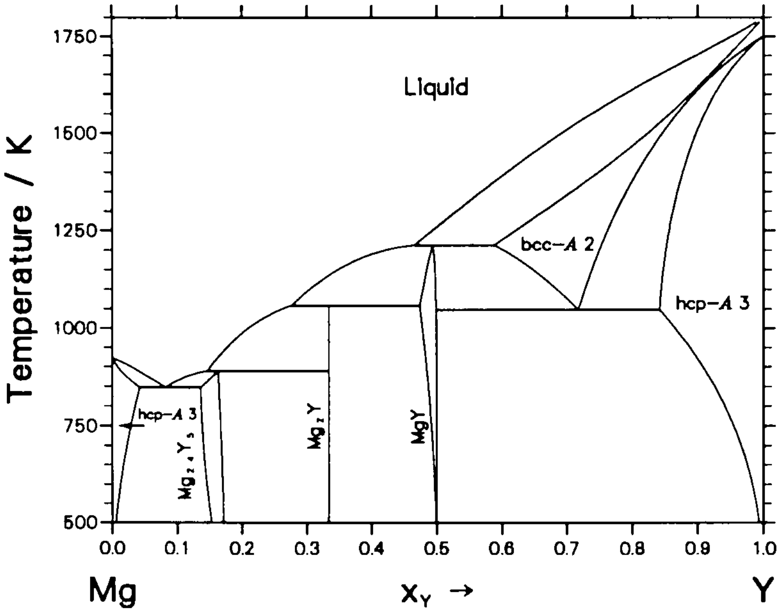


Table I - Invariant Reactions.

Reaction	Type	Compositions x_Y			T / K
Liquid + bcc-$A2 \rightleftharpoons$ MgY	Peritectic	.466	.588	.494	1213.3
Liquid + MgY $\rightleftharpoons Mg_2Y$	Peritectic	.276	.474	.333	1058.5
Liquid+ $Mg_2Y \rightleftharpoons Mg_{24}Y_5$	Peritectic	.146	.333	.163	889.4
Liquid $\rightleftharpoons$ hcp-$A3$ + $Mg_{24}Y_5$	Eutectic	.082	.042	.136	847.6
bcc-A2 $\rightleftharpoons$ MgY + hcp-$A3$	Eutectoid	.717	.499	.841	1048.0

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices		Comments
Mg-Y	(Mg)	Mg	$hP2$ $P6_3/mmc$	M	2	
	(Y)	W	$cI2$ $Im\bar{3}m$	M	4	
	(Y)	Mg	$hP2$ $P6_3/mmc$	M	2	
	$Mg_{24+x}Y_5$	α-Mn	$cI58$ $I\bar{4}3m$	M Mg_1 Mg_2 Y	2 24 24 8	cbcc-$A12$ designated as $Mg_{24}Y_5$
	Mg_2Y	$MgZn_2$	$hP12$ $P6_3/mmc$	Mg_1 Mg_2	2 6	
	$Mg_{1+x}Y$	CsCl	$cP2$ $Pm\bar{3}m$	Mg Y	1 1	bcc-$B2$ designated as MgY

System Mg–Zn

Solution Phases:

(stable) : Liquid, hcp–Zn, Laves–*C*14
(metastable) : bcc–*A*2, bcc–*B*2, fcc–*A*1, hcp–*A*3

Compounds:

(stable) Mg_2Zn_{11}, MgZn, Mg_2Zn_3, $Mg_{51}Zn_{20}$
(metastable) : AlMg–β, AlMg–ϵ, AlMg–γ, AlMgZn–ϕ
(metastable) : Laves–*C*15, Laves–*C*36

Modelling:

Liquid : Substitutional, Redlich–Kister
hcp–Zn : Substitutional, Redlich–Kister
bcc–*A*2 : see below
bcc–*B*2 : Sublattice model, $(Mg,Zn)_{0.5}(Mg,Zn)_{0.5}(\square)_3$ Two descriptions of the bcc–*A*2:bcc–*B*2 order-disorder transformation are given: one which includes the parameters of the order and disordered phases in a single description (equation 21 in the thermodynamic modelling chapter), and a second one where the order and disorder contributions are expressed by equation 23. For the second case, the parameters are in a frame.
fcc–*A*1 : Substitutional, Redlich–Kister
hcp–*A*3 : Substitutional, Redlich–Kister
Mg_2Zn_{11} : Stoichiometric, $(Mg)_2(Zn)_{11}$
MgZn : Stoichiometric, $(Mg)_{12}(Zn)_{13}$
Mg_2Zn_3 : Stoichiometric, $(Mg)_2(Zn)_3$
$Mg_{51}Zn_{20}$: Stoichiometric, $(Mg)_{51}(Zn)_{20}$
AlMgZn–ϕ : Stoichiometric, $(Mg)_6(Zn)_5$
AlMg–β : Stoichiometric, $(Mg)_{89}(Zn)_{104}$
AlMg–ϵ : Stoichiometric, $(Mg)_{23}(Zn)_{30}$
AlMg–γ : Sublattice model, $(Mg)_5(Mg,Zn)_{12}(Mg,Zn)_{12}$
Laves–*C*14 : Sublattice model, $(Mg,Zn)_2(Mg,Zn)$
Laves–*C*15 : Sublattice model, $(Mg,Zn)_2(Mg,Zn)$
Laves–*C*36 : Sublattice model, $(Mg,Zn)_2(Mg,Zn)$

Assessor and Date:

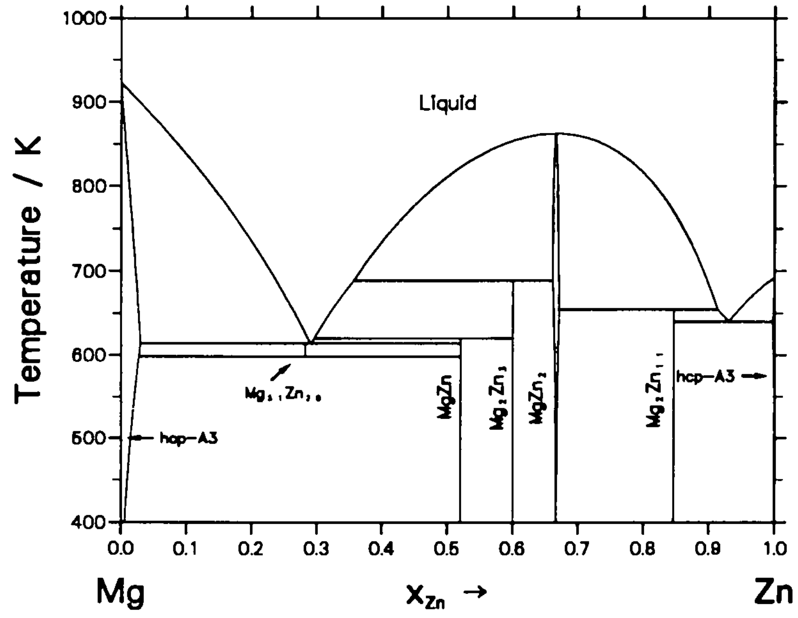
R. Agarwal, S.G. Fries, H.L. Lukas, G. Petzow,
F. Sommer, T.G. Chart, G. Effenberg

Publication:

Z. für Metallkde., 83, 4, 216-223 (1992).

Comments:

A reevaluation was performed in order to take into account the non-stoichiometry of the Laves-*C*14 phase.



Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase fcc-$A1$

$$L^{0,\text{fcc}-A1}_{\text{Mg,Zn}:\square} = -3056.82 + 5.63801\ T$$

$$L^{1,\text{fcc}-A1}_{\text{Mg,Zn}:\square} = -3127.26 + 5.65563\ T$$

Phase hcp–Zn

$$L^{0,\mathrm{hcp-Zn}}_{\mathrm{Mg,Zn:\square}} = -\,3056.82 + 5.63801\ T$$

$$L^{1,\mathrm{hcp-Zn}}_{\mathrm{Mg,Zn:\square}} = -\,3127.26 + 5.65563\ T$$

Phase hcp–$A3$

$$L^{0,\mathrm{hcp-}A3}_{\mathrm{Mg,Zn:\square}} = -\,3056.82 + 5.63801\ T$$

$$L^{1,\mathrm{hcp-}A3}_{\mathrm{Mg,Zn:\square}} = -\,3127.26 + 5.65563\ T$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Mg,Zn}} = -\,77729.24 + 680.52266\ T - 95.0\ T \cdot \ln T + 0.04\ T^2$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Mg,Zn}} = 3674.72 + 0.57139\ T$$

$$L^{2,\mathrm{liquid}}_{\mathrm{Mg,Zn}} = -\,1588.15$$

Phase AlMg–β

$$G^\circ(T) - 89.0\ H^{\mathrm{o,hcp-}A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) - 104.0\ H^{\mathrm{o,hcp-Zn}}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = 206100 + 89.0\ \mathrm{GHSER_{Mg}} + 104.0\ \mathrm{GHSER_{Zn}}$$

Phase AlMg–ϵ

$$G^\circ(T) - 23.0\ H^{\mathrm{o,hcp-}A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) - 30.0\ H^{\mathrm{o,hcp-Zn}}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = -\,318000 + 63.6\ T + 23.0\ \mathrm{GHSER_{Mg}} + 30.0\ \mathrm{GHSER_{Zn}}$$

Phase AlMg–γ

$$G^\circ(T) - 17.0\ H^{\mathrm{o,hcp-}A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) - 12.0\ H^{\mathrm{o,hcp-Zn}}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Mg{:}Zn)} = -\,145000 + 58\ T + 17.0\ \mathrm{GHSER_{Mg}} + 12.0\ \mathrm{GHSER_{Zn}}$$

$$G^\circ(T) - 17.0\ H^{\mathrm{o,hcp-}A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) - 12.0\ H^{\mathrm{o,hcp-Zn}}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Zn{:}Mg)} = 87000 + 29\ T + 17.0\ \mathrm{GHSER_{Mg}} + 12.0\ \mathrm{GHSER_{Zn}}$$

$$G^\circ(T) - 5.0\ H^{\mathrm{o,hcp-}A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) - 24.0\ H^{\mathrm{o,hcp-Zn}}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Zn{:}Zn)} = 290000.0 + 5.0\ \mathrm{GHSER_{Mg}} + 24.0\ \mathrm{GHSER_{Zn}}$$

$$L^{0,\mathrm{AlMg-}\gamma}_{\mathrm{Mg:Mg,Zn:Mg}} = L^{0,\mathrm{AlMg-}\gamma}_{\mathrm{Mg:Mg,Zn:Zn}} = -\,116000 + 58\ T$$

Phase $Mg_{51}Zn_{20}$

$$G^{\circ}(T) - 51.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) - 20.0\ H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = - 335741.54 + 35.5\ T + 51.0\ \mathrm{GHSER_{Mg}} + 20.0\ \mathrm{GHSER_{Zn}}$$

Phase MgZn

$$G^{\circ}(T) - 12.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) - 13.0\ H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = - 236980.84 + 59.24524\ T + 12.0\ \mathrm{GHSER_{Mg}} + 13.0\ \mathrm{GHSER_{Zn}}$$

Phase Mg_2Zn_3

$$G^{\circ}(T) - 2.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = - 54406.20 + 13.60156\ T + 2.0\ \mathrm{GHSER_{Mg}} + 3.0\ \mathrm{GHSER_{Zn}}$$

Phase Mg_2Zn_{11}

$$G^{\circ}(T) - 2.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) - 11.0\ H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = - 73818.32 + 18.45457\ T + 2.0\ \mathrm{GHSER_{Mg}} + 11.0\ \mathrm{GHSER_{Zn}}$$

Phase AlMgZn–ϕ

$$G^{\circ}(T) - 6.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) - 5.0\ H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = - 79530 + 20.9\ T + 6.0\ \mathrm{GHSER_{Mg}} + 5.0\ \mathrm{GHSER_{Zn}}$$

Phase Laves–$C14$

$$G^{\circ}(T) - 3.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Mg)} = 15000.0 + 3.0\ \mathrm{GHSER_{Mg}}$$

$$G^{\circ}(T) - 2.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) - H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Zn)} = 65355.45 - 8.83886\ T + 2.0\ \mathrm{GHSER_{Mg}} + \mathrm{GHSER_{Zn}}$$

$$G^{\circ}(T) - H_{\mathrm{Mg}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Zn{:}Mg)} = - 35355.45 + 8.83886\ T + \mathrm{GHSER_{Mg}} + 2.0\ \mathrm{GHSER_{Zn}}$$

$$G^{\circ}(T) - 3.0\ H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Zn{:}Zn)} = 15000.0 + 3.0\ \mathrm{GHSER_{Zn}}$$

$$L_{\mathrm{Mg,Zn:Mg}}^{0,\mathrm{Laves-}C14} = L_{\mathrm{Mg,Zn:Zn}}^{0,\mathrm{Laves-}C14} = 35000.0$$

$$L_{\mathrm{Mg:Mg,Zn}}^{0,\mathrm{Laves-}C14} = L_{\mathrm{Zn:Mg,Zn}}^{0,\mathrm{Laves-}C14} = 8000.0$$

Phase Laves–$C15$

$$G^{\circ}(T) - 3.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Mg)} = 15000.0 + 3.0\ \ \mathrm{GHSER_{Mg}}$$

$$G^{\circ}(T) - 2.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) - H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Zn)} = 55355.45 - 8.83886\ \ T + 2.0\ \ \mathrm{GHSER_{Mg}} + \mathrm{GHSER_{Zn}}$$

$$G^{\circ}(T) - H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) - 2.0\ \ H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Zn{:}Mg)} = -\ 25355.45 + 8.83886\ \ T + \mathrm{GHSER_{Mg}} + 2.0\ \ \mathrm{GHSER_{Zn}}$$

$$G^{\circ}(T) - 3.0\ \ H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Zn{:}Zn)} = 15000.0 + 3.0\ \ \mathrm{GHSER_{Zn}}$$

$$L_{\mathrm{Mg,Zn:Mg}}^{\mathrm{0,Laves-}C15} = L_{\mathrm{Mg,Zn:Zn}}^{\mathrm{0,Laves-}C15} = 35000.0$$

$$L_{\mathrm{Mg:Mg,Zn}}^{\mathrm{0,Laves-}C15} = L_{\mathrm{Zn:Mg,Zn}}^{\mathrm{0,Laves-}C15} = 8000.0$$

Phase Laves–$C36$

$$G^{\circ}(T) - 3.0\ \ H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Mg)} = 15000.0 + 3.0\ \ \mathrm{GHSER_{Mg}}$$

$$G^{\circ}(T) - 2.0\ \ H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) - H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Zn)} = 65355.45 - 8.83886\ \ T + 2.0\ \ \mathrm{GHSER_{Mg}} + \mathrm{GHSER_{Zn}}$$

$$G^{\circ}(T) - H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Zn{:}Mg)} = -35355.45 + 8.83886\ \ T + \mathrm{GHSER_{Mg}} + 2.0\ \ \mathrm{GHSER_{Zn}}$$

$$G^{\circ}(T) - 3.0\ \ H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Zn{:}Zn)} = 15000.0 + 3.0\ \ \mathrm{GHSER_{Zn}}$$

$$L_{\mathrm{Mg,Zn:Mg}}^{\mathrm{0,Laves-}C36} = L_{\mathrm{Mg,Zn:Zn}}^{\mathrm{0,Laves-}C36} = 35000.0$$

$$L_{\mathrm{Mg:Mg,Zn}}^{\mathrm{0,Laves-}C36} = L_{\mathrm{Zn:Mg,Zn}}^{\mathrm{0,Laves-}C36} = 8000.0$$

Phase bcc–$B2$

$$G_{\mathrm{Mg:Zn:\Box}}^{*} = 0.0$$

$$L_{\mathrm{Mg,Zn}}^{0} = -\ 2500.0$$

$$G^{\circ}(T) - H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G\ (Mg{:}Mg{:}\Box)} = \mathrm{GBCC_{Mg}}$$

$$G^{\circ}(T) - 0.5\ \ H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) - 0.5\ \ H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = \mathrm{G\ (Mg{:}Zn{:}\Box)} = G_{\mathrm{Mg:Zn:\Box}}^{*} + L_{\mathrm{Mg,Zn}}^{0} + 0.5\ \ \mathrm{GBCC_{Mg}} + 0.5\ \ \mathrm{GBCC_{Zn}}$$

$$G^{\circ}(T) - 0.5\ \ H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) - 0.5\ \ H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = \mathrm{G\ (Zn{:}Mg{:}\Box)} = G_{\mathrm{Mg:Zn:\Box}}^{*} + L_{\mathrm{Mg,Zn}}^{0} + 0.5\ \ \mathrm{GBCC_{Mg}} + 0.5\ \ \mathrm{GBCC_{Zn}}$$

$$G^{\circ}(T) - H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) = \mathrm{G\ (Zn{:}Zn{:}\Box)} = \mathrm{GBCC_{Zn}}$$

$$L_{\mathrm{Mg,Zn:Mg:\Box}}^{\mathrm{0,bcc-}B2} = L_{\mathrm{Mg:Mg,Zn:\Box}}^{\mathrm{0,bcc-}B2} = -\ G_{\mathrm{Mg:Zn:\Box}}^{*} + L_{\mathrm{Mg,Zn}}^{0}$$

$$L_{\mathrm{Mg,Zn:Zn:\Box}}^{\mathrm{0,bcc-}B2} = L_{\mathrm{Zn:Mg,Zn:\Box}}^{\mathrm{0,bcc-}B2} = -\ G_{\mathrm{Mg:Zn:\Box}}^{*} + L_{\mathrm{Mg,Zn}}^{0}$$

Phase bcc–$B2$

$G^{*}_{\mathrm{Mg:Zn:\square}} = 0.0$
$L^{0}_{\mathrm{Mg,Zn}} = -\ 2500.0$

$$G^{\circ}(T) - H^{\mathrm{o,hcp-}A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Mg:Mg:\square)} = 0.0$$

$$G^{\circ}(T) - 0.5\ H^{\mathrm{o,hcp-}A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) - 0.5\ H^{\mathrm{o,hcp-Zn}}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Mg:Zn:\square)} = 2.0\ G^{*}_{\mathrm{Mg:Zn:\square}}$$

$$G^{\circ}(T) - 0.5\ H^{\mathrm{o,hcp-}A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) - 0.5\ H^{\mathrm{o,hcp-Zn}}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Zn:Mg:\square)} = 2.0\ G^{*}_{\mathrm{Mg:Zn:\square}}$$

$$G^{\circ}(T) - H^{\mathrm{o,hcp-Zn}}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Zn:Zn:\square)} = 0.0$$

Phase bcc–$A2$

$L^{0,\mathrm{bcc-}A2}_{\mathrm{Mg,Zn:\square}} = 4.0\ L^{0}_{\mathrm{Mg,Zn}}$

Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Zn}			T / K
Liquid + hcp–$A3$ $\rightleftharpoons$ $\mathrm{Mg_{51}Zn_{20}}$	Peritectic	.295	.029	.289	614.1
Liquid $\rightleftharpoons$ $\mathrm{Mg_{51}Zn_{20}}$ + MgZn	Eutectic	.281	.290	.520	614.1
Liquid + $\mathrm{Mg_2Zn_3}$ $\rightleftharpoons$ MgZn	Peritectic	.196	.600	.520	620.1
Liquid + Laves–$C14$ $\rightleftharpoons$ $\mathrm{Mg_2Zn_3}$	Peritectic	.356	.661	.600	688.9
Liquid $\rightleftharpoons$ $\mathrm{MgZn_2}$	Congruent	.667	.667	....	864.0
Liquid + Laves–$C14$ $\rightleftharpoons$ $\mathrm{Mg_2Zn_{11}}$	Peritectic	.913	.661	.846	654.4
Liquid $\rightleftharpoons$ $\mathrm{Mg_2Zn_{11}}$ $\rightleftharpoons$ hcp–$A3$	Eutectic	.926	.846	.997	637.3
$\mathrm{Mg_{51}Zn_{20}}$ $\rightleftharpoons$ hcp–$A3$ + MgZn	Eutectoid	.282	.027	.520	598.1

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-Model	Comments
Mg-Zn	(Mg)	Mg	*hP2* $P6_3/mmc$	M 2	
	(Zn)	Mg	*hP2* $P6_3/mmc$	M 2	
	$MgZn_2$	$MgZn_2$	*hP12* $P6_3/mmc$	Mg 4 Zn_1 2 Zn_3 6	Laves-*C*14
	Mg_2Zn_{11}	Mg_2Zn_{11}	*cP39* $Pm\bar{3}$		
	MgZn				
	Mg_2Zn_3		*mC110* $B2/m$		
	Mg_7Zn_3	Ta_3B_4	*oI142* $Immm$		designated as $Mg_{51}Zn_{20}$

System Mg-Zr

Solution Phases:

(stable)	Liquid, bcc–$A2$, hcp–$A3$
(metastable)	fcc–$A1$

Modelling:

Liquid	:	Substitutional, Redlich-Kister
bcc–$A2$	:	Substitutional, Redlich-Kister
fcc–$A1$	:	Substitutional, Redlich-Kister
hcp–$A3$	:	Substitutional, Redlich-Kister

Assessor and Date:

M. Hämäläinen 1991

Thermodynamic properties of the solution phases (J.mol^{-1})

Phase bcc–$A2$

$$L^{0,\text{bcc}-A2}_{\text{Mg,Zr}:\square} = 5720.44 + 50.11642\ T$$

Phase fcc–$A1$

$$L^{0,\text{fcc}-A1}_{\text{Mg,Zr}:\square} = 42063.55 + 1.01789\ T$$

$$L^{1,\text{fcc}-A1}_{\text{Mg,Zr}:\square} = -2885.9$$

Phase hcp–$A3$

$$L^{0,\text{hcp}-A3}_{\text{Mg,Zr}:\square} = 42063.55 + 1.01789\ T$$

$$L^{1,\text{hcp}-A3}_{\text{Mg,Zr}:\square} = -2885.9$$

Phase liquid

$$L^{0,\text{liquid}}_{\text{Mg,Zr}} = 14003.84 + 29.34205\ T$$

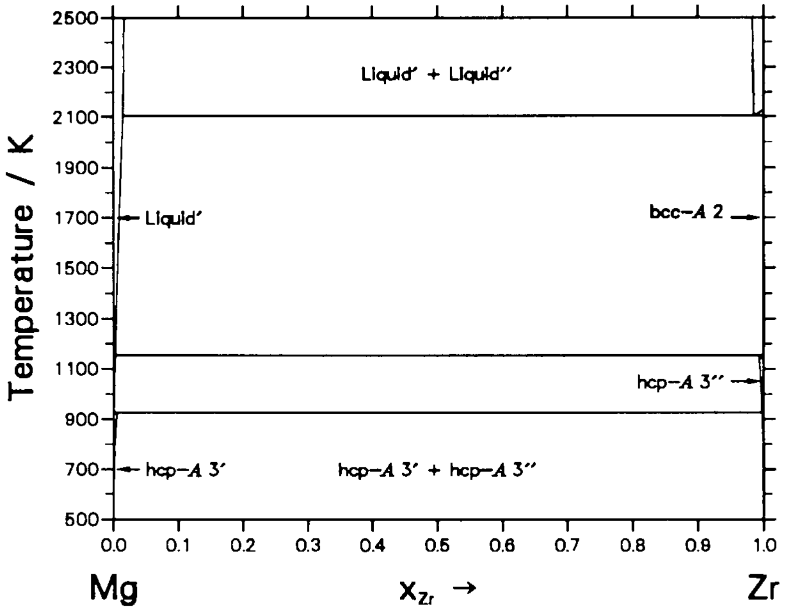


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Zr}			T / K
Liquid' + bcc-$A2$ ⇌ hcp-$A3$	Peritectic	.003	1.000	.993	1154.6
Liquid" ⇌ Liquid' + bcc-$A2$	Monotectic	.985	.015	.999	2104.8
Liquid' + hcp-$A3$" ⇌ hcp-$A3$'	Peritectic	.001	.997	.006	926.6

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group
Mg-Zr	(Mg)	Mg	*hP2* $P6_3/mmc$
	(Zr)	Mg	*hP2* $P6_3/mmc$
	(Zr)	W	*cI2* $Im\bar{3}m$

System Mn–Si

Solution Phases:

Liquid, bcc–$A2$, cbcc–$A12$, cub–$A13$, fcc–$A1$

Compounds:

(stable) Mn_6Si, Mn_9Si_2, Mn_3Si, Mn_5Si_3 MnSi, $Mn_{11}Si_{19}$

(metastable) Al_8Mn_5–$D8_{10}$

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc–$A2$: Substitutional, Redlich-Kister
cbcc–$A12$: Substitutional, Redlich-Kister
cub–$A13$: Substitutional, Redlich-Kister
fcc–$A1$: Substitutional, Redlich-Kister
Mn_6Si : Stoichiometric, $(Mn)_{17}(Si)_3$
Mn_9Si_2 : Stoichiometric,$(Mn)_{33}(Si)_7$
Mn_3Si : Stoichiometric, $(Mn)_3(Si)$
Mn_5Si_3 : Stoichiometric, $(Mn)_5(Si)_3$
MnSi : Stoichiometric, (Mn)(Si)
$Mn_{11}Si_{19}$: Stoichiometric, $(Mn)_{11}(Si)_{19}$
Al_8Mn_5–$D8_{10}$: Sublattice model, $(Si)_{12}(Mn)_4(Mn)_{10}$

Assessor and Date:

J.E. Tibballs, 1991

Publication:

SI-report, 890221-5, 1991

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase Mn_3Si

$$G^\circ(T) - 3.0\ H_{\mathrm{Mn}}^{\mathrm{o,cbcc-}A12\mathrm{,para}}(298.15\ \mathrm{K}) - H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) =$$

$$298.15 < T < 950.00 : -124189.87 + 782.4373\ T - 131.682\ T\cdot \ln T - 0.00777\ T^2 + 1657200\ T^{-1}$$

$$950.00 < T < 2000.00 : -119740.6 + 777.7538\ T - 131.682\ T\cdot \ln T - 0.00777\ T^2 + 1657200\ T^{-1}$$

Phase MnSi

$$\begin{aligned} &G^{\circ}(T) - H_{\text{Mn}}^{\text{o,cbcc}-A12\text{,para}}(298.15\ \text{K}) - H_{\text{Si}}^{\text{o,diamond}}(298.15\ \text{K}) = \\ &\quad - 78135.144 + 308.2488\ T - 52.42121\ T\cdot \ln T - 0.006903355\ T^{2} \\ &\quad + 876442.9\ T^{-1} \end{aligned}$$

Phase $\text{Mn}_{11}\text{Si}_{19}$

$$\begin{aligned} &G^{\circ}(T) - 11.0\ H_{\text{Mn}}^{\text{o,cbcc}-A12\text{,para}}(298.15\ \text{K}) - 19.0\ H_{\text{Si}}^{\text{o,diamond}}(298.15\ \text{K}) = \\ &\quad - 636300.0 + 1624.93\ T - 378.694\ T\cdot \ln T - 0.16391\ T^{2} \\ &\quad - 15432618\ T^{-1} \end{aligned}$$

Phase Mn_6Si

$$G^{\circ}(T) - 17.0\ H_{\text{Mn}}^{\text{o,cbcc}-A12\text{,para}}(298.15\ \text{K}) - 3.0\ H_{\text{Si}}^{\text{o,diamond}}(298.15\ \text{K}) =$$

$$\begin{array}{rcl} 298.15 < T < 1519.00 & : & - 250180.6 + 84.8444\ T - 12.07755\ T\cdot \ln T \\ & & - 0.02850984\ T^{2} + 7514\ T^{-1} \\ & & + 17.0\ \text{GHSER}_{\text{Mn}} + 3.0\ \text{GHSER}_{\text{Si}} \\ 1519.00 < T < 3000.00 & : & - 282008.6 - 32.58304\ T + 12.06754\ T\cdot \ln T \\ & & - 0.05879165\ T^{2} + 3.928228\text{E}{+}31\ T^{-9} \\ & & + 17.0\ \text{GHSER}_{\text{Mn}} + 3.0\ \text{GHSER}_{\text{Si}} \end{array}$$

Phase Mn_9Si_2

$$G^{\circ}(T) - 33.0\ H_{\text{Mn}}^{\text{o,cbcc}-A12\text{,para}}(298.15\ \text{K}) - 7.0\ H_{\text{Si}}^{\text{o,diamond}}(298.15\ \text{K}) =$$

$$\begin{array}{rcl} 298.15 < T < 1519.00 & : & - 578208.4 + 381.294\ T - 56.86988\ T\cdot \ln T \\ & & - 0.0500355\ T^{2} + 1458600\ T^{-1} \\ & & + 33.0\ \text{GHSER}_{\text{Mn}} + 7.0\ \text{GHSER}_{\text{Si}} \\ 298.15 < T < 1519.00 & : & - 639992.0 + 153.3464\ T - 10.0\ T\cdot \ln T \\ & & - 0.1\ T^{2} + 7.625384\text{E}{+}31\ T^{-9} \\ & & + 33.0\ \text{GHSER}_{\text{Mn}} + 7.0\ \text{GHSER}_{\text{Si}} \end{array}$$

Phase Mn_5Si_3

$$\begin{aligned} &G^{\circ}(T) - 5.0\ H_{\text{Mn}}^{\text{o,cbcc}-A12\text{,para}}(298.15\ \text{K}) - 3.0\ H_{\text{Si}}^{\text{o,diamond}}(298.15\ \text{K}) = \\ &\quad - 261930.32 + 1170.778\ T - 211.150\ T\cdot \ln T - 0.015293\ T^{2} \\ &\quad - 149263.11\ T^{-1} \end{aligned}$$

Phase Al_8Mn_5–$D8_{10}$

$$\begin{aligned} &G^{\circ}(T) - 14.0\ H_{\text{Mn}}^{\text{o,cbcc}-A12\text{,para}}(298.15\ \text{K}) - 12.0\ H_{\text{Si}}^{\text{o,diamond}}(298.15\ \text{K}) = \\ &\quad + 14.0\ \text{GHSER}_{\text{Mn}} + 12.0\ \text{GHSER}_{\text{Si}} \end{aligned}$$

Phase bcc–$A2$

$$L_{\text{Mn,Si}:\square}^{0,\text{bcc}-A2} = - 89620.7 + 2.94097\ T$$

$$L_{\text{Mn,Si}:\square}^{1,\text{bcc}-A2} = - 7500.0$$

Phase cbcc–*A*12

$$L^{0,\mathrm{cbcc}-A12}_{\mathrm{Mn,Si:\square}} = -142743.62 + 22.3961\ T$$

$$L^{1,\mathrm{cbcc}-A12}_{\mathrm{Mn,Si:\square}} = 16440.608 - 3.5300332\ T$$

Phase cub–*A*13

$$L^{0,\mathrm{cub}-A13}_{\mathrm{Mn,Si:\square}} = -142343.62 + 21.892610\ T$$

$$L^{1,\mathrm{cub}-A13}_{\mathrm{Mn,Si:\square}} = 16440.608 - 3.5300332\ T$$

Phase fcc–*A*1

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Mn,Si:\square}} = -95600 + 2.94097\ T$$

$$L^{1,\mathrm{fcc}-A1}_{\mathrm{Mn,Si:\square}} = -7500$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Mn,Si}} = -139817 + 29.86137\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Mn,Si}} = -34917.2 + 3.20488\ T$$

$$L^{2,\mathrm{liquid}}_{\mathrm{Mn,Si}} = 46782.4 - 1.8.1897\ T$$

$$L^{3,\mathrm{liquid}}_{\mathrm{Mn,Si}} = 16168.2$$

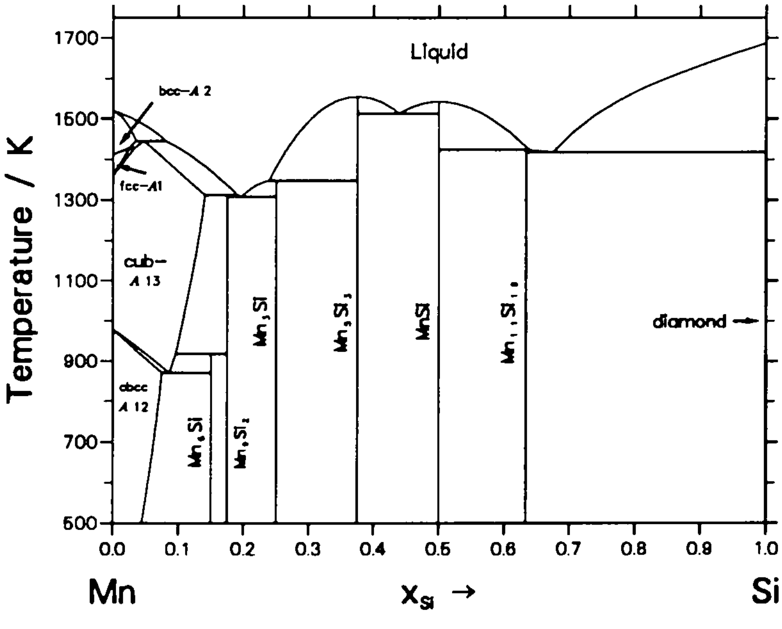


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Si}			T / K
Liquid + bcc–$A2$ ⇌ cub–$A13$	Peritectic	.080	.035	.046	1445.3
bcc–$A2$ + cub–$A13$ ⇌ fcc–$A1$	Peritectic	.024	.024	.033	1426.6
Liquid + cub–$A13$ ⇌ Mn_9Si_2	Peritectic	.191	.140	.175	1312.7
Liquid ⇌ Mn_9Si_2 + Mn_3Si	Eutectic	.197	.175	.250	1309.3
Liquid + Mn_5Si_3 ⇌ Mn_3Si	Peritectic	.239	.375	.250	1348.0
Mn_5Si_3 ⇌ Liquid	Congruent	.375	.375	.....	1556.0
Liquid ⇌ Mn_5Si_3 + MnSi	Eutectic	.439	.375	.500	1513.4
MnSi ⇌ Liquid	Congruent	.500	.500	.....	1544.0
Liquid + MnSi ⇌ $Mn_{11}Si_{19}$	Peritectic	.639	.500	.633	1423.4
Liquid ⇌ diamond + $Mn_{11}Si_{19}$	Eutectic	.674	.633	1.000	1417.1
cub–$A13$ + Mn_9Si_2 ⇌ Mn_6Si	Peritectoid	.096	.170	.150	918.0
cbcc–$A12$ ⇌ cub–$A13$ + Mn_6Si	Eutectoid	.086	.075	.150	870.6

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Mn–Si	α–Mn	α–Mn	$c58$ $I\bar{4}3m$		cbcc–$A12$
	β–Mn	β–Mn	$cP20$ $P4_1323m$		cub–$A13$
	γ–Mn	Cu	$cF4$ $Fm3m$		
	δ–Mn	W	$cI2$ $Im\bar{3}m$		
	(Si)	diamond	$cF8$ $Fd\bar{3}m$	M 8	
	MnSi	FeSi	$cP8$ $P2_13$	Mn 4 Si 4	
	Mn_3Si–α			M_1 4	transformation not considered
	Mn_3Si–β	BiF_3	$cF16$ $Fm\bar{3}m$	M_1 4 M_2 4 M_3 8	
	Mn_5Si_2	Mn_5Si_2	$tP56$ $P4_12_12$		

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
	$Mn_{11}Si_{19}$	$Mn_{11}Si_{19}$	*tP120* $P\bar{4}n2$		$MnSi_{1.75-x}$ in [90Mas]
	$Mn_{44}Si_9$	Mo	*hR53* $R\bar{3}$	M_1 1 M_2 2 M_3 6 M_5 6 M_6 6 Mn_1 2 Mn_2 6 Mn_3 6 Mn_4 6 Mn_5 6	approximated as Mn_6Si
	Mn_5Si_3	Mn_5Si_3	*hP16* $P6_3/mcm$	Mn_1 4 Mn_2 6 Si 6	

System Mn–Ti

Solution Phases:

Liquid, bcc-*A*2, fcc-*A*1, hcp-*A*3, cbcc-*A*12, cub-*A*13

Compounds:

Mn_4Ti, Mn_3Ti, MnTi-α, MnTi-β,Laves-*C*14

Modelling:

Liquid : Substitutional, Redlich–Kister
bcc-*A*2 : Substitutional, Redlich–Kister
cbcc-*A*12 : Substitutional, Redlich–Kister
cub-*A*13 : Substitutional, Redlich–Kister
fcc-*A*1 : Substitutional, Redlich–Kister
hcp-*A*3 : Substitutional, Redlich–Kister
Laves-*C*14 : Sublattice model: $(Mn,Ti)_2(Mn,Ti)$
Mn_4Ti : Stoichiometric, $(Mn)_{0.815}(Ti)_{0.185}$
MnTi-α : Stoichiometric, (Mn)(Ti)
MnTi-β : Stoichiometric, $(Mn)_{0.515}(Ti)_{0.485}$

Assessor and Date:

N. Saunders, 1993

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase bcc–*A*2

$$L^{0,bcc-A2}_{Mn,Ti:\square} = -23200 + 20\ T$$

$$L^{1,bcc-A2}_{Mn,Ti:\square} = -1000$$

Phase cbcc–*A*12

$$L^{0,cbcc-A12}_{Mn,Ti:\square} = -29500 + 20\ T$$

$$L^{1,cbcc-A12}_{Mn,Ti:\square} = -3635 - 5\ T$$

Phase cub–*A*13

$$L^{0,cub-A13}_{Mn,Ti:\square} = -34000 + 20\ T$$

Phase fcc-$A1$

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Mn,Ti:\square}} = -26200 + 20\ T$$

Phase hcp–$A3$

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Mn,Ti:\square}} = 22100$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Mn,Ti}} = -34000 + 21.5\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Mn,Ti}} = 1400$$

Phase Mn$_4$Ti

$$G^{\circ}(T) - 0.815\ H^{\circ,\mathrm{cbcc}-A12,\mathrm{para}}_{\mathrm{Mn}}(298.15\ \mathrm{K}) - 0.185\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \\ -2445.0 - 2.9\ T + 0.815\ \mathrm{GHSER_{Mn}} + 0.185\ \mathrm{GHSER_{Ti}}$$

Phase Mn$_3$Ti

$$G^{\circ}(T) - 3.0\ H^{\circ,\mathrm{cbcc}-A12,\mathrm{para}}_{\mathrm{Mn}}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \\ -18552.0 - 9.12\ T + 3.0\ \mathrm{GHSER_{Mn}} + \mathrm{GHSER_{Ti}}$$

Phase MnTi–α

$$G^{\circ}(T) - H^{\circ,\mathrm{cbcc}-A12,\mathrm{para}}_{\mathrm{Mn}}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \\ -11478.0 + \mathrm{GHSER_{Mn}} + \mathrm{GHSER_{Ti}}$$

Phase MnTi–β

$$G^{\circ}(T) - 0.515\ H^{\circ,\mathrm{cbcc}-A12,\mathrm{para}}_{\mathrm{Mn}}(298.15\ \mathrm{K}) - 0.485\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \\ -5540.0 - 2.29\ T + 0.515\ \mathrm{GHSER_{Mn}} + 0.485\ \mathrm{GHSER_{Ti}}$$

Phase Laves–C14

$$G^{\circ}(T) - 3.0\ H^{\circ,\mathrm{cbcc}-A12,\mathrm{para}}_{\mathrm{Mn}}(298.15\ \mathrm{K}) = \mathrm{G(Mn{:}Mn)} = 3000.0 + 3.0\ \mathrm{GHSER_{Mn}}$$

$$G^{\circ}(T) - 2.0\ H^{\circ,\mathrm{cbcc}-A12,\mathrm{para}}_{\mathrm{Mn}}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Mn{:}Ti)} = \\ -26400.0 + 2.0\ \mathrm{GHSER_{Mn}} + \mathrm{GHSER_{Ti}}$$

$$G^{\circ}(T) - H^{\circ,\mathrm{cbcc}-A12,\mathrm{para}}_{\mathrm{Mn}}(298.15\ \mathrm{K}) - 2.0\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Mn)} = \\ 3000.0 + \mathrm{GHSER_{Mn}} + 2.0\ \mathrm{GHSER_{Ti}}$$

$$G^{\circ}(T) - 3.0\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Ti)} = \\ 15000.0 + 3.0\ \mathrm{GHSER_{Ti}}$$

$$L^{0,\mathrm{Laves}-C14}_{\mathrm{Mn:Mn,Ti}} = L^{0,\mathrm{Laves}-C14}_{\mathrm{Ti:Mn,Ti}} = 15000$$

$$L^{0,\mathrm{Laves}-C14}_{\mathrm{Mn,Ti:Mn}} = L^{0,\mathrm{Laves}-C14}_{\mathrm{Mn,Ti:Ti}} = 27000$$

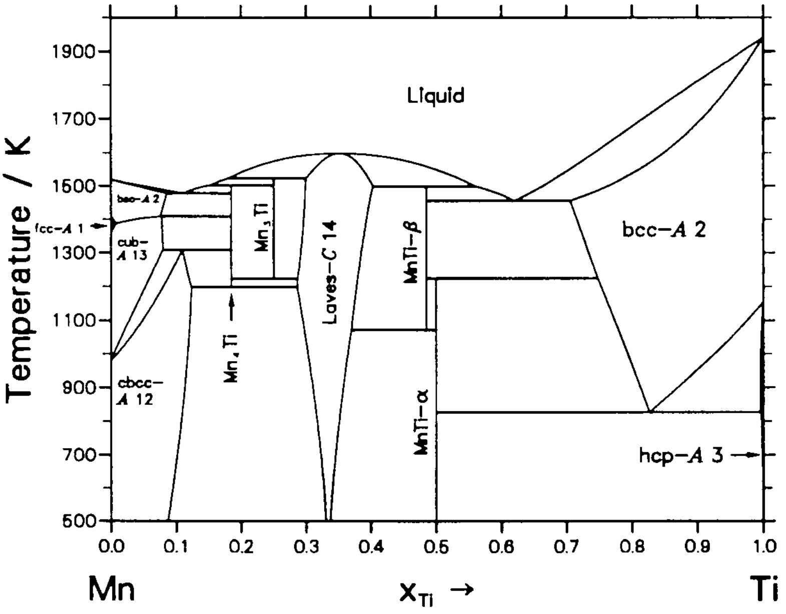


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Ti}			T / K
Liquid ⇌ bcc-$A2$ + Mn_4Ti	Eutectic	.111	.086	.185	1478.0
Liquid + Mn_3Ti ⇌ Mn_4Ti	Peritectic	.153	.250	.185	1502.8
Liquid + Laves-$C14$ ⇌ Mn_3Ti	Peritectic	.180	.300	.250	1523.5
Mn_3Ti ⇌ Mn_4Ti+ Laves-$C14$	Eutectoid	.250	.185	.287	1222.3
Mn_4Ti ⇌ cbcc-$A12$ + Laves-$C14$	Eutectoid	.185	.124	.286	1198.4
cbcc-$A12$ + Mn_4Ti ⇌ cub-$A13$	Peritectoid	.080	.185	.110	1309.3
bcc-$A2$ + Mn_4Ti ⇌ cub-$A13$	Peritectoid	.076	.185	.078	1408.6
bcc-$A2$ ⇌ fcc-$A1$ + cub-$A13$	Eutectoid	.008	.005	.009	1387.6
Laves-$C14$ ⇌ Liquid	Congruent	.344	.344	....	1598.0
Liquid + Laves-$C14$ ⇌ MnTi-β	Peritectic	.560	.485	.403	1500.2
MnTi-β ⇌ Laves-$C14$ + MnTi-α	Eutectoid	.485	.369	.500	1071.3
MnTi-β + bcc-$A2$ ⇌ MnTi-α	Peritectoid	.485	.748	.500	1224.0
bcc-$A2$ ⇌ MnTi-α + hcp-$A3$	Eutectoid	.827	.500	.996	827.6
Liquid ⇌ MnTi-β + bcc-$A2$	Eutectic	.620	.485	.706	1455.5

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattice	Comments
Mn–Ti	α–Mn	α–Mn	$c584$ $I\bar{4}3m$		cbcc–$A12$
	β-Mn	β-Mn	$cP20$ $P4_1323m$		cub–$A13$
	γ–Mn	Cu	$cF4$ $Fm3m$	M 4	fcc–$A1$
	δ–Mn	W	$cI2$ $Im\bar{3}m$	M 2	bcc–$A2$
	(Ti)	Mg	$hP2$ $P6_3/mmc$	M 2	
	(Ti)	W	$cI2$ $Im\bar{3}m$	M 2	
	MnTi–α		$t*58$		
	MnTi–β				
	Mn_3Ti				
	Mn_2Ti	$MgZn_2$	$hP12$ $P6_3/mmc$	Mn_1 2 Mn_2 6 Ti 4	Laves-$C14$
	Mn_4Ti	$\sim\delta$(Mo,Ni)	$hR53$ $R\bar{3}$		

System Mn–Zr

Solution Phases:

Liquid, bcc-$A2$, cbcc-$A12$, cub-$A13$, fcc-$A1$, hcp-$A3$

Compound:

Mn_2Zr

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-$A2$: Substitutional, Redlich-Kister
cbcc-$A12$: Substitutional, Redlich-Kister
cub-$A13$: Substitutional, Redlich-Kister
fcc-$A1$: Substitutional, Redlich-Kister
hcp-$A3$: Substitutional, Redlich-Kister
Mn_2Zr : Stoichiometric, $(Mn)_2(Zr)$

Assessor and Date:

K. Hack, GTT, Germany (1997).

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase Mn_2Zr

$$G^\circ(T) - 3.0\ H_{\mathrm{Mn}}^{\mathrm{o,cbcc-}A12\mathrm{,para}}(298.15\ \mathrm{K}) = \mathrm{G(Mn{:}Mn)} =$$

$$298.15 < T < 1519.00 : - 021345.84 + 390.177\ T - 70.3746\ T\cdot \ln T - 0.02204304\ T^2 + 209481.3\ T^{-1}$$

$$1519.00 < T < 2000.00 : - 83200.23 + 936.7944\ T - 144\ T\cdot \ln T + 4.970541\mathrm{E}{+}30\ T^{-9}$$

$$G^\circ(T) - 2.0\ H_{\mathrm{Mn}}^{\mathrm{o,cbcc-}A12\mathrm{,para}}(298.15\ \mathrm{K}) - H_{\mathrm{Zr}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \mathrm{G(Mn{:}Zr)} =$$

$$298.15 < T < 1900.00 : - 79282.375 + 386.94271\ T -71.0782\ T\cdot \ln T - 0.01907327\ T^2 + 174625.2\ T^{-1}$$

$$1900.00 < T < 2000.00 : - 119446.65 + 750.75589\ T - 120.1618\ T\cdot \ln T - 0.00437791\ T^2 + 34971\ T^{-1} + 3.313694\mathrm{E}{+}30\ T^{-9}$$

$G^{\circ}(T) - H_{\mathrm{Mn}}^{\mathrm{o,cbcc}-A12,\mathrm{para}}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Zr}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Zr{:}Mn)} =$

$298.15 < T < 1519.00 : - 8770.8146 + 381.3571\ T - 71.7818\ T \cdot \ln T - 0.0161035\ T^{2} + 139769.1\ T^{-1}$

$1519.00 < T < 2000.00 : - 29388.945 + 563.56289\ T - 96.3236\ T \cdot \ln T - 0.00875582\ T^{2} + 69942\ T^{-1} + 1.656847\mathrm{E}{+}30\ T^{-9}$

$G^{\circ}(T) - 3.0\ H_{\mathrm{Zr}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Zr{:}Zr)} =$

$298.15 < T < 2128.00 : - 8482.785 + 376.94715\ T - 72.4854\ T \cdot \ln T - 0.01313373\ T^{2} + 104913\ T^{-1}$

$2128.00 < T < 6000.00 : - 63257.763 + 788.17255\ T - 126.432\ T \cdot \ln T -4.028685\mathrm{E}{+}31\ T^{-9}$

$L_{\mathrm{Mn,Zr:Mn}}^{0,\mathrm{Mn_2Zr}} = 18442.56 + 14.090471\ T$

$L_{\mathrm{Zr:Mn,Zr}}^{0,\mathrm{Mn_2Zr}} = 18442.56 + 14.090471\ T$

$L_{\mathrm{Mn:Mn,Zr}}^{0,\mathrm{Mn_2Zr}} = 1066.4675 + 10.504933\ T$

$L_{\mathrm{Mn,Zr:Zr}}^{0,\mathrm{Mn_2Zr}} = 1066.4675 + 10.504933\ T$

Phase bcc–*A*2

$L_{\mathrm{Mn,Zr:\square}}^{0,\mathrm{bcc}-A2} = - 2135.3475 - 0.13258\ T$

$L_{\mathrm{Mn,Zr:\square}}^{1,\mathrm{bcc}-A2} = - 4084$

Phase cbcc–*A*12

$L_{\mathrm{Mn,Zr:\square}}^{0,\mathrm{cbcc}-A12} = 20000$

Phase cub–*A*13

$L_{\mathrm{Mn,Zr:\square}}^{0,\mathrm{cub}-A13} = 24000$

Phase fcc–*A*1

$L_{\mathrm{Mn,Zr:\square}}^{0,\mathrm{fcc}-A1} = 20000$

Phase hcp–*A*3

$L_{\mathrm{Mn,Zr:\square}}^{0,\mathrm{hcp}-A3} = 25000$

Phase liquid

$L_{\mathrm{Mn,Zr}}^{0,\mathrm{liquid}} = - 35187.553 + 2.6983563\ T$

$L_{\mathrm{Mn,Zr}}^{1,\mathrm{liquid}} = - 1305.986$

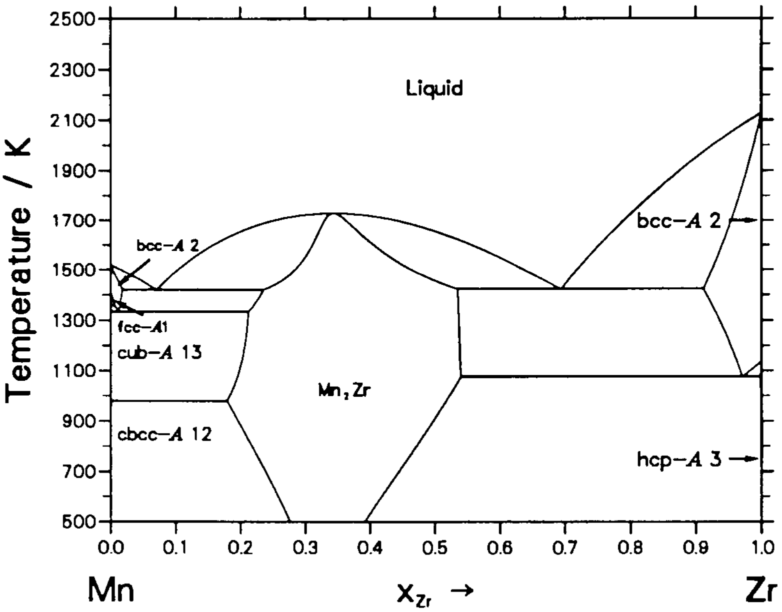


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Zr}			T / K
Liquid $\rightleftharpoons$ bcc–$A2$ + Mn$_2$Zr	Eutectic	.071	.018	.236	1421.9
bcc–$A2$ $\rightleftharpoons$ + cub–$A13$ + Mn$_2$Zr	Eutectoid	.012	.000	.213	1334.5
fcc–$A1$ $\rightleftharpoons$ bcc–$A2$ + cub–$A13$	Metatectic	.0003	.0002	.0062	1359.1
cub–$A13$ $\rightleftharpoons$ cbcc–$A12$ + Mn$_2$Zr	Degenerate	.000	.000	.179	980.1
Liquid $\rightleftharpoons$ Mn$_2$Zr + bcc–$A2$	Eutectic	.694	.535	.911	1424.1
bcc–$A2$ $\rightleftharpoons$ Mn$_2$Zr + hcp–$A3$	Eutectoid	.971	.540	.998	1075.4
Mn$_2$Zr $\rightleftharpoons$ Liquid	Congruent	.345	.345	.....	1730.0

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Mn-Zr	α-Mn	α-Mn	$c58$ $I\bar{4}3m$		cbcc-$A12$
	β-Mn	β-Mn	$cP20$ $P4_1323m$		cub-$A13$
	γ-Mn	Cu	$cF4$ $Fm3m$		
	δ-Mn	W	$cI2$ $Im\bar{3}m$		
	(Zr)	Mg	$hP2$ $P6_3/mmc$	M 2	
	(Zr)	W	$cI2$ $Im\bar{3}m$	M 4	
	Mn_2Zr	$MgZn_2$	$hP12$ $P6_3/mmc$	Mn 2 Mn 6 Zr 4	Laves-$C14$

System Mo–Ti

Solution Phases:

(stable)	Liquid, bcc-$A2$, hcp-$A3$
(metastable)	bcc-$B2$, fcc-$A1$

Compounds:

(metastable)	AlM-$D0_{19}$, AlM-$D0_{22}$, AlTi-$L1_0$

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-$A2$: Substitutional, Redlich-Kister
bcc-$B2$: Sublattice model, $(\mathrm{Mo,Ti})_{0.5}(\mathrm{Mo,Ti})_{0.5}(\square)_3$
The thermodynamic description of the bcc-B2 takes into account the ordering reaction bcc-$A2 \rightleftharpoons$ bcc-$B2$.
Two descriptions are given: one using equations 23 and 27, the other using equations 23 and 28.
For the latter, the parameters are given in a frame.
fcc-$A1$: Substitutional, Redlich-Kister
hcp-$A3$: Substitutional, Redlich-Kister
AlM-$D0_{19}$: Sublattice model, $(\mathrm{Mo,Ti})(\mathrm{Mo,Ti})_3$
AlM-$D0_{22}$: Sublattice model, $(\mathrm{Mo,Ti})_3(\mathrm{Mo,Ti})$
AlTi-$L1_0$: Sublattice model, $(\mathrm{Mo,Ti})(\mathrm{Mo,Ti})$

Assessor and Date:

N. Saunders, 1995

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Mo,Ti}} = -9000 + 2\ T$$

Phase fcc-$A1$

$$L^{0,\mathrm{fcc-}A1}_{\mathrm{Mo,Ti:\square}} = 16500$$

Phase hcp–$A3$

$L^{0,\text{hcp}-A3}_{\text{Mo,Ti}:\square} = 22760 - 6\ T$

Phase bcc–$A2$

$L^{0,\text{bcc}-A2}_{\text{Mo,Ti}:\square} = 2000$

$L^{1,\text{bcc}-A2}_{\text{Mo,Ti}:\square} = -\ 2000$

Phase bcc–$B2$

$G^{\circ}(T) - H^{\circ,\text{bcc}-A2}_{\text{Mo}}(298.15\ \text{K}) = \text{G(Mo:Mo)} = 0.0$
$G^{\circ}(T) - 0.5\ H^{\circ,\text{bcc}-A2}_{\text{Mo}}(298.15\ \text{K}) - 0.5\ H^{\circ,\text{hcp}-A3}_{\text{Ti}}(298.15\ \text{K}) = \text{G(Mo:Ti)} = 5000$
$G^{\circ}(T) - 0.5\ H^{\circ,\text{bcc}-A2}_{\text{Mo}}(298.15\ \text{K}) - 0.5\ H^{\circ,\text{hcp}-A3}_{\text{Ti}}(298.15\ \text{K}) = \text{G(Ti:Mo)} = 5000$
$G^{\circ}(T) - H^{\circ,\text{hcp}-A3}_{\text{Ti}}(298.15\ \text{K}) = \text{G(Ti:Ti)} = 0$
$L^{0,\text{bcc}-B2}_{\text{Mo,Ti:Mo}:\square} = L^{0,\text{bcc}-B2}_{\text{Mo,Ti:Ti}:\square} = -\ 5000$

$L^{0,\text{bcc}-B2}_{\text{Mo:Mo,Ti}:\square} = L^{0,\text{bcc}-B2}_{\text{Ti:Mo,Ti}:\square} = -\ 5000$

Phase bcc–$B2$

$G^{*}_{\text{Mo:Ti}:\square} = 5000$

$G^{\circ}(T) - H^{\circ,\text{bcc}-A2}_{\text{Mo}}(298.15\ \text{K}) = \text{G(Mo:Mo:}\square\text{)} = 0.0$

$G^{\circ}(T) - 0.5\ H^{\circ,\text{bcc}-A2}_{\text{Mo}}(298.15\ \text{K}) - 0.5\ H^{\circ,\text{hcp}-A3}_{\text{Ti}}(298.15\ \text{K}) = \text{G(Mo:Ti:}\square\text{)} = 2.0\ \text{G}^{*}_{\text{Mo:Ti}:\square}$

$\text{G}^{\circ}(T) - 0.5\ H^{\circ,\text{bcc}-A2}_{\text{Mo}}(298.15\ \text{K}) - 0.5\ H^{\circ,\text{hcp}-A3}_{\text{Ti}}(298.15\ \text{K}) = \text{G(Ti:Mo:}\square\text{)} = 2.0\ G^{*}_{\text{Mo:Ti}:\square}$

$G^{\circ}(T) - H^{\circ,\text{hcp}-A3}_{\text{Ti}}(298.15\ \text{K}) = \text{G(Ti:Ti:}\square\text{)} = 0.0$

Phase bcc–$A2$

$L^{0,\text{bcc}-A2}_{\text{Mo,Ti}:\square} = 2000$

$L^{1,\text{bcc}-A2}_{\text{Mo,Ti}:\square} = -\ 2000$

Phase AlM-$D0_{19}$

$G^\circ(T) - 4.0\ H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Mo}}(298.15\ \mathrm{K}) = \mathrm{G(Mo{:}Mo)} = 4.0\ \mathrm{GHCP_{Mo}}$
$G^\circ(T) - 3.0\ H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Mo}}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Mo{:}Ti)} =$
$17072 - 4.5\ T + 3.0\ \mathrm{GHCP_{Mo}} + \mathrm{GHSER_{Ti}}$
$G^\circ(T) - H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Mo}}(298.15\ \mathrm{K}) - 3.0\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Mo)} =$
$17072 - 4.5\ T + \mathrm{GHCP_{Mo}} + 3.0\ \mathrm{GHSER_{Ti}}$
$G^\circ(T) - 4.0\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Ti)} = 4.0 + 4.0\ \mathrm{GHSER_{Ti}}$

Phase AlM-$D0_{22}$

$G^\circ(T) - 4.0\ H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Mo}}(298.15\ \mathrm{K}) = \mathrm{G(Mo{:}Mo)} = 4.0\ \mathrm{GFCC_{Mo}}$
$G^\circ(T) - 3.0\ H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Mo}}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Mo{:}Ti)} =$
$3.0\ \mathrm{GFCC_{Mo}} + \mathrm{GFCC_{Ti}}$
$G^\circ(T) - H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Mo}}(298.15\ \mathrm{K}) - 3.0\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Mo)} =$
$\mathrm{GFCC_{Mo}} + 3.0\ \mathrm{GFCC_{Ti}}$
$G^\circ(T) - 4.0\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Ti)} = 4.0\ \mathrm{GFCC_{Ti}}$

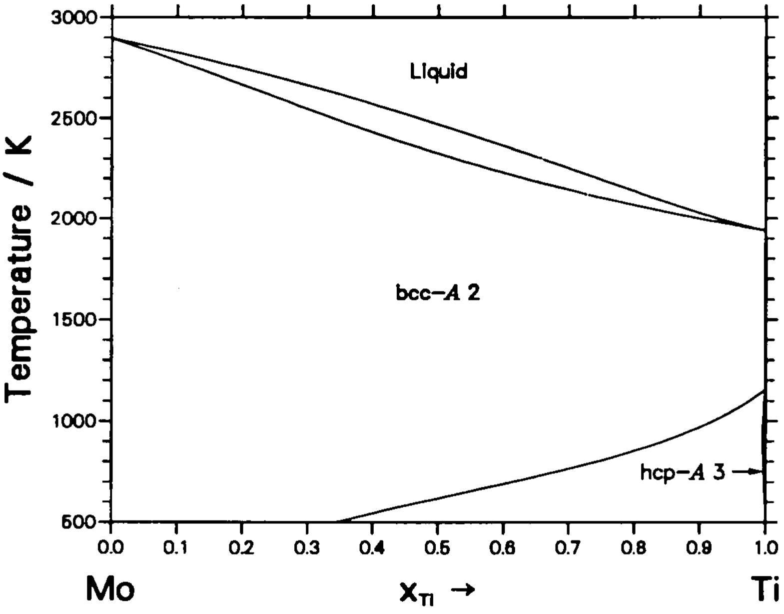
Phase AlTi–$L1_0$

$G^\circ(T) - 2.0\ H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Mo}}(298.15\ \mathrm{K}) = \mathrm{G(Mo{:}Mo)} = 2.0\ \mathrm{GFCC_{Mo}}$
$G^\circ(T) - H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Mo}}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Mo{:}Ti)} =$
$8250 + \mathrm{GFCC_{Mo}} + \mathrm{GFCC_{Ti}}$
$G^\circ(T) - H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Mo}}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Mo)} =$
$8250 + \mathrm{GFCC_{Mo}} + \mathrm{GFCC_{Ti}}$
$G^\circ(T) - 2.0\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Ti)} = 2.0\ \mathrm{GFCC_{Ti}}$
$L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Mo,Ti:Mo}} = L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Mo:Mo,Ti}} = 8250$

$L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Mo,Ti:Ti}} = L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Ti:Mo,Ti}} = 8250$

Table I – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Comments
Mo–Ti	(Mo)	W	*cI2* $Im\bar{3}m$	
	(Ti)	Mg	*hP2* $P6_3/mmc$	
	(Ti)	W	*cI2* $Im\bar{3}m$	


Temperature / K
3000
2500
2000
1500
1000
500
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
Mo
x_{Ti} →
Ti
Liquid
bcc-A 2
hcp-A 3

System N–Ti

Solution Phases:

Liquid, hcp-*A*3, bcc-*A*2, fcc-*A*1 (Ti_xN_{1-x})

Compound:

Ti_2N, Ti_3N_2, Ti_4N_3

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-*A*2 : Sub-lattice, (Ti)(N,□)
hcp-*A*3 : Sub-lattice, (Ti)(N,□)
fcc-*A*1 : Sub-lattice, (Ti)(N,□)
Ti_2N : Stoichiometric, $(Ti)_2(N)$
Ti_3N_2 : Stoichiometric, $(Ti)_{0.29}(N)_{0.71}$
Ti_4N_3 : Stoichiometric, $(Ti)_{0.315}(N)_{0.685}$

Assessor and Date:

K. Zeng and R. Schmid-Fetzer, Univ. Clausthal, Germany, 1997

Comments:

The value of $GHSER_{TiN}$ is taken from S. Jonsson, Thesis, Royal Institute of Technology, Stockholm, Sweden (1993)

Thermodynamic properties of the solution and compound phases ($J.mol^{-1}$)

Phase fcc–*A*1

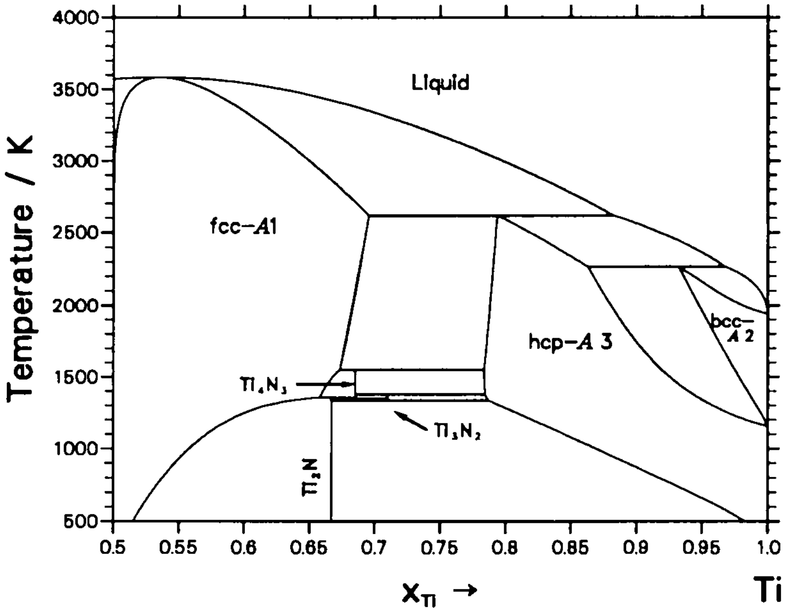
$$G^\circ(T) - H^{\circ,\mathrm{gas}}_{0.5\mathrm{N}_2}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{GHSER}_{\mathrm{TiN}} = - 357905.0 + 330.498\ T - 52.4587\ T\cdot \ln T - 9.28\mathrm{E}{-}04\ T^2 - 2.41\mathrm{E}{+}09\ T^{-3} + 871000.0\ T^{-1}$$

$$L^{0,\mathrm{fcc}-\mathrm{A1}}_{\mathrm{Ti:C}\square} = - 42704.41$$

$$L^{1,\mathrm{fcc}-\mathrm{A1}}_{\mathrm{Ti:C}\square} = - 13989.34$$

Phase Ti_4N_3

$$G^\circ(T) - 0.315\ H^{\circ,\mathrm{gas}}_{0.5\mathrm{N}_2}(298.15\ \mathrm{K}) - 0.685\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = - 5956.8633 - 3.2749\ T + 0.37\ \mathrm{GHSER}_{\mathrm{Ti}} + 0.315\ \mathrm{GHSER}_{\mathrm{TiN}}$$



Phase bcc–$A2$

$$G^{\circ}(T) - 3.0\ H^{\circ,\mathrm{gas}}_{0.5\mathrm{N}_2}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}N)} =$$
$$2604201.62 + 118.04\ T + \mathrm{GHSER}_{\mathrm{TiN}} + 2.0\ \mathrm{GHSER}_{\mathrm{N}}$$
$$L^{0,\mathrm{bcc}-\mathrm{A2}}_{\mathrm{Ti:N,\square}} = -3215338.17$$

Phase hcp–$A3$

$$G^{\circ}(T) - 0.5\ H^{\circ,\mathrm{gas}}_{0.5\mathrm{N}_2}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}N)} =$$
$$-6046.53 - 2.653\ T + 0.5\ \mathrm{GHSER}_{\mathrm{TiN}} + 0.5\ \mathrm{GHSER}_{\mathrm{Ti}}$$
$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Ti:\square}} = -13501$$

Phase Ti_2N

$$G^{\circ}(T) - H^{\circ,\mathrm{gas}}_{0.5\mathrm{N}_2}(298.15\ \mathrm{K}) - 2.0\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) =$$
$$-67116 + 26.5395533\ T + \mathrm{GHSER}_{\mathrm{Ti}} + \mathrm{GHSER}_{\mathrm{TiN}}$$

Phase Ti_3N_2

$$G^{\circ}(T) - 0.29\ H^{\circ,\mathrm{gas}}_{0.5\mathrm{N}_2}(298.15\ \mathrm{K}) - 0.71\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) =$$
$$-8190.34 - 1.54816\ T + 0.42\ \mathrm{GHSER}_{\mathrm{Ti}} + 0.29\ \mathrm{GHSER}_{\mathrm{TiN}}$$

Phase liquid

$L^{0,\mathrm{liquid}}_{\mathrm{N,Ti}}$ = - 376354.145

$L^{1,\mathrm{liquid}}_{\mathrm{N,Ti}}$ = - 98242.2945

Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Ti}			T / K
fcc-$A1$ + hcp-$A3$ ⇌ Ti_4N_3	Peritectoid	.673	.784	.685	1551.1
Ti_4N_3 + hcp-$A3$ ⇌ Ti_3N_2	Peritectoid	.685	.784	.710	1376.8
Ti_3N_2 ⇌ Ti_2N + hcp-$A3$	Eutectoid	.710	.667	.787	1336.2
Ti_4N_3 ⇌ Ti_2N + Ti_3N_2	Eutectoid	.685	.667	.710	1348.5
fcc-$A1^*$ + Ti_3N_2 ⇌ Ti_2N	Peritectoid	.658	.685	.667	1354.8
Liquid + fcc-$A1^*$ ⇌ hcp-$A3$	Peritectic	.882	.695	.793	2618.0
Liquid + hcp-$A3$ ⇌ bcc-$A2$	Peritectic	.967	.863	.932	2268.6
fcc-$A1$ ⇌ Liquid	Congruent	.533	.541	....	3585.0

* fcc-$A1$ ≡ Ti_xN_{1-x}

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattice	Comments
N-Ti	$0.5N_2$	gas			
	(Ti)	Mg	$hP2$ $P6_3/mmc$	M 2	
	(Ti)	W	$cI2$ $Im\bar{3}m$	M 2	
	TiN	ClNa	$cF8$ $Fm\bar{3}m$	N 4 Ti 4	modelled as fcc-$A1$
	Ti_2N	anti-O_2Ti (rutile)	$tP6$ $P4_2/mnm$	N 2 Ti 4	
	Ti_4N_3	Ti_7S_{12}	$hR8$ $R\bar{3}m$	N_1 3 N_2 3 N_3 6 Ti_1 6 Ti_2 6	
	Ti_3N_2				not indicated in [91Vil] nor in [90Mas]

System Nb–Ti

Solution Phases:

(stable)	Liquid, bcc-*A*2, hcp-*A*3
(metastable)	bcc-*B*2, fcc-*A*1

Compounds:

(metastable)	AlM-*D*0_{19}, AlM-*D*0_{22}, AlTi-*L*1_0, Cr_3Si-*A*15

Modelling:

Liquid : Substitutional, Redlich-Kister

bcc-*A*2 : Substitutional, Redlich-Kister

bcc-*B*2 : Sublattice model, $(Nb,Ti)_{0.5}(Nb,Ti)_{0.5}(\square)_3$
The thermodynamic description of the bcc-B2 takes into account the ordering reaction bcc-*A*2 $\rightleftharpoons$ bcc-*B*2. Two descriptions are given: one using equations 23 and 27, the other using equations 23 and 28. For the latter, the parameters are given in a frame.

fcc-*A*1 : Substitutional, Redlich-Kister

hcp-*A*3 : Substitutional, Redlich-Kister

AlM-*D*0_{19} : Sublattice model, $(Nb,Ti)(Nb,Ti)_3$

AlM-*D*0_{22} : Sublattice model, $(Ti)_3(Nb,Ti)$

AlTi-*L*1_0 : Sublattice model, $(Nb,Ti)(Nb,Ti)$

Cr_3Si-*A*15 : Sublattice model, $(Nb,Ti)_3(Nb)$

Assessor and Date:

N. Saunders, 1995

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Nb,Ti}} = 8500$$

Phase fcc–*A*1

$L^{0,\mathrm{fcc}-A1}_{\mathrm{Nb,Ti:\square}} = 13600$

$L^{1,\mathrm{fcc}-A1}_{\mathrm{Nb,Ti:\square}} = 1\mathrm{E}\text{-}04$

$L^{2,\mathrm{fcc}-A1}_{\mathrm{Nb,Ti:\square}} = 2500$

Phase hcp–*A*3

$L^{0,\mathrm{hcp}-A3}_{\mathrm{Nb,Ti:\square}} = 13600$

$L^{1,\mathrm{hcp}-A3}_{\mathrm{Nb,Ti:\square}} = 1\mathrm{E}\text{-}04$

$L^{2,\mathrm{hcp}-A3}_{\mathrm{Nb,Ti:\square}} = 2500$

Phase $\mathrm{Cr_3Si}$–*A*15

$$G^{\circ}(T) - 4.0\ H^{\mathrm{o,bcc}-A2}_{\mathrm{Nb}}(298.15\ \mathrm{K}) = \mathrm{G(Nb{:}Nb)} = \\ 20000 + 10\ T + 4.0\ \mathrm{GFCC_{Nb}}$$

$$G^{\circ}(T) - H^{\mathrm{o,bcc}-A2}_{\mathrm{Nb}}(298.15\ \mathrm{K}) - 3.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Nb)} = \\ 20000 + 10\ T + 3.0\ \mathrm{GFCC_{Nb}} + \mathrm{GFCC_{Ti}}$$

Phase bcc–*A*2

$L^{0,\mathrm{bcc}-A2}_{\mathrm{Nb,Ti:\square}} = 14000$

$L^{1,\mathrm{bcc}-A2}_{\mathrm{Nb,Ti:\square}} = 1.0\mathrm{E}\text{-}4$

$L^{2,\mathrm{bcc}-A2}_{\mathrm{Nb,Ti:\square}} = 2500$

Phase bcc–*B*2

$$G^{*}_{\mathrm{Nb:Ti:\square}} = 5500$$

$$G^{\circ}(T) - H^{\mathrm{o,bcc}-A2}_{\mathrm{Nb}}(298.15\ \mathrm{K}) = \mathrm{G(Nb{:}Nb\square)} = 0.0$$

$$G^{\circ}(T) - 0.5\ H^{\mathrm{o,bcc}-A2}_{\mathrm{Nb}}(298.15\ \mathrm{K}) - 0.5\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \\ \mathrm{G(Nb{:}Ti{:}\square)} = G^{*}_{\mathrm{Nb:Ti:\square}}$$

$$G^{\circ}(T) - 0.5\ H^{\mathrm{o,bcc}-A2}_{\mathrm{Nb}}(298.15\ \mathrm{K}) - 0.5\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \\ \mathrm{G(Ti{:}Nb{:}\square)} = G^{*}_{\mathrm{Nb:Ti:\square}}$$

$$G^{\circ}(T) - H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Ti\square)} = 0.0$$

$L^{0,\mathrm{bcc}-B2}_{\mathrm{Nb,Ti:Nb:\square}} = L^{0,\mathrm{bcc}-B2}_{\mathrm{Nb,Ti:Ti:\square}} = -5500$

$L^{0,\mathrm{bcc}-B2}_{\mathrm{Nb:Nb,Ti:\square}} = L^{0,\mathrm{bcc}-B2}_{\mathrm{Ti:Nb,Ti:\square}} = -5500$

Phase bcc–$B2$

$G^{\bullet}_{\mathrm{Nb:Ti:\square}} = 5500$

$G^{\circ}(T) - H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Nb}}(298.15\ \mathrm{K}) = \mathrm{G(Nb:Nb:\square)} = 0.0$

$G^{\circ}(T) - 0.5\ H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Nb}}(298.15\ \mathrm{K}) - 0.5\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Nb:Ti:\square)} = 2.0\ G^{\bullet}_{\mathrm{Nb:Ti:\square}}$

$G^{\circ}(T) - 0.5\ H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Nb}}(298.15\ \mathrm{K}) - 0.5\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti:Nb:\square)} = 2.0\ G^{\bullet}_{\mathrm{Nb:Ti:\square}}$

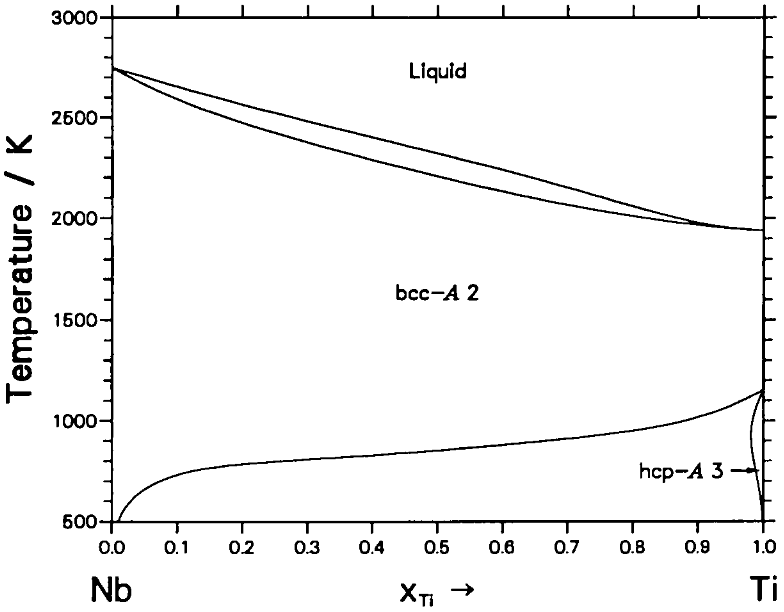
$G^{\circ}(T) - H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti:Ti:\square)} = 0.0$

Phase bcc–$A2$

$L^{0,\mathrm{bcc}-A2}_{\mathrm{Nb,Ti:\square}} = 14000$

$L^{1,\mathrm{bcc}-A2}_{\mathrm{Nb,Ti:\square}} = 1.0\mathrm{E}{-4}$

$L^{2,\mathrm{bcc}-A2}_{\mathrm{Nb,Ti:\square}} = 2500$



Phase AlM-$D0_{19}$

$G^{\circ}(T) - 4.0\ H^{\mathrm{o,bcc-}A2}_{\mathrm{Nb}}(298.15\ \mathrm{K}) = \mathrm{G(Nb:Nb)} = 4.0\ \ \mathrm{GHCP_{Nb}}$

$G^{\circ}(T) - 3.0\ H^{\mathrm{o,bcc-}A2}_{\mathrm{Nb}}(298.15\ \mathrm{K}) -\ H^{\mathrm{o,hcp-}A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Nb:Ti)} =$
$10668 + 3.0\ \ \mathrm{GHCP_{Nb}} + \mathrm{GHSER_{Ti}}$

$G^{\circ}(T) - H^{\mathrm{o,bcc-}A2}_{\mathrm{Nb}}(298.15\ \mathrm{K}) - 3.0\ \ H^{\mathrm{o,hcp-}A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti:Nb)} =$
$10668 + \mathrm{GHCP_{Nb}} + 3.0\ \ \mathrm{GHSER_{Ti}}$

$G^{\circ}(T) - 4.0\ \ H^{\mathrm{o,hcp-}A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti:Ti)} = 4.0 + 4.0\ \ \mathrm{GHSER_{Ti}}$

$L^{0,\mathrm{AlM-}D0_{19}}_{\mathrm{Nb,Ti:Nb}} = 30248$

$L^{1,\mathrm{AlM-}D0_{19}}_{\mathrm{Nb,Ti:Nb}} = 4220$

$L^{2,\mathrm{AlM-}D0_{19}}_{\mathrm{Nb,Ti:Nb}} = 3164$

$L^{0,\mathrm{AlM-}D0_{19}}_{\mathrm{Nb,Ti:Ti}} = 30248$

$L^{1,\mathrm{AlM-}D0_{19}}_{\mathrm{Nb,Ti:Ti}} = -\ 4220$

$L^{2,\mathrm{AlM-}D0_{19}}_{\mathrm{Nb,Ti:Ti}} = 3164$

$L^{0,\mathrm{AlM-}D0_{19}}_{\mathrm{Nb:Nb,Ti}} = 4924$

$L^{1,\mathrm{AlM-}D0_{19}}_{\mathrm{Nb:Nb,Ti}} = 468$

$L^{2,\mathrm{AlM-}D0_{19}}_{\mathrm{Nb:Nb,Ti}} = 40$

$L^{0,\mathrm{AlM-}D0_{19}}_{\mathrm{Ti:Nb,Ti}} = 4924$

$L^{1,\mathrm{AlM-}D0_{19}}_{\mathrm{Ti:Nb,Ti}} = -\ 468$

$L^{2,\mathrm{AlM-}D0_{19}}_{\mathrm{Ti:Nb,Ti}} = 40$

Phase AlM-$D0_{22}$

$G^{\circ}(T) - H^{\mathrm{o,bcc-}A2}_{\mathrm{Nb}}(298.15\ \mathrm{K}) - 3.0\ \ H^{\mathrm{o,hcp-}A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti:Nb)} =$
$\mathrm{GFCC_{Nb}} + 3.0\ \ \mathrm{GFCC_{Ti}}$

$G^{\circ}(T) - 4.0\ \ H^{\mathrm{o,hcp-}A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti:Ti)} = 4.0\ \ \mathrm{GFCC_{Ti}}$

Phase AlTi-$L1_0$

$G^{\circ}(T) - 2.0\ \ H^{\mathrm{o,bcc-}A2}_{\mathrm{Nb}}(298.15\ \mathrm{K}) = \mathrm{G(Nb:Nb)} = 2.0\ \ \mathrm{GFCC_{Nb}}$

$G^{\circ}(T) - H^{\mathrm{o,bcc-}A2}_{\mathrm{Nb}}(298.15\ \mathrm{K}) -\ H^{\mathrm{o,hcp-}A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Nb:Ti)} =$
$13600 + \mathrm{GFCC_{Nb}} + \mathrm{GFCC_{Ti}}$

$$G^\circ(T) - H_{\mathrm{Nb}}^{\mathrm{o,bcc-}A2}(298.15\ \mathrm{K}) - H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Nb)} = 6800 + \mathrm{GFCC_{Nb}} + \mathrm{GFCC_{Ti}}$$

$$G^\circ(T) - 2.0\ H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Ti)} = 2.0\ \ \mathrm{GFCC_{Ti}}$$

$$L_{\mathrm{Nb,Ti:Nb}}^{0,\mathrm{AlTi-}L1_0} = 7738$$

$$L_{\mathrm{Nb,Ti:Nb}}^{1,\mathrm{AlTi-}L1_0} = 1250$$

$$L_{\mathrm{Nb,Ti:Nb}}^{2,\mathrm{AlTi-}L1_0} = 312$$

$$L_{\mathrm{Nb,Ti:Ti}}^{0,\mathrm{AlTi-}L1_0} = 7738$$

$$L_{\mathrm{Nb,Ti:Ti}}^{1,\mathrm{AlTi-}L1_0} = -\ 1250$$

$$L_{\mathrm{Nb,Ti:Ti}}^{2,\mathrm{AlTi-}L1_0} = 312$$

$$L_{\mathrm{Nb:Nb,Ti}}^{0,\mathrm{AlTi-}L1_0} = 7738$$

$$L_{\mathrm{Nb:Nb,Ti}}^{1,\mathrm{AlTi-}L1_0} = 1250$$

$$L_{\mathrm{Nb:Nb,Ti}}^{2,\mathrm{AlTi-}L1_0} = 312$$

$$L_{\mathrm{Ti:Nb,Ti}}^{0,\mathrm{AlTi-}L1_0} = 7738$$

$$L_{\mathrm{Ti:Nb,Ti}}^{1,\mathrm{AlTi-}L1_0} = -\ 1250$$

$$L_{\mathrm{Ti:Nb,Ti}}^{2,\mathrm{AlTi-}L1_0} = 312$$

$$L_{\mathrm{Nb,Ti:Nb,Ti}}^{0,\mathrm{AlTi-}L1_0} = -\ 7500$$

Table I – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Comments
Nb-Ti	(Nb)	W	*cI2* $Im\bar{3}m$	
	(Ti)	Mg	*hP2* $P6_3/mmc$	
	(Ti)	W	*cI2* $Im\bar{3}m$	

System Ni–V

Solution Phases:

Liquid, bcc–$A2$, fcc–$A1$, σ

Compounds:

Ni_2V, Ni_3V, Ni_2V_7

Modelling:

Liquid : Substitutional, Redlich–Kister
bcc–$A2$: Substitutional, Redlich–Kister
fcc–$A1$: Substitutional, Redlich–Kister
Ni_2V : Stoichiometric, $(Ni)_2(V)$
Ni_3V : Stoichiometric, $(Ni)_3(V)$
Ni_2V_7 : Stoichiometric, $(Ni)_2(V)_7$
σ : Sublattice model, $(Ni)_8(V)_4(Ni,V)_{18}$

Publication:

J. Korb, and K. Hack, GTT, Germany (1997).

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase bcc–$A2$

$$L^{0,bcc-A2}_{Ni,V:\square} = -30513.8 + 12.6138\ T$$

Phase fcc–$A1$

$$L^{0,fcc-A1}_{Ni,V:\square} = -36365.6 + 3.75677\ T$$

$$L^{1,fcc-A1}_{Ni,V:\square} = 11860.7 - 9.0302\ T$$

$$L^{2,fcc-A1}_{Ni,V:\square} = -10647.5 + 7.00954\ T$$

Phase liquid

$$L^{0,liquid}_{Ni,V} = -51927 + 14.99\ T$$

Phase Ni_2V

$$G^{\circ}(T) - 2.0\ H_{\mathrm{Ni}}^{\mathrm{o,fcc-}A1\mathrm{,para}}(298.15\ \mathrm{K}) - H_{\mathrm{V}}^{\mathrm{o,bcc-}A2}(298.15\ \mathrm{K}) = - 38032.065 + 337.2614\ T - 64.6973\ T \cdot \ln T - 0.01512\ T^{2} - 13.75326\ T^{-1}$$

Phase Ni_3V

$$G^{\circ}(T) - 3.0\ H_{\mathrm{Ni}}^{\mathrm{o,fcc-}A1\mathrm{,para}}(298.15\ \mathrm{K}) - H_{\mathrm{V}}^{\mathrm{o,bcc-}A2}(298.15\ \mathrm{K}) = - 45524.96 + 529.01852\ T - 99.74166\ T \cdot \ln T - 0.00824\ T^{2} - 13753.332\ T^{-1}$$

Phase Ni_2V_7

$$G^{\circ}(T) - 2.0\ H_{\mathrm{Ni}}^{\mathrm{o,fcc-}A1\mathrm{,para}}(298.15\ \mathrm{K}) - 7.0\ H_{\mathrm{V}}^{\mathrm{o,bcc-}A2}(298.15\ \mathrm{K}) = - 190634.14 + 1333.90548\ T - 233.55668\ T \cdot \ln T - 0.00482\ T^{2} - 5.196308\mathrm{E}{-}06\ T^{3} + 844557.21\ T^{-1}$$

Phase σ

$$G^{\circ}(T) - 26.0\ H_{\mathrm{Ni}}^{\mathrm{o,fcc-}A1\mathrm{,para}}(298.15\ \mathrm{K}) - 4.0\ H_{\mathrm{V}}^{\mathrm{o,bcc-}A2}(298.15\ \mathrm{K}) = \mathrm{G(Ni{:}V{:}Ni)} =$$

$$298.15 < T < 790.00 : - 161645.05 + 3532.8443\ T - 671.032\ T \cdot \ln T - 0.1382502\ T^{2} + 4.87\mathrm{E}{-}07\ T^{3} + 277840\ T^{-1}$$

$$790.00 < T < 1728.00 : - 161794.7 + 3572.6245\ T - 678.096\ T \cdot \ln T - 0.1256082\ T^{2} - 2.72\mathrm{E}{-}06\ T^{3}$$

$$G^{\circ}(T) - 8.0\ H_{\mathrm{Ni}}^{\mathrm{o,fcc-}A1\mathrm{,para}}(298.15\ \mathrm{K}) - 22.0\ H_{\mathrm{V}}^{\mathrm{o,bcc-}A2}(298.15\ \mathrm{K}) = \mathrm{G(Ni{:}V{:}V)} =$$

$$298.15 < T < 790.00 : - 663330.65 + 4012.7719\ T - 707.716\ T \cdot \ln T - 0.1068816\ T^{2} + 2.6785\mathrm{E}{-}06\ T^{3} + 1528120\ T^{-1}$$

$$790.00 < T < 1728.00 : - 664153.72 + 4231.5628\ T - 746.568\ T \cdot \ln T - 0.0373506\ T^{2} - 1.496\mathrm{E}{-}05\ T^{3}$$

Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Zr}			T / K
Liquid + bcc-$A2$ $\rightleftharpoons$ σ	Peritectic	.626	.769	.662	1552.3
σ + bcc-$A2$ $\rightleftharpoons$ Ni_2V_7	Peritectoid	.727	.922	.778	1171.9
Liquid $\rightleftharpoons$ fcc-$A1$ + σ	Eutectic	.501	.443	.578	1485.7
fcc-$A1$ $\rightleftharpoons$ Ni_2V + σ	Eutectoid	.368	.333	.554	1150.9
fcc-$A1$ $\rightleftharpoons$ Ni_3V + Ni_2V	Eutectoid	.313	.250	.333	1175.5
Ni_3V $\rightleftharpoons$ fcc-$A1$	Congruent	.250	.250	....	1324.0
Ni_2V $\rightleftharpoons$ fcc-$A1$	Congruent	.333	.333	....	1190.0

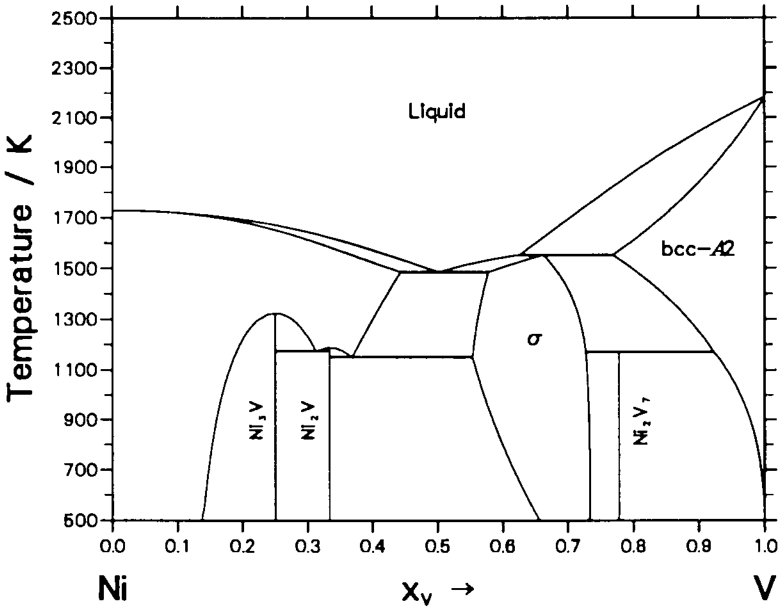


Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub–lattices	Comments
Ni-V	(Ni)	Cu	*cF4* $Fm\bar{3}m$	M 4	
	(V)	W	*cI2* $Im\bar{3}m$		
	Ni_8V	$NbNi_8$	*tI18*		
	Ni_3V	Al_3Ti	*tI8* $I4/mmm$	Ni_1 2 Ni_2 4 V 2	
	Ni_2V	$MoPt_2$	*oI6*		
	σ	σ CrFe	*tP30* $P4_2/mnm$		High and low forms given in [90Mas] assumed to be Ni_2V_7 by the assessors
	NiV_3	Cr_3Si	*cP8* $Pm\bar{3}n$	Cr 6 Si 2	

System Si–Sn

Solution Phases:

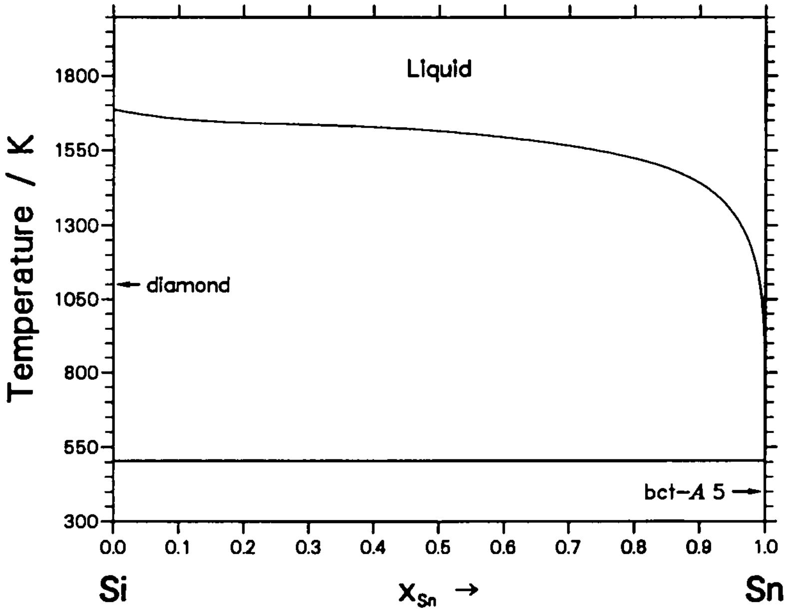
Liquid, diamond

Modelling:

Liquid	:	Substitutional, Redlich–Kister
diamond	:	Substitutional, Redlich–Kister

Assessor and Date:

H.L. Lukas 1993



Thermodynamic properties of the solution phases ($\mathrm{J.mol^{-1}}$)

Phase diamond

$$L^{0,\mathrm{diamond}}_{\mathrm{Si,Sn}} = 25265.65 + 23.84\ T$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Si,Sn}} = 25364.6$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Si,Sn}} = 3148.8$$

$$L^{2,\mathrm{liquid}}_{\mathrm{Si,Sn}} = 4460.9$$

Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Sn}	T / K
Liquid ⇌ bct-$A5$ + diamond	Degenerate	.000 .000 1.000	505.1

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group
Si-Sn	(Si)	diamond	*cF8* *Fd3m*
	(Sn)	β-Sn	*tI4* $I4_1/amd$

System Si–Ti

Solution Phases:

Liquid, bcc-$A2$, hcp-$A3$

Compounds:

Si_2Ti, Si_4Ti_5, SiTi, $SiTi_3$, Si_3Ti_5

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-$A2$: Substitutional, Redlich-Kister
hcp-$A3$: Substitutional, Redlich-Kister
Si_2Ti : Stoichiometric $(Si)_2(Ti)$
Si_4Ti_5 : Stoichiometric $(Si)_4(Ti)_5$
SiTi : Stoichiometric, (Si)(Ti)
$SiTi_3$: Stoichiometric, $(Si)(Ti)_3$
Si_3Ti_5 : Sublattice model, $(Si,Ti)_2(Si,Ti)_3(Ti)_3$
:

Assessor and Date:

H. Seifert

Publication:

Thesis, Univ. Stuttgart, Germany (1994)

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase Si_2Ti

$$G^\circ(T) - 2.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) - H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \\ -175038.5 + 4.54\ T + 2.0\ \mathrm{GHSER_{Si}} + \mathrm{GHSER_{Ti}}$$

Phase Si_4Ti_5

$$G^\circ(T) - 4.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) - 5.0\ H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \\ -711000.0 + 22.37355\ T + 4.0\ \mathrm{GHSER_{Si}} + 5.0\ \mathrm{GHSER_{Ti}}$$

Phase SiTi

$$G^\circ(T) - H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) - H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \\ -155061.7 + 7.6345\ T + \mathrm{GHSER_{Si}} + \mathrm{GHSER_{Ti}}$$

Phase Si_3Ti_5

$$G^\circ(T) - 5.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \mathrm{G(Si{:}Si{:}Ti)} = \\ -\ 206191.45 + 16.4953\ T + 5.0\ \mathrm{GHSER_{Si}} + 3.0\ \mathrm{GHSER_{Ti}}$$

$$G^\circ(T) - 3.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) - 5.0\ H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Si{:}Ti)} = \\ -\ 583564.31 + 2.68514\ T + 3.0\ \mathrm{GHSER_{Si}} + 5.0\ \mathrm{GHSER_{Ti}}$$

$$G^\circ(T) - 2.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) - 6.0\ H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \mathrm{G(Si{:}Ti{:}Ti)} = \\ 417372.85 + 33.81017\ T + 2.0\ \mathrm{GHSER_{Si}} + 6.0\ \mathrm{GHSER_{Ti}}$$

$$G^\circ(T) - 8.0\ H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Ti{:}Ti)} = \\ 40000.0 + 20.0\ T + 8.0\ \mathrm{GHSER_{Ti}}$$

$$L_{\mathrm{Si,Ti{:}Si{:}Ti}}^{0,\mathrm{Si_3Ti_5}} = -500000 + 40.0\ T$$

$$L_{\mathrm{Si,Ti{:}Ti{:}Ti}}^{0,\mathrm{Si_3Ti_5}} = -500000 + 40.0\ T$$

$$L_{\mathrm{Si{:}Si,Ti{:}Ti}}^{0,\mathrm{Si_3Ti_5}} = 43024.29 - 3.44194\ T$$

$$L_{\mathrm{Ti{:}Si,Ti{:}Ti}}^{0,\mathrm{Si_3Ti_5}} = 43024.29 - 3.44194\ T$$

Phase $SiTi_3$

$$G^\circ(T) - H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \\ -\ 200000.0 + 3.19924\ T + \mathrm{GHSER_{Si}} + 3.0\ \mathrm{GHSER_{Ti}}$$

Phase bcc–$A2$

$$L_{\mathrm{Si,Ti{:}\square}}^{0,\mathrm{bcc-}A2} = -\ 275629.1 + 42.5094\ T$$

$$L_{\mathrm{Si,Ti{:}\square}}^{1,\mathrm{bcc-}A2} = 25025.35 - 2.00203\ T$$

$$L_{\mathrm{Si,Ti{:}\square}}^{2,\mathrm{bcc-}A2} = 83940.65 - 6.71526\ T$$

Phase diamond

$$L_{\mathrm{Si,Ti}}^{0,\mathrm{diamond}} = 80\ T$$

Phase hcp–$A3$

$$L_{\mathrm{Si,Ti{:}\square}}^{0,\mathrm{hcp-}A3} = -\ 302731.04 + 69.08469\ T$$

$$L_{\mathrm{Si,Ti{:}\square}}^{1,\mathrm{hcp-}A3} = 25025.35 - 2.00203\ T$$

$$L_{\mathrm{Si,Ti{:}\square}}^{2,\mathrm{hcp-}A3} = 83940.65 - 6.71526\ T$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Si,Ti}} = -255852.17 + 21.87411\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Si,Ti}} = 25025.35 - 2.00203\ T$$

$$L^{2,\mathrm{liquid}}_{\mathrm{Si,Ti}} = 83940.65 - 6.71526\ T$$

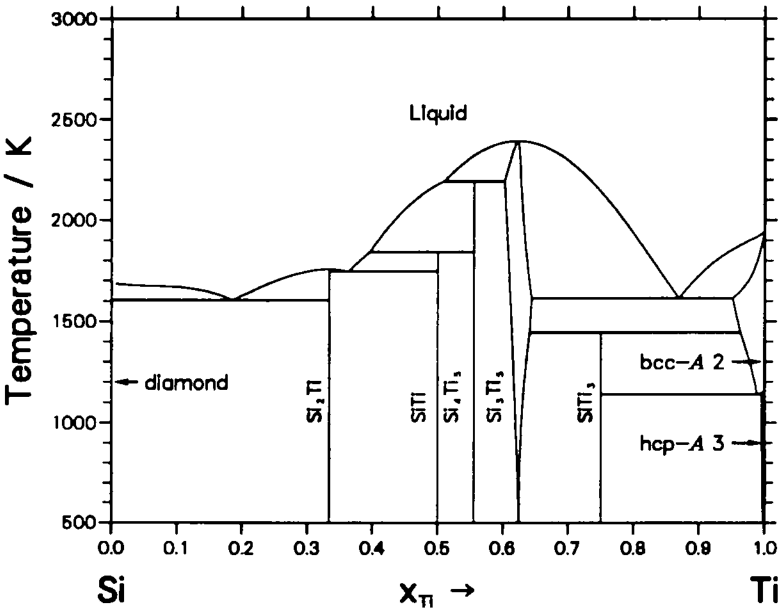


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Ti}			T / K
Liquid $\rightleftharpoons$ diamond + Si_2Ti	Eutectic	.185	.000	.333	1604.3
Liquid $\rightleftharpoons$ Si_2Ti + SiTi	Eutectic	.363	.333	.500	1747.4
Si_2Ti $\rightleftharpoons$ Liquid	Congruent	.333	.333	....	1757.0
Liquid + Si_4Ti_5 $\rightleftharpoons$ SiTi	Peritectic	.396	.556	.500	1842.8
Liquid + Si_3Ti_5 $\rightleftharpoons$ Si_4Ti_5	Peritectic	.509	.602	.555	2192.6
Si_3Ti_5 $\rightleftharpoons$ Liquid	Congruent	.625	.625	....	2394.0
Liquid $\rightleftharpoons$ Si_3Ti_5 + bcc-$A2$	Eutectic	.869	.644	.951	1613.0
Si_3Ti_5 + bcc-$A2$ $\rightleftharpoons$ $SiTi_3$	Peritectoid	.641	.963	.750	1443.2
bcc-$A2$ $\rightleftharpoons$ $SiTi_3$ + hcp-$A3$	Eutectoid	.988	.750	.995	1139.4

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Si–Ti	(Si)	diamond	*cF*8 *Fd*$\bar{3}$*m*		
	(Ti)	Mg	*hP*2 $P6_3/mmc$		
	(Ti)	W	*cI*2 *Im*$\bar{3}$*m*		
	$TiSi_2$	$TiSi_2$	*oF*24 *Fddd*		
	TiSi	TiSi	*oP*8 *Pmm*2	Si_1 2 Si_2 2 Ti_1 1 Ti_2 1 Ti_3 1 Ti_4 1	
	TiSi	FeB	*oP*8 *Pnma*		also given in [90Mas]
	Ti_3Si	PTi_3	*tP*32 $P4_2/n$		
	Ti_5Si_3	Mn_5Si_3	*hP*16 $P6_3/mcm$	Si 6 Ti_1 4 Ti_2 6	
	Ti_5Si_4	Si_4Zr_5	*tP*36 $P4_12_12$		

System Si–V

Solution Phases:

Liquid, bcc–$A2$

Compounds:

Si_2V, Si_3V_5, Si_5V_6, SiV_3

Modelling:

Liquid : Substitutional, Redlich–Kister
bcc–$A2$: Substitutional, Redlich–Kister
SiV_3 : Sublattice model, $(Si,V)(Si,V)_3$
Si_2V : Stoichiometric $(Si)_2(V)$
Si_3V_5 : Stoichiometric $(Si)_3(V)_5$
Si_5V_6 : Stoichiometric $(Si)_5(V)_6$

Assessor and Date:

M.H. Rand, and N. Saunders 1994

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase Si_2V

$$G^{\circ}(T) - 2.0\ H_{\mathrm{Si}}^{\circ,\mathrm{diamond}}(298.15\ \mathrm{K}) - H_{\mathrm{V}}^{\circ,\mathrm{bcc}-A2}(298.15\ \mathrm{K}) = - 143160.0 + 401.98\ T - 67.8\ T\cdot \ln T - 0.0075\ T^2 + 330000.0\ T^{-1}$$

Phase Si_3V_5

$$G^{\circ}(T) - 3.0\ H_{\mathrm{Si}}^{\circ,\mathrm{diamond}}(298.15\ \mathrm{K}) - 5.0\ H_{\mathrm{V}}^{\circ,\mathrm{bcc}-A2}(298.15\ \mathrm{K}) = - 504000.0 + 1259.03\ T - 211.04\ T\cdot \ln T - 0.00748\ T^2 + 1680000.0\ T^{-1}$$

Phase Si_5V_6

$$G^{\circ}(T) - 5.0\ H_{\mathrm{Si}}^{\circ,\mathrm{diamond}}(298.15\ \mathrm{K}) - 6.0\ H_{\mathrm{V}}^{\circ,\mathrm{bcc}-A2}(298.15\ \mathrm{K}) = - 641675.0 + 1665.98\ T - 280.28\ T\cdot \ln T - 0.013915\ T^2 + 2310000.0\ T^{-1}$$

Phase SiV_3

$$G^{\circ}(T) - 4.0 \ H^{\circ,\text{diamond}}_{\text{Si}}(298.15 \text{ K}) = \text{G(Si:Si)} = $$
$$208000.0 - 80.0 \ T + 4.0 \ \text{GHSER}_{\text{Si}}$$

$$G^{\circ}(T) - H^{\circ,\text{diamond}}_{\text{Si}}(298.15 \text{ K}) - 3.0 \ H^{\circ,\text{bcc}-A2}_{\text{V}}(298.15 \text{ K}) = \text{G(Si:V)} =$$
$$- 216397.0 + 516.532 \ T - 90.44 \ T \cdot \ln T - 0.008346 \ T^2$$
$$+ 358000 \ T^{-1}$$

$$G^{\circ}(T) - 3.0 \ H^{\circ,\text{diamond}}_{\text{Si}}(298.15 \text{ K}) - H^{\circ,\text{bcc}-A2}_{\text{V}}(298.15 \text{ K}) = \text{G(V:Si)} =$$
$$166000.0 - 60.0 \ T + 3.0 \ \text{GHSER}_{\text{Si}} + \text{GHSER}_{\text{V}}$$

$$G^{\circ}(T) - 4.0 \ H^{\circ,\text{bcc}-A2}_{\text{V}}(298.15 \text{ K}) = \text{G(V:V)} =$$
$$+ 18000.0 + 10.0 \ T + 4.0 \ \text{GHSER}_{\text{V}}$$

$$L^{0,\text{SiV}_3}_{\text{Si,V:Si}} = 9794.5 - 21.8 \ T$$

$$L^{0,\text{SiV}_3}_{\text{Si,V:V}} = 9794.5 - 21.8 \ T$$

$$L^{0,\text{SiV}_3}_{\text{Si:Si,V}} = - 150000$$

$$L^{0,\text{SiV}_3}_{\text{V:Si,V}} = 0.0$$

Phase bcc–$A2$

$$L^{0,\text{bcc}-A2}_{\text{Si,V}:\square} = - 164505 + 30.1 \ T$$

$$L^{1,\text{bcc}-A2}_{\text{Si,V}:\square} = 37000$$

$$L^{2,\text{bcc}-A2}_{\text{Si,V}:\square} = 20000$$

Phase liquid

$$L^{0,\text{liquid}}_{\text{Si,V}} = - 180900 + 40 \ T$$

$$L^{1,\text{liquid}}_{\text{Si,V}} = 37000$$

$$L^{2,\text{liquid}}_{\text{Si,V}} = 20000$$

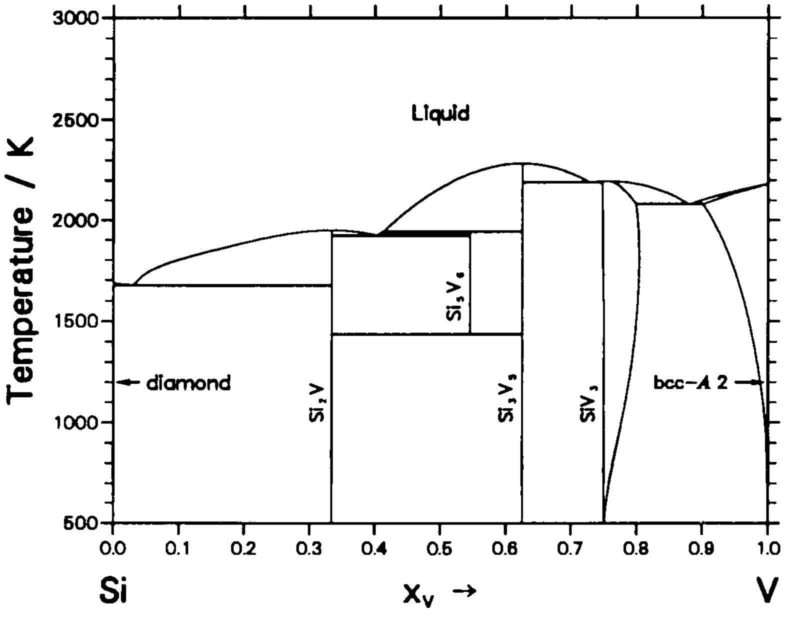


Table I – Invariant Reactions.

Reaction	Type	Compositions x_V			T / K
Liquid ⇌ diamond + Si_2V	Eutectic	.031	.000	.333	1675.1
Si_2V ⇌ Liquid	Congruent	.333	.333	....	1952.0
Liquid ⇌ Si_2V + Si_5V_6	Eutectic	.403	.333	.545	1923.9
Liquid + Si_3V_5 ⇌ Si_5V_6	Peritectic	.412	.625	.545	1943.1
Si_3V_5 ⇌ Liquid	Congruent	.625	.625	....	2284.0
Liquid ⇌ Si_3V_5 + SiV_3	Eutectic	.727	.625	.748	2190.8
SiV_3 ⇌ Liquid	Congruent	.750	.750	....	2196.0
Liquid ⇌ SiV_3 + bcc-A2	Eutectic	.879	.799	.901	2081.1
Si_5V_6 ⇌ Si_2V + Si_3V_5	Eutectoid	.545	.333	.625	1434.7

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Si-V	(Si)	diamond	$cF8$ $Fd\bar{3}m$	M 8	
	(V)	W	$cI2$ $Im\bar{3}m$	M 2	
	SiV_3	Cr_3Si	$cP8$ $Pm\bar{3}n$	Si 2 V 6	
	Si_2V	$CrSi_2$	$hP9$ $P6_222$	Si 6 V 4	
	Si_3V_5	Si_3W_5	$tI32$ $I4/mcm$		
	Si_5V_6	Nb_6Sn_5	$oI44$ $Immm$	Si_1 4 Si_2 8 Si_3 8 V_1 8 V_2 8 V_3 8	Ge_5Ti_6 , *Ibam* in [91Vil]

System Si–Y

Solution Phases:

Liquid, bcc-*A*2, hcp-*A*3

Compounds:

Si_2Y-R, Si_2Y-H, Si_5Y_3-R, Si_5Y_3-H, SiY, Si_3Y_5, Si_4Y_5

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-*A*2 : Substitutional, Redlich-Kister
hcp-*A*3 : Substitutional, Redlich-Kister
Si_2Y-H : Stoichiometric, $(Si)_2(Y)$-H
Si_2Y-R : Stoichiometric, $(Si)_2(Y)$-R
Si_5Y_3-H : Stoichiometric $(Si)_5(Y)_3$-H
Si_5Y_3-R : Stoichiometric $(Si)_5(Y)_3$-R
SiY : Stoichiometric, (Si)(Y)
Si_3Y_5 : Stoichiometric, $(Si)_3(Y)_5$
Si_4Y_5 : Stoichiometric, $(Si)_4(Y)_5$

Assessor and Date:

H.L. Lukas 1991

Thermodynamic properties of the solution and compound phases ($J.mol^{-1}$)

Phase Si_2Y–H

$$G^{\circ}(T) - 2.0\ H_{\mathrm{Si}}^{\circ,\mathrm{diamond}}(298.15\ \mathrm{K}) - H_{\mathrm{Y}}^{\circ,\mathrm{hcp}-A3}(298.15\ \mathrm{K}) = - 21463.0 + 28.5\ T + 2.0\ \mathrm{GHSER_{Si}} + \mathrm{GHSER_{Y}}$$

Phase Si_2Y–R

$$G^{\circ}(T) - 2.0\ H_{\mathrm{Si}}^{\circ,\mathrm{diamond}}(298.15\ \mathrm{K}) - H_{\mathrm{Y}}^{\circ,\mathrm{hcp}-A3}(298.15\ \mathrm{K}) = - 219201.0 + 31.5\ T + 2.0\ \mathrm{GHSER_{Si}} + \mathrm{GHSER_{Y}}$$

Phase Si_3Y_5

$$G^{\circ}(T) - 3.0\ H_{\mathrm{Si}}^{\circ,\mathrm{diamond}}(298.15\ \mathrm{K}) - 5.0\ H_{\mathrm{Y}}^{\circ,\mathrm{hcp}-A3}(298.15\ \mathrm{K}) = -588000.0 + 76.0\ T + 3.0\ \mathrm{GHSER_{Si}} + 5.0\ \mathrm{GHSER_{Y}}$$

Phase Si_4Y_5

$$G^{\circ}(T) - 4.0\ H_{\mathrm{Si}}^{\circ,\mathrm{diamond}}(298.15\ \mathrm{K}) - 5.0\ H_{\mathrm{Y}}^{\circ,\mathrm{hcp}-A3}(298.15\ \mathrm{K}) = -697950.0 + 86.72688\ T + 4.0\ \mathrm{GHSER_{Si}} + 5.0\ \mathrm{GHSER_{Y}}$$

Phase SiY

$$G^{\circ}(T) - H_{\mathrm{Si}}^{\circ,\mathrm{diamond}}(298.15\ \mathrm{K}) - H_{\mathrm{Y}}^{\circ,\mathrm{hcp}-A3}(298.15\ \mathrm{K}) = -160700.0 + 19.8\ T + \mathrm{GHSER_{Si}} + \mathrm{GHSER_{Y}}$$

Phase Si_5Y_3–H

$$G^{\circ}(T) - 5.0\ H_{\mathrm{Si}}^{\circ,\mathrm{diamond}}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Y}}^{\circ,\mathrm{hcp}-A3}(298.15\ \mathrm{K}) = -601572.0 + 76.0\ T + 5.0\ \mathrm{GHSER_{Si}} + 3.0\ \mathrm{GHSER_{Y}}$$

Phase Si_5Y_3–R

$$G^{\circ}(T) - 5.0\ H_{\mathrm{Si}}^{\circ,\mathrm{diamond}}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Y}}^{\circ,\mathrm{hcp}-A3}(298.15\ \mathrm{K}) = -607356.0 + 84.0\ T + 5.0\ \mathrm{GHSER_{Si}} + 3.0\ \mathrm{GHSER_{Y}}$$

Phase bcc–$A2$

$$L_{\mathrm{Si,Y:\square}}^{0,\mathrm{bcc}-A2} = 80\ T$$

Phase hcp–$A3$

$$L_{\mathrm{Si,Y:\square}}^{0,\mathrm{hcp}-A3} = 80\ T$$

Phase liquid

$$L_{\mathrm{Si,Y}}^{0,\mathrm{liquid}} = -212656.12 + 25.83471\ T$$

$$L_{\mathrm{Si,Y}}^{1,\mathrm{liquid}} = 13977.08 - 31.08941\ T$$

$$L_{\mathrm{Si,Y}}^{2,\mathrm{liquid}} = 62049.23 - 50.31476\ T$$

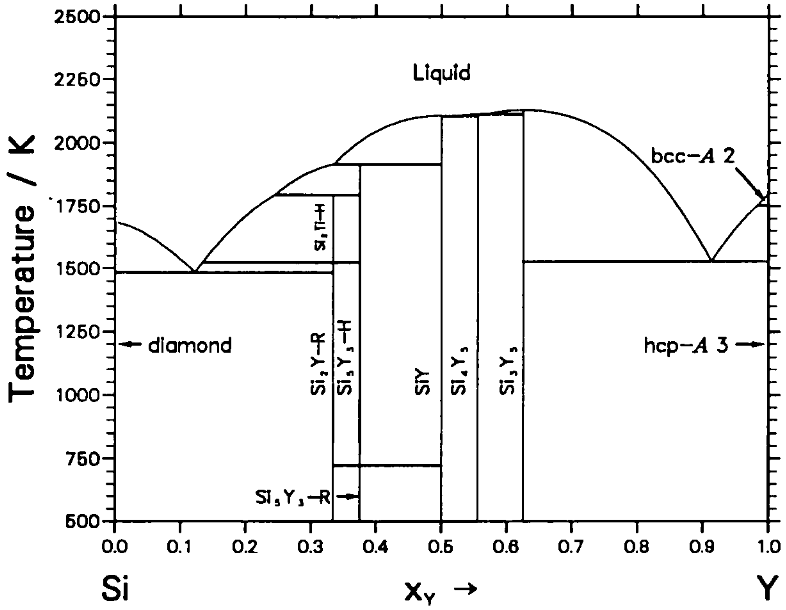


Table I – Invariant Reactions.

Reaction	Type	Compositions x_Y			T / K
Liquid ⇌ diamond + Si_2Y-R	Eutectic	.122	.000	.333	1485.3
Si_2Y-R ⇌ Si_2Y-H	Polymorphic	.333	.333	....	1523.0
Liquid + Si_5Y_3-H ⇌ Si_2Y-H	Peritectic	.244	.375	.333	1793.2
Liquid + SiY ⇌ Si_5Y_3-H	Peritectic	.335	.500	.375	1915.3
SiY ⇌ Liquid	Congruent	.500	.500	....	2108.0
Liquid ⇌ SiY + Si_4Y_5	Eutectic	.518	.500	.556	2107.0
Si_4Y_5 ⇌ Liquid	Congruent	.556	.556	....	2114.5
Liquid ⇌ Si_4Y_5 + Si_3Y_5	Eutectic	.567	.556	.625	2113.9
Si_3Y_5 ⇌ Liquid	Congruent	.625	.625	....	2132.0
Liquid ⇌ Si_3Y_5 + hcp-A3	Eutectic	.913	.625	1.000	1527.9
hcp-A3 ⇌ bcc-A2	Allotropic	1.000	1.000	....	1752.0
Si_5Y_3-R ⇌ Si_5Y_3-H	Polymorphic	.375	.375	....	723.0

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Si-Y	(Si)	C(diamond)	*cF8* $Fd\bar{3}m$	M 8	
	(Y)	Mg	*hP2* $P6_3/mmc$	M 2	
	(Y)	W	*cI2* $Im\bar{3}m$	M 2	
	Si_2Y-α	AlB_2	*hP3* $P6/mmm$		designated as Si_2Y-R
	Si_2Y-β	Si_2Th	*oI12* $Imma$		designated as Si_2Y-H Gd_2Si_3-type in [91Vil]
	Si_3Y_5	Mn_5Si_3	*hP16* $P6_3/mcm$	Si 6 Y_1 4 Y_2 6	
	Si_4Y_5	Si_4Y_5	*tP36* $P4_12_12$	Si_1 8 Si_2 8 Zr_1 4 Zr_2 8 Zr_3 8	
	Si_5Y_3-α	AlB2	*hP3* $P6/mmm$	Si 2 Y 1	designated as Si_5Y_3-R
	Si_5Y_3-β	$ThSi_2$			designated as Si_5Y_3-H
	SiY	CrB	*oC8* $Cmcm$	Si 4 Y 4	

System Si–Zn

Solution Phases:

Liquid, diamond, hcp–Zn

Modelling:

Liquid : Substitutional, Redlich–Kister
diamond : Substitutional, Redlich–Kister
hcp–Zn : Substitutional, Redlich–Kister

Assessor and Date:

M. Jacobs 1993

Thermodynamic properties of the solution phases (J.mol^{-1})

Phase diamond

$L^{0,\mathrm{diamond}}_{\mathrm{Si,Zn}} = 100\ T$

Phase hcp–Zn

$L^{0,\mathrm{hcp-Zn}}_{\mathrm{Si,Zn}} = 80\ T$

Phase liquid

$L^{0,\mathrm{liquid}}_{\mathrm{Si,Zn}} = 7829.25$

$L^{1,\mathrm{liquid}}_{\mathrm{Si,Zn}} = -3338.18$

$L^{2,\mathrm{liquid}}_{\mathrm{Si,Zn}} = -891.33$

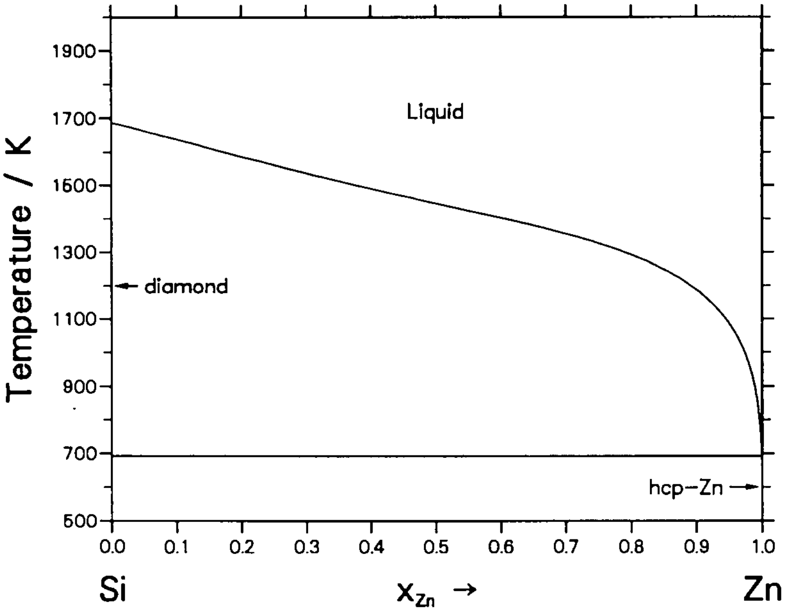


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Zn}	T / K
Liquid ⇌ diamond + hcp–Zn	Degenerate	1.000 .000 1.000	692.1

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group
Si–Zn	(Si)	diamond	*cF8* *Fd3m*
	(Zn)	Mg	*hP2* $P6_3/mmc$

System Si–Zr

Solution Phases:

Liquid

Compounds:

Si_2Zr, Si_2Zr_3, Si_3Zr_5, Si_4Zr_5, SiZr, $SiZr_2$, $SiZr_3$

Modelling:

Liquid	:	Substitutional, Redlich–Kister
Si_2Zr	:	Stoichiometric $(Si)_2(Zr)$
Si_2Zr_3	:	Stoichiometric $(Si)_2(Zr)_3$
Si_3Zr_5	:	Stoichiometric $(Si)_3(Zr)_5$
Si_4Zr_5	:	Stoichiometric $(Si)_4(Zr)_5$
SiZr	:	Stoichiometric (Si)(Zr)
$SiZr_2$	:	Stoichiometric, $(Si)(Zr)_2$
$SiZr_3$	:	Stoichiometric $(Si)(Zr)_3$

Assessor and Date:

C. Gueneau, C. Servant, I. Ansara, and N. Dupin

Publication:

Calphad, **18**, 3, 319-327 (1994)

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase liquid

$$L^{0,\text{liquid}}_{\text{Si,Zr}} = -190000.0 + 16.8955\ T$$

$$L^{1,\text{liquid}}_{\text{Si,Zr}} = 14.52575\ T$$

Phase Si_2Zr

$$G^\circ(T) - 2.0\ H^{\circ,\text{diamond}}_{\text{Si}}(298.15\text{ K}) - H^{\circ,\text{hcp}-A3}_{\text{Zr}}(298.15\text{ K}) = -189332.0 + 354.937\ \text{T} - 63.16867\ T\cdot\ln T - 7.67745\text{E-}03\ T^2 - 1.972048\text{E-}11\ T^3 + 139751.1\ T^{-1}$$

Phase SiZr

$$G^{\circ}(T) - H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) - H_{\mathrm{Zr}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \\ - 182203.4 + 258.514\ T - 45.18631\ T \cdot \ln T - 4.393865\mathrm{E}{-}03\ T^{2} \\ + 5.49699\mathrm{E}{-}11\ T^{3} + 148517.5 T^{-1}$$

Phase Si_4Zr_5

$$G^{\circ}(T) - 4.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) - 5.0\ H_{\mathrm{Zr}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \\ - 880743.11 + 1433.658\ T - 240.256\ T \cdot \ln T - 0.0109481\ T^{2} \\ + 6.591183\mathrm{E}{-}07\ T^{3} + 2006425\ T^{-1}$$

Phase Si_2Zr_3

$$G^{\circ}(T) - 2.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Zr}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \\ - 493990.62 + 844.448\ T - 140.103\ T \cdot \ln T - 0.003701\ T^{2} \\ + 1.028333\mathrm{E}{-}07\ T^{3} + 1167755\ T^{-1}$$

Phase Si_3Zr_5

$$G^{\circ}(T) - 3.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) - 5.0\ H_{\mathrm{Zr}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \\ - 685146.78 + 1044.78\ T - 187\ T \cdot \ln T - 0.0161754\ T^{2} \\ + 5.22283\mathrm{E}{-}08\ T^{3} + 381210\ T^{-1}$$

Phase $SiZr_2$

$$G^{\circ}(T) - H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Zr}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \\ - 255317.83 + 411.767\ T - 72.43244\ T \cdot \ln T - 5.46177\mathrm{E}{-}03\ T^{2} \\ - 4.0442633\mathrm{E}{-}09\ T^{3} + 306730.45\ T^{-1}$$

Phase $SiZr_3$

$$G^{\circ}(T) - H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Zr}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \\ - 270398.16 + 457.33\ T - 82.328\ T \cdot \ln T - 0.0263963\ T^{2} \\ + 1.54326\mathrm{E}{-}06\ T^{3} - 34700\ T^{-1}$$

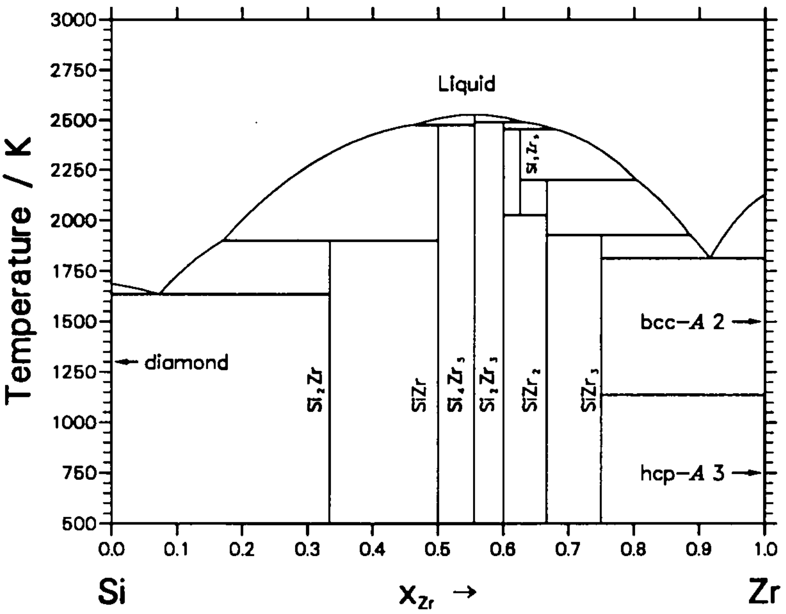


Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Zr}			T / K
Liquid ⇌ diamond + Si_2Zr	Eutectic	.073	.000	.333	1634.6
Liquid + SiZr ⇌ Si_2Zr	Peritectic	.170	.500	.333	1900.3
Liquid + Si_4Zr_5 ⇌ SiZr	Peritectic	.463	.555	.500	2477.0
Liquid + Si_4Zr_5 ⇌ Si_2Zr_3	Peritectic	.629	.555	.600	2491.5
Liquid + Si_2Zr_3 ⇌ Si_3Zr_5	Peritectic	.677	.600	.675	2455.4
Liquid + Si_3Zr_5 ⇌ $SiZr_2$	Peritectic	.803	.625	.666	2200.0
Liquid + $SiZr_2$ ⇌ $SiZr_3$	Peritectic	.886	.666	.750	1927.4
Liquid ⇌ $SiZr_3$ + bcc-A2	Eutectic	.916	.750	1.000	1814.2
hcp-A3 ⇌ bcc-A2	Allotropic	1.000	1.000	....	1139.4
Si_3Zr_5 ⇌ Si_2Zr_3 + $SiZr_2$	Eutectoid	.625	.600	.666	2025.2
Liquid ⇌ Si_4Zr_5	Congruent	.556	.556	....	2527.0

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Si-Zr	(Si)	diamond	*cF8* $Fd\bar{3}m$	M 8	
	(Zr)	Mg	*hP2* $P6_3/mmc$	M 2	
	(Zr)	W	*cI2* $Im\bar{3}m$	M 4	
	SiZr-α	BFe	*oP8*	Si 4	transformation not considered
	SiZr-β	BCr	*oC8* *Cmcm*	Zr 4	
	$SiZr_2$	Al_2Cu	*tI12* $I4/mcm$	Si 8 Zr 4	
	$SiZr_3$	PTi_3	*tP32* $P4_2/n$		
	Si_2Zr	Si_2Zr	*oC12* *Cmcm*	Si_1 4 Si2 4 Zr 4	
	Si_2Zr_3	Si_2U_3	*tP10* $P4/mbm$		
	Si_3Zr_5	Mn_5Si_3	*hP16* $P6_3/mcm$	Si 6 Zr_1 4 Zr_2 6	
	Si_4Zr_5-α	Si_4Zr_5	*tP36* $P4_12_12$	Si_1 8 Si_2 8 Zr_1 4 Zr_2 8 Zr_3 8	transformation not considered
	Si_4Zr_5-β	Si_4Zr_5			

System Sn–Ti

Solution Phases:

Liquid, bcc–$A2$, hcp–$A3$, bct–$A5$

Compounds:

Sn_5Ti_6, Sn_3Ti_5, $SnTi_2$, $SnTi_3$

Modelling:

Liquid : Substitutional, Redlich–Kister
bcc–$A2$: Substitutional, Redlich–Kister
bct–$A5$: Substitutional, Redlich–Kister
hcp–$A3$: Substitutional, Redlich–Kister
$SnTi_3$: Sublattice model: $(Sn,Ti)(Sn,Ti)_3$
Sn_5Ti_6 : Stoichiometric, $(Sn)_5(Ti)_6$
Sn_3Ti_5 : Stoichiometric, $(Sn)_3(Ti)_5$
$SnTi_2$: Stoichiometric, $(Sn)(Ti)_2$

Assessor and Date:

F. Hayes, 1992

Thermodynamic properties of the solution and compound phases ($J.mol^{-1}$)

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Sn,Ti:\square}} = -\,115000.00 + 6.77583\ T$$

$$L^{1,\mathrm{bcc}-A2}_{\mathrm{Sn,Ti:\square}} = 45000.00 + 1.58018\ T$$

Phase bct–$A5$

$$L^{0,\mathrm{bct}-A5}_{\mathrm{Sn,Ti}} = 50000.0$$

Phase hcp–$A3$

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Sn,Ti:\square}} = -\,111502.08 + 1.8068\ T$$

$$L^{1,\mathrm{hcp}-A3}_{\mathrm{Sn,Ti:\square}} = 43871.41 + 2.08175\ T$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Sn,Ti}} = -\,90206.13 - 5.55089\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Sn,Ti}} = 44395.59 - 6.09746\ T$$

Phase SnTi$_3$

$$G^\circ(T) - 4.0\ H^{\mathrm{o,bct}-A5}_{\mathrm{Sn}}(298.15\ \mathrm{K}) = \mathrm{G(Sn{:}Sn)} =$$
$$4.0\ \mathrm{GHSER_{Sn}}$$

$$G^\circ(T) - H^{\mathrm{o,bct}-A5}_{\mathrm{Sn}}(298.15\ \mathrm{K}) - 3.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Sn{:}Ti)} =$$
$$-\,193466.8 + 35.74052\ T + \mathrm{GLIQ_{Sn}} + 3.0\ \mathrm{GLIQ_{Ti}}$$

$$G^\circ(T) - 3.0\ H^{\mathrm{o,bct}-A5}_{\mathrm{Sn}}(298.15\ \mathrm{K}) - H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Sn)} =$$
$$300000 - 200\ T + 3.0\ \mathrm{GLIQ_{Sn}} + \mathrm{GLIQ_{TI}}$$

$$G^\circ(T) - 4.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Ti)} =$$
$$4.0\ \mathrm{GHSER_{Ti}}$$

$$L^{0,\mathrm{SnTi_3}}_{\mathrm{Sn:Sn,Ti}} = 400000 - 40.0\ T$$

$$L^{0,\mathrm{SnTi_3}}_{\mathrm{Ti:Sn,Ti}} = 600000 + 40.0\ T$$

$$L^{0,\mathrm{SnTi_3}}_{\mathrm{Sn,Ti:Sn}} = 400000$$

$$L^{0,\mathrm{SnTi_3}}_{\mathrm{Sn,Ti:Ti}} = 200000 - 108.000\ T$$

Phase SnTi$_2$

$$G^\circ(T) - H^{\mathrm{o,bct}-A5}_{\mathrm{Sn}}(298.15\ \mathrm{K}) - 2.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) =$$
$$-\,152700.00 + 26.80539\ T + \mathrm{GLIQ_{Sn}} + 2.0\ \mathrm{GLIQ_{Ti}}$$

Phase Sn$_3$Ti$_5$

$$G^\circ(T) - 3.0\ H^{\mathrm{o,bct}-A5}_{\mathrm{Sn}}(298.15\ \mathrm{K}) - 5.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) =$$
$$-\,398000.00 + 64.8\ T + 3.0\ \mathrm{GLIQ_{Sn}} + 5.0\ \mathrm{GLIQ_{Ti}}$$

Phase Sn$_5$Ti$_6$

$$G^\circ(T) - 5.0\ H^{\mathrm{o,bct}-A5}_{\mathrm{Sn}}(298.15\ \mathrm{K}) - 6.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) =$$
$$-\,525800.00 + 77.0\ T + 5.0\ \mathrm{GLIQ_{Sn}} + 6.0\ \mathrm{GLIQ_{Ti}}$$

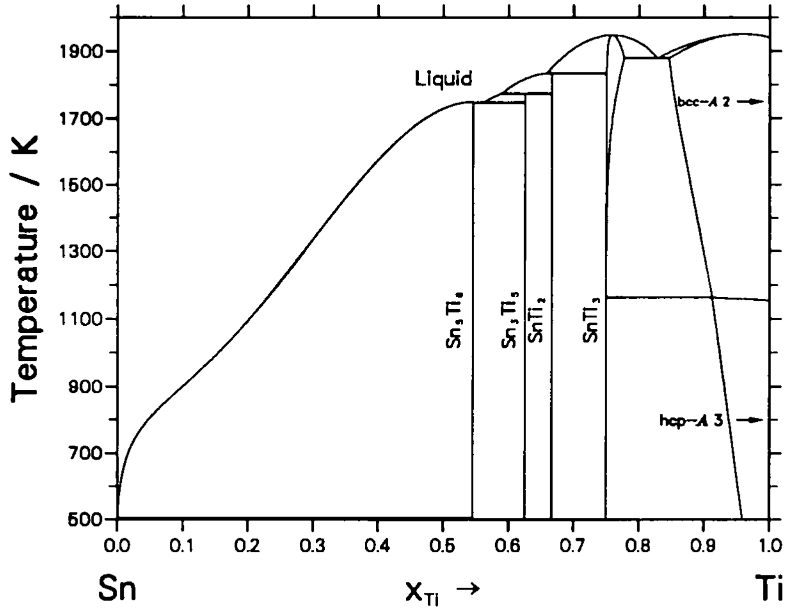


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Ti}			T / K
bcc-$A2$ + $SnTi_3$ ⇌ hcp-$A3$	Peritectic	.913	.750	.912	1163.3
Liquid ⇌ $SnTi_3$ + bcc-$A2$	Eutectic	.828	.777	.846	1879.8
$SnTi_3$ ⇌ Liquid	Congruent	.750	.750	....	1947.0
Liquid + $SnTi_3$ ⇌ $SnTi_2$	Peritectic	.659	.750	.667	1835.9
Liquid + $SnTi_2$ ⇌ + Sn_3Ti_5	Peritectic	.589	.667	.625	1774.7
Liquid ⇌ Sn_5Ti_6 + Sn_3Ti_5	Eutectic	.561	.545	.625	1746.9
Sn_5Ti_6 ⇌ Liquid	Congruent	.545	.545	....	1750.0
Liquid ⇌ bct-$A5$ + Sn_5Ti_6	Degenerate	.001	.000	.545	504.8

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub–lattices	Comments
Sn–Ti	(Sn)	β-Sn	*tI4* $I4_1/amd$	M 2	
	(Ti)	Mg	*hP2* $P6_3/mmc$	M 2	
	(Ti)	W	*cI2* $Im\bar{3}m$	M 2	
	Sn_5Ti_6-α	Nb_6Sn_5	*oI44* *Immm3*		transformation not considered
	Sn_5Ti_6-β	......	*hP22* $P6_3/mmc$	Sn 3 Ti 6	
	Sn_3Ti_5	Mn_5Si_3	*hP16* $P6_3/mcm$	Sn 6 Ti 4	
	$SnTi_2$	$InNi_2$	*hP6* $P6_3/mmc$		
	$SnTi_3$	Ni_3Sn	*hP8* $P6_3/mmc$	Sn 2 Ti 6 Si_1 4 Si_2 8	

System Sn–Zn

Solution Phases:

(stable) Liquid, bct–*A*5, hcp–Zn
(metastable) bcc–*A*2

Modelling:

Liquid : Substitutional, Redlich–Kister
bcc–*A*2 : Substitutional, Redlich–Kister
bct–*A*5 : Substitutional, Redlich–Kister
hcp–Zn : Substitutional, Redlich–Kister

Assessor and Date:

S. Fries, and H.L. Lukas

Publication:

"Cost507 New Light Alloys", Leuven Proceedings,
Ed. G. Effenberg (1991)

Thermodynamic properties of the solution phases (J.mol^{-1})

Phase bct–*A*5

$$L^{0,\text{bct}-A5}_{\text{Sn,Zn}:\square} = 6514.76 + 25.70957\ T$$

Phase bcc–*A*2

$$L^{0,\text{bcc}-A2}_{\text{Sn,Zn}:\square} = 6514.76 + 25.70957\ T$$

Phase hcp–Zn

$$L^{0,\text{hcp}-\text{Zn}}_{\text{Sn,Zn}:\square} = 33433.94 - 11.14466\ T$$

Phase liquid

$$L^{0,\text{liquid}}_{\text{Sn,Zn}} = 19314.64 - 75.89939\ T + 8.751396\ T\cdot \ln T$$

$$L^{1,\text{liquid}}_{\text{Sn,Zn}} = -5696.28 + 4.20198\ T$$

$$L^{2,\text{liquid}}_{\text{Sn,Zn}} = 1037.22 + 0.98362\ T$$

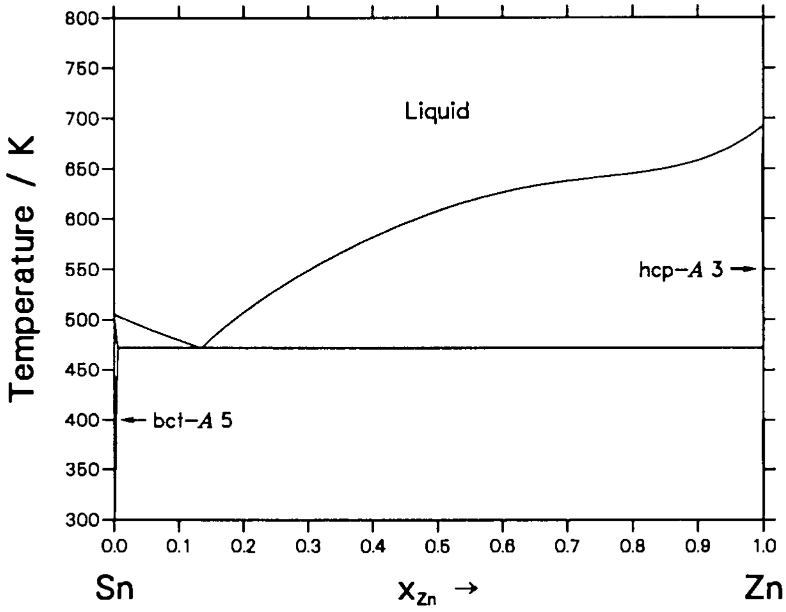


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Zn}			T / K
Liquid ⇌ bct-*A*5 + hcp-Zn	Eutectic	0.135	.006	1.000	471.7

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group
Sn–Zn	(Sn)	β-Sn	*tI4* $I4_1/amd$
	(Zn)	Mg	*hP2* $P6_3/mmc$

System Sn – Zr

Solution Phases

Liquid, bcc–$A2$, bct–$A5$, hcp–$A3$

Compounds:

$SnZr_4$, Sn_3Zr_5, Sn_2Zr

Modelling:

Liquid : Substitutional, Redlich–Kister
bcc–$A2$: Substitutional, Redlich–Kister
hcp–$A3$: Substitutional, Redlich–Kister
$SnZr_4$: Stoichiometric, $(Sn)(Zr)_4$
Sn_3Zr_5 : Stoichiometric, $(Sn)_3(Zr)_5$
Sn_2Zr : Stoichiometric, $(Sn)_2(Zr)$

Asessor and date:

J. Korb, and K. Hack, GTT, Germany (1996).

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Sn,Zr}} = -45520 - 95.46\ T$$

$$L^{1,\mathrm{Liquid}}_{\mathrm{Sn,Zr}} = -80000 + 82.115\ T$$

$$L^{2,\mathrm{Liquid}}_{\mathrm{Sn,Zr}} = -120000 + 80.0273\ T$$

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Sn,Zr}:\square} = -101200 - 71.13\ T$$

$$L^{1,\mathrm{bcc}-A2}_{\mathrm{Sn,Zr}:\square} = 55000$$

$$L^{2,\mathrm{bcc}-A2}_{\mathrm{Sn,Zr}:\square} = 26102.3$$

Phase hcp-$A3$

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Sn,Zr:\square}} = -160000 - 31\ T$$

$$L^{1,\mathrm{hcp}-A3}_{\mathrm{Sn,Zr:\square}} = 151800$$

$$L^{2,\mathrm{hcp}-A3}_{\mathrm{Sn,Zr:\square}} = 129900$$

Phase $\mathrm{SnZr_4}$

$$G^{\circ}(T) - H^{\mathrm{o,bct}-A5}_{\mathrm{Sn}}(298.15\ \mathrm{K}\ ) - 4.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Zr}}(298.15\ \mathrm{K}) = -270456.8 + 602.125\ T - 123.0\ T\cdot \ln T - 0.00883\ T^2$$

Phase $\mathrm{Sn_3Zr_5}$

$$G^{\circ}(T) - 3.0\ H^{\mathrm{o,bct}-A5}_{\mathrm{Sn}}(298.15\ \mathrm{K}) - 5.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Zr}}(298.15\ \mathrm{K}) = -769380 + 1131.86\ T - 217.118\ T\cdot \ln T - 0.02404\ T^2 + 1648000\ T^{-1}$$

Phase $\mathrm{Sn_2Zr}$

$$G^{\circ}(T) - 2.0\ H^{\mathrm{o,bct}-A5}_{\mathrm{Sn}}(298.15\ \mathrm{K}) - H^{\mathrm{o,hcp}-A3}_{\mathrm{Zr}}(298.15\ \mathrm{K}) = -267104.8 + 492.1\ T - 86.404\ T\cdot \ln T - 0.002226\ T^2 + 618000\ T^{-1}$$

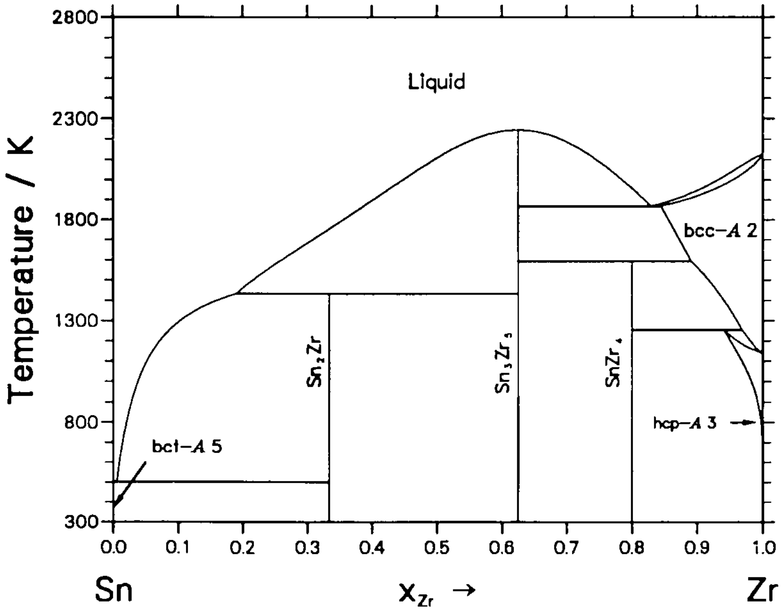


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{Zr}			T / K
Liquid $\rightleftharpoons$ bcc-$A2$ + Sn_3Zr_5	Eutectic	.892	.844	.625	1868.5
bcc-$A2$ + Sn_3Zr_5 $\rightleftharpoons$ $SnZr_4$	Peritectoid	.891	.625	.800	1595.5
bcc-$A2$ + $SnZr_4$ $\rightleftharpoons$ hcp-$A3$	Peritectoid	.968	.800	.941	1254.0
Liquid + Sn_3Zr_5 $\rightleftharpoons$ Sn_2Zr	Peritectoid	.189	.625	.333	1433.3
Liquid $\rightleftharpoons$ Sn_2Zr + bct-$A5$	Eutectic	.0056	.333	.000	502.0
Liquid $\rightleftharpoons$ Sn_3Zr_5	Congruent	.625	.625	....	2245.0

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices
Sn-Zr	(Sn)	β-Sn	*tI4* $I4_1/amd$	M 2
	(Zr)	Mg	*hP2* $P6_3/mmc$	M 2
	(Zr)	W	*cI2* $Im\bar{3}m$	M 2
	$SnZr_4$	Cr_3Si	*cP8* $Pm\bar{3}n$	
	Sn_3Zr_5	Mn_5Si_3	*hP16* $P6_3/mcm$	
	Sn_2Zr	$SiTi_2$	*oF24* *Fddd*	

System Ta–Ti

Solution Phases:

(stable) Liquid, bcc-$A2$, hcp-$A3$
(metastable) bcc-$B2$, fcc-$A1$

Compounds:

(metastable) AlM-$D0_{19}$, AlM-$D0_{22}$, AlTi-$L1_0$

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-$A2$: see below
bcc-$B2$: Sublattice model, $(\mathrm{Ta,Ti})_{0.5}(\mathrm{Ta,Ti})_{0.5}(\square)_3$
The thermodynamic description of the bcc-B2 takes
into account the ordering reaction bcc-$A2$ $\rightleftharpoons$ bcc-$B2$.
Two descriptions are given: one using equations
23 and 27, the other using equations 23 and 28.
For the latter, the parameters are given in a frame.
fcc-$A1$: Substitutional, Redlich-Kister
hcp-$A3$: Substitutional, Redlich-Kister
AlM-$D0_{19}$: Sublattice model, $(\mathrm{Ta,Ti})(\mathrm{Ta,Ti})_3$
AlM-$D0_{22}$: Sublattice model, $(\mathrm{Ti})_3(\mathrm{Ta,Ti})$
AlTi-$L1_0$: Sublattice model, $(\mathrm{Ta,Ti})(\mathrm{Ta,Ti})$
:

Assessor and Date:

N. Saunders, 1997.

Thermodynamic properties of the solution phases ($\mathrm{J.mol^{-1}}$)

Phase fcc–$A1$

$$L^{0,\mathrm{fcc-}A1}_{\mathrm{Ta,Ti:\square}} = 8500$$

Phase hcp–$A3$

$$L^{0,\mathrm{hcp-}A3}_{\mathrm{Ta,Ti:\square}} = 8500$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Ta,Ti}} = 1000$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Ta,Ti}} = -7000$$

Phase AlM–$D0_{19}$

$$G^\circ(T) - 4.0\ H^{\mathrm{o,bcc}-A2}_{\mathrm{Ta}}(298.15\ \mathrm{K}) = \mathrm{G(Ta{:}Ta)} = 4.0\ \mathrm{GHCP_{Ta}}$$

$$G^\circ(T) - 3.0\ H^{\mathrm{o,bcc}-A2}_{\mathrm{Ta}}(298.15\ \mathrm{K}) - H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ta{:}Ti)} = 6376 + 3.0\ \mathrm{GHCP_{Ta}} + \mathrm{GHSER_{Ti}}$$

$$G^\circ(T) - H^{\mathrm{o,bcc}-A2}_{\mathrm{Ta}}(298.15\ \mathrm{K}) - 3.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Ta)} = 6376 + \mathrm{GHCP_{Ta}} + 3.0\ \mathrm{GHSER_{Ti}}$$

$$G^\circ(T) - 4.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Ti)} = 4.0 + 4.0\ \mathrm{GHSER_{Ti}}$$

$$L^{0,\mathrm{AlM}-D0_{19}}_{\mathrm{Ta,Ti:Ta}} = L^{0,\mathrm{AlM}-D0_{19}}_{\mathrm{Ta,Ti:Ti}} = 19128$$

$$L^{0,\mathrm{AlM}-D0_{19}}_{\mathrm{Ta:Ta,Ti}} = L^{0,\mathrm{AlM}-D0_{19}}_{\mathrm{Ti:Ta,Ti}} = 2128$$

Phase AlM–$D0_{22}$

$$G^\circ(T) - H^{\mathrm{o,bcc}-A2}_{\mathrm{Ta}}(298.15\ \mathrm{K}) - 3.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Ta)} = \mathrm{GFCC_{Ta}} + 3.0\ \mathrm{GFCC_{Ti}}$$

$$G^\circ(T) - 4.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Ti)} = 4.0\ \mathrm{GFCC_{Ti}}$$

Phase AlTi–$L1_0$

$$G^\circ(T) - 2.0\ H^{\mathrm{o,bcc}-A2}_{\mathrm{Ta}}(298.15\ \mathrm{K}) = \mathrm{G(Ta{:}Ta)} = 2.0\ \mathrm{GFCC_{Ta}}$$

$$G^\circ(T) - H^{\mathrm{o,bcc}-A2}_{\mathrm{Ta}}(298.15\ \mathrm{K}) - H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ta{:}Ti)} = 4250 + \mathrm{GFCC_{Ta}} + \mathrm{GFCC_{Ti}}$$

$$G^\circ(T) - H^{\mathrm{o,bcc}-A2}_{\mathrm{Ta}}(298.15\ \mathrm{K}) - H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Ta)} = 4250 + \mathrm{GFCC_{Ta}} + \mathrm{GFCC_{Ti}}$$

$$G^\circ(T) - 2.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Ti)} = 2.0\ \mathrm{GFCC_{Ti}}$$

$$L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Ta,Ti:Ta}} = L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Ta:Ta,Ti}} = 4250$$

$$L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Ta,Ti:Ti}} = L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Ti:Ta,Ti}} = 4250$$

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Ta,Ti}:\square} = 12000$$

$$L^{1,\mathrm{bcc}-A2}_{\mathrm{Ta,Ti}:\square} = -2500$$

Phase bcc–$B2$

$G^{\bullet}_{\mathrm{Ti:Ta:\square}} = -\ 2500$
$G^{\circ}(T) - H^{\mathrm{o,bcc}-A2}_{\mathrm{Ta}}(298.15\ \mathrm{K}) = \mathrm{G(Ta:Ta:\square)} = 0.0$
$G^{\circ}(T) - 0.5\ H^{\mathrm{o,bcc}-A2}_{\mathrm{Ta}}(298.15\ \mathrm{K}) - 0.5\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ta:Ti:\square)} = G^{\bullet}_{\mathrm{Ta:Ti:\square}}$
$G^{\circ}(T) - 0.5\ H^{\mathrm{o,bcc}-A2}_{\mathrm{Ta}}(298.15\ \mathrm{K}) - 0.5\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ta:Ti:\square)} = G^{\bullet}_{\mathrm{Ti:Ta:\square}}$
$G^{\circ}(T) - H^{\mathrm{o,hcp}_{A}3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti:Ti:\square)} = 0.0$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Ta,Ti:Ta:\square}} = L^{0,\mathrm{bcc}-B2}_{\mathrm{Ta,Ti:Ti:\square}} = -\ G^{\bullet}_{\mathrm{Ti:Ta:\square}}$$
$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Ta:Ta,Ti:\square}} = L^{0,\mathrm{bcc}-B2}_{\mathrm{Ti:Ta,Ti:\square}} = -\ G^{\bullet}_{\mathrm{Ti:Ta:\square}}$$

Phase bcc–$B2$

$G^{\bullet}_{\mathrm{Ti:Ta:\square}} = 2500$

$G^{\circ}(T) - H^{\mathrm{o,bcc}-A2}_{\mathrm{Ta}}(298.15\ \mathrm{K}) = \mathrm{G(Ta:Ta:\square)} = 0.0$

$G^{\circ}(T) - 0.5\ H^{\mathrm{o,bcc}-A2}_{\mathrm{Ta}}(298.15\ \mathrm{K}) - 0.5\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ta:Ti:\square)} = 2.0\ G^{\bullet}_{\mathrm{Ti:Ta:\square}}$

$G^{\circ}(T) - 0.5\ H^{\mathrm{o,bcc}-A2}_{\mathrm{Ta}}(298.15\ \mathrm{K}) - 0.5\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti:Ta:\square)} = 2.0\ G^{\bullet}_{\mathrm{Ti:Ta:\square}}$

$G^{\circ}(T) - H^{\mathrm{o,hcp}_{A}3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti:Ti:\square)} = 0.0$

Phase bcc–$A2$

$L^{0,\mathrm{bcc}-A2}_{\mathrm{Ta,Ti:\square}} = 12000$

$L^{1,\mathrm{bcc}-A2}_{\mathrm{Ta,Ti:\square}} = -2500$

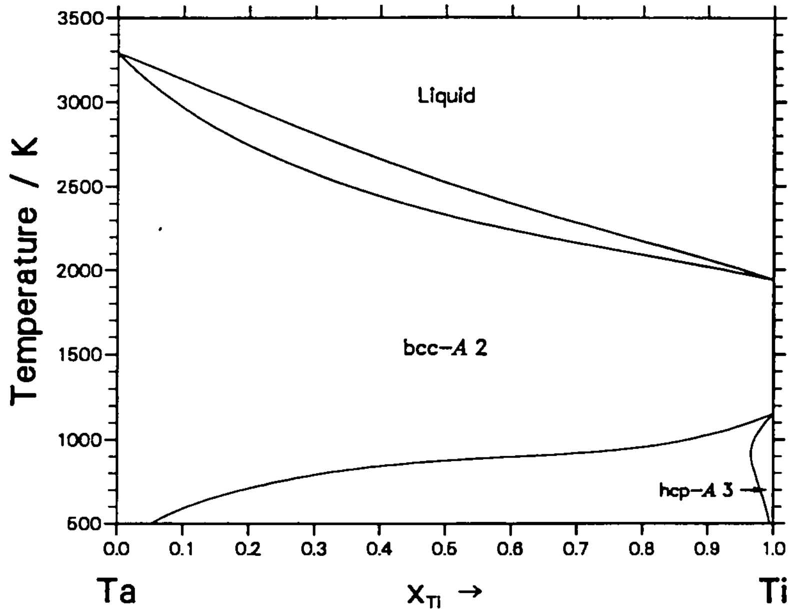


Table I – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group
Ta–Ti	(V)	W	*cI2* $Im\bar{3}m$
	(Ti)	Mg	*hP2* $P6_3/mmc$
	(Ti)	W	*cI2* $Im\bar{3}m$

System Ti–V

Solution Phases:

Liquid, bcc–$A2$, hcp–$A3$

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc–$A2$: Substitutional, Redlich-Kister
hcp–$A3$: Substitutional, Redlich-Kister
:

Assessor and Date:

N. Saunders (1990)

Thermodynamic properties of the solution phases (J.mol^{-1})

Phase bcc–$A2$

$$L^{0,\mathrm{bcc-}A2}_{\mathrm{Ti,V:\square}} = 10500 - 1.5\ T$$

$$L^{1,\mathrm{bcc-}A2}_{\mathrm{Ti,V:\square}} = 2000$$

$$L^{2,\mathrm{bcc-}A2}_{\mathrm{Ti,V:\square}} = 1000$$

Phase hcp–$A3$

$$L^{0,\mathrm{hcp-}A3}_{\mathrm{Ti,V:\square}} = 20000$$

Phase liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Ti,V}} = 1400$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Ti,V}} = 4100$$

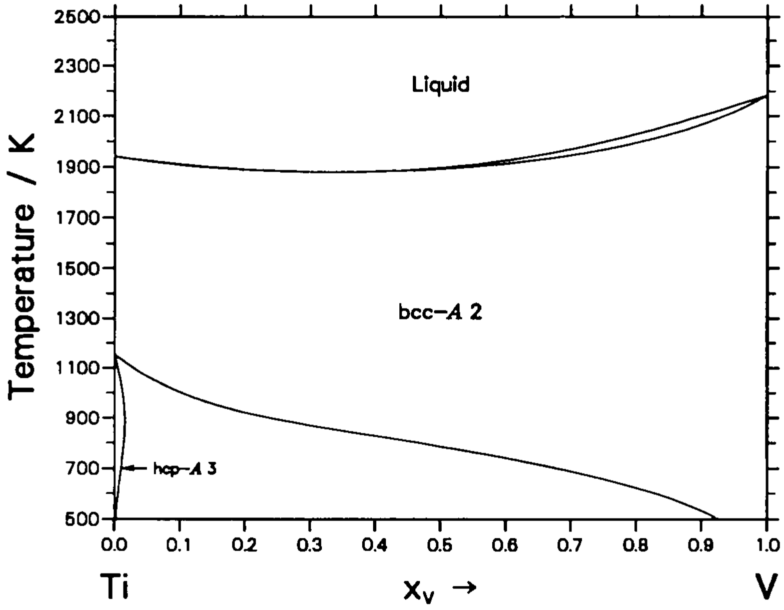


Table I – Invariant Reactions.

Reaction	Type	Compositions x_V	T / K
bcc-$A2$ ⇌ Liquid	Congruent	0.333 0.333	1881.0

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group
Ti-V	(Ti)	Mg	$hP2$ $P6_3/mmc$
	(Ti)	W	$cI2$ $Im\bar{3}m$
	(V)	W	$cI2$ $Im\bar{3}m$

System Ti–W

Solution Phases:

(stable) Liquid, bcc–$A2$, hcp–$A3$
(metastable) : bcc–$B2$, fcc–$A1$

Compounds:

(metastable) : AlM-$D0_{19}$, AlTi–$L1_0$

Modelling:

Liquid : Substitutional, Redlich–Kister
bcc–$A2$: see above
bcc–$B2$: Sublattice model, $(\mathrm{Ti,W})_{0.5}(\mathrm{Ti,W})_{0.5}(\square)_3$
The thermodynamic description of the bcc–B2 takes into account the ordering reaction bcc–$A2 \rightleftharpoons$ bcc–$B2$. Two descriptions are given: one using equations 23 and 27, the other using equations 23 and 28. For the latter, the parameters are given in a frame.
fcc–$A1$: Substitutional, Redlich–Kister
hcp–$A3$: Substitutional, Redlich–Kister
AlM–$D0_{19}$: Sublattice model, $(\mathrm{Ti,W})(\mathrm{Ti,W})_3$
AlTi–$L1_0$: Sublattice model, (Ti,W)(Ti,W)
:

Assessor and Date:

N. Saunders, 1997.

Thermodynamic properties of the solution phases (J.mol^{-1})

Phase fcc–$A1$

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Ti,W}:\square} = 33825$$

Phase hcp–$A3$

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Ti,W}:\square} = 35774$$

Phase liquid

$$L^{0,\text{liquid}}_{\text{Ti,W}} = 28392$$

$$L^{1,\text{liquid}}_{\text{Ti,W}} = -4282$$

Phase AlM-$D0_{19}$

$$G^\circ(T) - 4.0\ H^{\circ,\text{hcp}-A3}_{\text{Ti}}(298.15\text{ K}) = \text{G(Ti:Ti)} = 4.0 + 4.0\ \text{GHSER}_{\text{Ti}}$$

$$G^\circ(T) - 3.0\ H^{\circ,\text{hcp}-A3}_{\text{Ti}}(298.15\text{ K}) - H^{\circ,\text{bcc}-A2}_{\text{W}}(298.15\text{ K}) = \text{G(Ti:W)} = 26832 + 3.0\ \text{GHCP}_{\text{W}} + \text{GHSER}_{\text{Ti}}$$

$$G^\circ(T) - H^{\circ,\text{hcp}-A3}_{\text{Ti}}(298.15\text{ K}) - 3.0\ H^{\circ,\text{bcc}-A2}_{\text{W}}(298.15\text{ K}) = \text{G(W:Ti)} = 26832 + \text{GHCP}_{\text{W}} + 3.0\ \text{GHSER}_{\text{Ti}}$$

$$G^\circ(T) - 4.0\ H^{\circ,\text{bcc}-A2}_{\text{W}}(298.15\text{ K}) = \text{G(W:W)} = 4.0\ \text{GHCP}_{\text{W}}$$

$$L^{0,\text{AlM}-D0_{19}}_{\text{Ti,W:Ti}} = L^{0,\text{AlM}-D0_{19}}_{\text{Ti,W:Wi}} = 80492$$

$$L^{0,\text{AlM}-D0_{19}}_{\text{Ti:Ti,W}} = L^{0,\text{AlM}-D0_{19}}_{\text{W:Ti,W}} = 8944$$

Phase AlTi–$L1_0$

$$G^\circ(T) - 4.0\ H^{\circ,\text{hcp}-A3}_{\text{Ti}}(298.15\text{ K}) = \text{G(Ti:Ti)} = 2.0\ \text{GFCC}_{\text{Ti}}$$

$$G^\circ(T) - H^{\circ,\text{hcp}-A3}_{\text{Ti}}(298.15\text{ K}) - H^{\circ,\text{bcc}-A2}_{\text{W}}(298.15\text{ K}) = \text{G(Ti:W)} = 4250 + \text{GFCC}_{\text{Ti}} + \text{GFCC}_{\text{W}}$$

$$G^\circ(T) - H^{\circ,\text{hcp}-A3}_{\text{Ti}}(298.15\text{ K}) - H^{\circ,\text{bcc}-A2}_{\text{W}}(298.15\text{ K}) = \text{G(W:Ti)} = 4250 + \text{GFCC}_{\text{Ti}} + \text{GFCC}_{\text{W}}$$

$$G^\circ(T) - 2.0\ H^{\circ,\text{bcc}-A2}_{\text{W}}(298.15\text{ K}) = \text{G(W:W)} = 2.0\ \text{GFCC}_{\text{W}}$$

$$L^{0,\text{AlTi}-L1_0}_{\text{Ti,W:Ti}} = L^{0,\text{AlTi}-L1_0}_{\text{Ti:Ti,W}} = 16914$$

$$L^{0,\text{AlTi}-L1_0}_{\text{Ti,W:W}} = L^{0,\text{AlTi}-L1_0}_{\text{W:Ti,W}} = 16914$$

Phase bcc–$A2$

$$L^{0,\text{bcc}-A2}_{\text{Ti,W:}\square} = 3957{+}13.033\ T$$

$$L^{1,\text{bcc}-A2}_{\text{Ti,W:}\square} = 10640{-}4.464\ T$$

Phase bcc–$B2$

$$G^{*}_{\text{Ti:W:}\square} = 0$$

$$G^\circ(T) - H^{\circ,\text{hcp}-A3}_{\text{Ti}}(298.15\text{ K}) = \text{G(Ti:Ti:}\square\text{)} = 0.0$$

$$G^\circ(T) - 0.5\ H^{\circ,\text{hcp}-A3}_{\text{Ti}}(298.15\text{ K}) - 0.5\ H^{\circ,\text{bcc}-A2}_{\text{W}}(298.15\text{ K}) = \text{G(Ti:W:}\square = G^{*}_{\text{Ti:W:}\square}$$

$$G^\circ(T) - 0.5\ H^{\circ,\text{hcp}-A3}_{\text{Ti}}(298.15\text{ K}) - 0.5\ H^{\circ,\text{bcc}-A2}_{\text{W}}(298.15\text{ K}) = \text{G(W:Ti:}\square\text{)} = G^{*}_{\text{Ti:W:}\square}$$

$$G^\circ(T) - H^{\circ,\text{bcc}-A2}_{\text{W}}(298.15\text{ K}) = \text{G(W:W:}\square\text{)} = 0.0$$

$$L^{0,\text{bcc}-B2}_{\text{Ti,W:W:}\square} = L^{0,\text{bcc}-B2}_{\text{Ti,W:Ti:}\square} = -G^{*}_{\text{Ti:W:}\square}$$

$$L^{0,\text{bcc}-B2}_{\text{W:Ti,W:}\square} = L^{0,\text{bcc}-B2}_{\text{Ti:Ti,W:}\square} = -G^{*}_{\text{Ti:W:}\square}$$

Phase bcc–$B2$

$G^{*}_{\mathrm{Ti:W:\square}} = 0$

$G^{\circ}(T) - H^{\mathrm{o,bcc-}A2}_{\mathrm{W}}(298.15\ \mathrm{K}) = \mathrm{G(W{:}W{:}\square)} = 0.0$

$G^{\circ}(T) - 0.5\ H^{\mathrm{o,bcc-}A2}_{\mathrm{W}}(298.15\ \mathrm{K}) - 0.5\ H^{\mathrm{o,hcp-}A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(W{:}Ti{:}\square)} = 2.0\ G^{*}_{\mathrm{Ti:W:\square}}$

$G^{\circ}(T) - 0.5\ H^{\mathrm{o,bcc-}A2}_{\mathrm{W}}(298.15\ \mathrm{K}) - 0.5\ H^{\mathrm{o,hcp-}A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}W{:}\square)} = 2.0\ G^{*}_{\mathrm{Ti:W:\square}}$

$G^{\circ}(T) - H^{\mathrm{o,hcp}_{A}3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Ti{:}Ti{:}\square)} = 0.0$

Phase bcc–$A2$

$L^{0,\mathrm{bcc-}A2}_{\mathrm{Ti,W:\square}} = 3957{+}13.033\ T$

$L^{1,\mathrm{bcc-}A2}_{\mathrm{Ti,W:\square}} = 10640{-}4.464\ T$

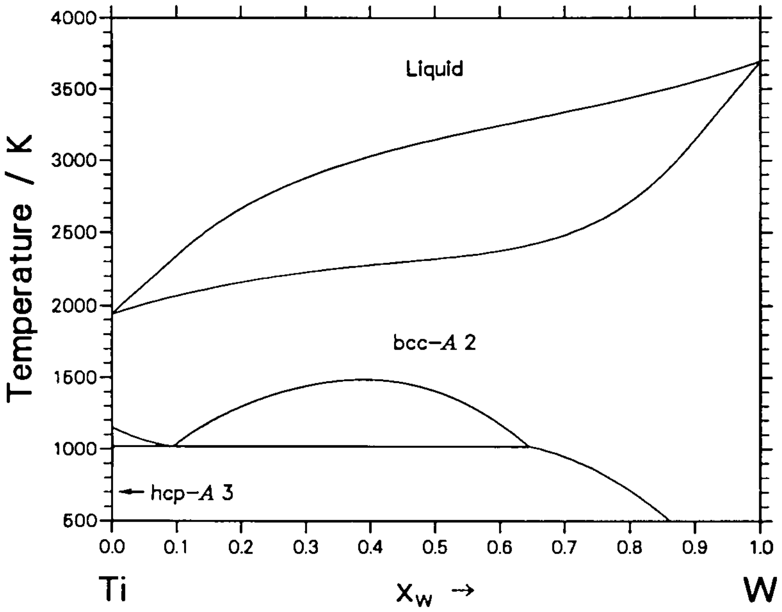


Table I – Invariant Reactions.

Reaction	Type	Compositions x_{W}	T / K
hcp–$A3$ bcc–$A2$' $\rightleftharpoons$ bcc–$A2$"	Monotectoid	.002 .645 .095	1019.5

Table II – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group
Ti–W	(V)	W	$cI2$ $Im\bar{3}m$
	(Ti)	Mg	$hP2$ $P6_3/mmc$
	(Ti)	W	$cI2$ $Im\bar{3}m$

System V-Zr

Solution Phases:

Liquid, bcc-*A*2, hcp-*A*3

Compound:

V_2Zr

Modelling:

bcc-*A*2	:	Substitutional, Redlich-Kister
hcp-*A*3	:	Substitutional, Redlich-Kister
Liquid	:	Substitutional, Redlich-Kister
V_2Zr	:	Sublattice model, $(V)_2(Zr)$

Assessor and Date:

J. Korb, and K. Hack, GTT, Germany (1995).

Thermodynamic properties of the solution and compound phases ($J.mol^{-1}$)

Phase V_2Zr

$$G^\circ(T) - 2.0\ H_V^{o,bcc-A2}(298.15\text{ K}) - H_{Zr}^{o,hcp-A3}(298.15\text{ K}) = - 63100 + 26.83\ T + 2.0\ \text{GLIQ}_V + \text{GLIQ}_{Zr}$$

Phase liquid

$$L_{V,Zr}^{0,liquid} = - 23986 + 19.338\ T$$

$$L_{V,Zr}^{1,liquid} = - 2058.35 + 3.289\ T$$

Phase bcc-*A*2

$$L_{V,Zr:\square}^{0,bcc-A2} = 21876 + 7.76081\ T$$

$$L_{V,Zr:\square}^{1,bcc-A2} = 8995.72 - 0.8968\ T$$

Phase hcp-*A*3

$$L_{V,Zr:\square}^{0,hcp-A3} = 29007 - 7.2944\ T$$

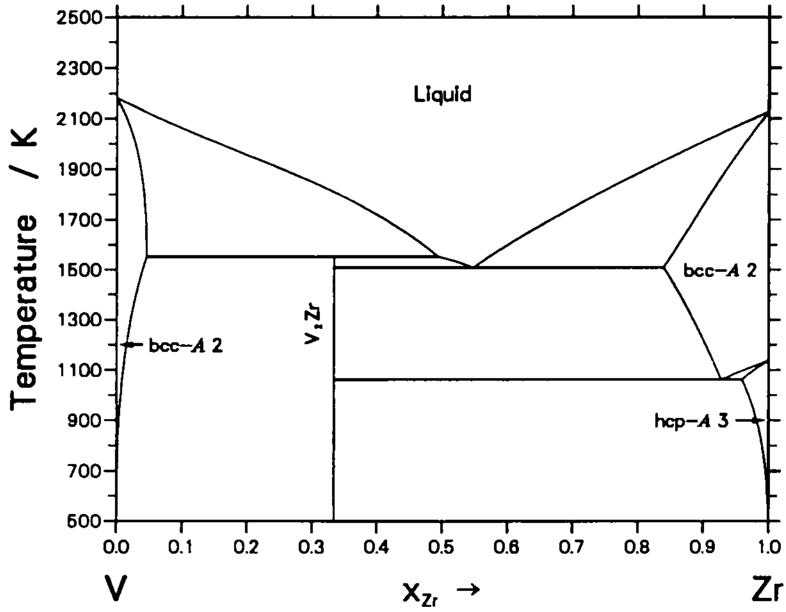


Table I - Invariant Reactions.

Reaction	Type	Compositions x_{Zr}			T / K
bcc–A2 +Liquid $\rightleftharpoons$ V_2Zr	Peritectic	.046	.494	.333	1552.7
Liquid $\rightleftharpoons$ V_2Zr + bcc–A2	Eutectic	.548	.333	.839	1510.2
bcc–A2 $\rightleftharpoons$ V_2Zr + hcp–A3	Eutectoid	.927	.333	.959	1062.9

Table II - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
V-Zr	(V)	W	*cI2* $Im\bar{3}m$	M 2	
	(Zr)	Mg	*hP2* $P6_3/mmc$	M 2	
	(Zr)	W	*cI2* $Im\bar{3}m$	M 4	
	V_2Zr	Cu_2Mg	*cF24* $Fd\bar{3}m$	M_1 8 M_2 16	Laves-*C*15

TERNARY SYSTEMS

System Al–C–Si

Ternary Solution Phases:

Liquid, fcc-*A*1

Ternary Compounds:

Al_4SiC_4, Al_8SiC_7

Quasi-binary phase:

$(Al,Si)_4C_3$

Modelling:

Liquid : Substitutional, Redlich-Kister
fcc-*A*1 : Substitutional, Redlich-Kister
Al_4C_3 : Quasi-binary, $(Al,Si)_4(C)_3$
Al_4SiC_4 : $(Al)_4(Si)_1(C)_4$
Al_8SiC_7 : $(Al)_8(Si)_1(C)_7$

Comments:

Liquid and fcc-*A*1 phases assumed to be ideal
Al and Si behave ideally in the Al_4C_3 phase
No ternary compounds

Assessor and Date:

J. Gröbner, H. L. Lukas, and F. Aldinger.

Publication:

Calphad **20**, 2 (1996) 247-254.

Thermodynamic properties of the solution and compound phases ($J.mol^{-1}$)

Phase Al_4SiC_4

$$G^{\circ}(T) - 4.0\ H_{Al}^{o,fcc-A1}(298.15\ K) - 4.0\ H_{C}^{o,graphite}(298.15\ K) - H_{Si}^{o,diamond}(298.15\ K) = - 380700.0 + 1233\ T - 193.902723\ T\cdot \ln T - 0.017517573\ T^2 + 3240000\ T^{-1} + 9E\text{-}07\ T^3$$

Phase Al_8SiC_7

$$G^{\circ}(T) - 8.0\ H_{Al}^{o,fcc-A1}(298.15\ K) - 7.0\ H_{C}^{o,graphite}(298.15\ K) - H_{Si}^{o,diamond}(298.15\ K) = - 686400.0 + 2212.8\ T - 344.434112\ T\cdot \ln T - 0.04544832\ T^2 + 5680000\ T^{-1} + 3.2E\text{-}06\ T^3$$

Table I - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices
Al-C-Si	(Al)	Cu	*cF4* $Fm\bar{3}m$	M 4
	(C)	graphite		
	(Si)	diamond	*cF8* $Fd3m$	
	Al_4SiC_4	Al_5C_3N	*hP18* $P6_3mc$	
	Al_8SiC_7		*hP16*	
	$(Al,Si)_4C_3$	Al_4C_3	*hP7* $R\bar{3}m$	

System Al–Cu–Li

Ternary Solution Phases:

Liquid, fcc-$A1$, bcc-$A2$

Ternary Compounds:

AlCuLi-R, AlCuLi-T1, AlCuLi-T2, AlCuLi-TB

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-$A2$: Substitutional, Redlich-Kister
fcc-$A1$: Substitutional, Redlich-Kister
AlCuLi-R : Stoichiometric, $(\mathrm{Al})_{0.55}(\mathrm{Cu})_{0.117}(\mathrm{Li})_{0.333}$
AlCuLi-T1 : Stoichiometric, $(\mathrm{Al})_{0.5}(\mathrm{Cu})_{0.25}(\mathrm{Li})_{0.25}$
AlCuLi-T2 : Stoichiometric, $(\mathrm{Al})_{0.57}(\mathrm{Cu})_{0.11}(\mathrm{Li})_{0.32}$
AlCuLi-TB : Stoichiometric, $(\mathrm{Al})_{0.60}(\mathrm{Cu})_{0.32}(\mathrm{Li})_{0.08}$

Assessor and Date:

N. Saunders, 1994.

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase AlCuLi–R

$$
\begin{aligned}
&G^{\circ}(T) - 0.55\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - 0.117\ H_{\mathrm{Cu}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K})\\
&- 0.333\ H_{\mathrm{Li}}^{\circ,\mathrm{bcc}-A2}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Cu{:}Li)} =\\
&\qquad - 20983.0 + 6.0\ T + 0.55\ \mathrm{GHSER_{Al}} + 0.117\ \mathrm{GHSER_{Cu}}\\
&\qquad + 0.333\ \mathrm{GHSER_{Li}}
\end{aligned}
$$

Phase AlCuLi–T1

$$
\begin{aligned}
&G^{\circ}(T) - 0.5\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - 0.25\ H_{\mathrm{Cu}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K})\\
&- 0.25\ H_{\mathrm{Li}}^{\circ,\mathrm{bcc}-A2}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Cu{:}Li)} =\\
&\qquad - 24560.0 + 6.0\ T + 0.25\ \mathrm{GHSER_{Al}} + 0.25\ \mathrm{GHSER_{Cu}}\\
&\qquad + 0.25\ \mathrm{GHSER_{Li}}
\end{aligned}
$$

Phase AlCuLi–T2

$$
\begin{aligned}
&G^{\circ}(T) - 0.57\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - 0.11\ H_{\mathrm{Cu}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K})\\
&- 0.32\ H_{\mathrm{Li}}^{\circ,\mathrm{bcc}-A2}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Cu{:}Li)} =\\
&\qquad - 20000.0 + 5.497\ T + 0.57\ \mathrm{GHSER_{Al}} + 0.11\ \mathrm{GHSER_{Cu}}\\
&\qquad + 0.32\ \mathrm{GHSER_{Li}}
\end{aligned}
$$

Phase AlCuLi–TB

$$
\begin{aligned}
&G^{\circ}(T) - 0.60\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - 0.32\ H_{\mathrm{Cu}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K})\\
&- 0.08\ H_{\mathrm{Li}}^{\circ,\mathrm{bcc}-A2}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Cu{:}Li)} =\\
&\qquad - 19918.0 + 4.0\ T + 0.60\ \mathrm{GHSER_{Al}} + 0.32\ \mathrm{GHSER_{Cu}}\\
&\qquad + 0.08\ \mathrm{GHSER_{Li}}
\end{aligned}
$$

Table I – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub–lattices	Comments
Al-Cu-Li	(Al)	Cu	*cF4* $Fm\bar{3}m$	M 4	
	(Cu)	Cu	*cF4*	M 4	
	(Li)	W	*cI2* $Im\bar{3}m$	M 2	
	$Al_{7.5}Cu_4Li$	CaF_2	*cF*12 $Fm\bar{3}m$		AlCuLi-TB
	Al_2CuLi	Al_2CuLi	*hP*12 $P6/mmm$		AlCuLi-T1
	Al_6CuLi_3				AlCuLi-T2 quasicrystal
	Al_5CuLi_3	$Mg_{23}(Zn,Al_{49}$	*cI*162 $Im\bar{3}$		AlCuLi-TR

System Al–Cu–Mg

Ternary Solution Phases:

Liquid, fcc-*A*1, hcp-*A*3

Ternary Compounds:

Laves-*C*14, Laves-*C*15, Laves-*C*36, Q-Phase, S-Phase, τ, V-Phase

Modelling:

Liquid : Substitutional, Redlich-Kister
fcc-*A*1 : Substitutional, Redlich-Kister
hcp-*A*3 : Substitutional, Redlich-Kister
Laves-*C*14 : Sublattice model, $(Al,Cu,Mg)(Al,CuMg)_2$
Laves-*C*15 : Sublattice model, $(Al,Cu,Mg)(Al,Cu,Mg)_2$
Laves-*C*36 : Sublattice model, $(Al,Cu,Mg)(Al,Cu,Mg)_2$
τ : Sublattice model, $(Mg)_{26}(Al, Mg)_6(Al,Cu,Mg)_{48}(Al)$
Q-Phase : Stoichiometric, $(Al)_7(Cu)_3(Mg)_6$
S-Phase : Stoichiometric, $(Al)_2(Cu)(Mg)$
V-Phase : Stoichiometric, $(Al)_5(Cu)_6(Mg)_2$

Assessor and Date:

T. Bühler, RWTH, Germany, (1997).

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase Q-Phase

$$G^{\circ}(T) - 7.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K})$$
$$- 6.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Cu{:}Mg)} =$$
$$- 221500 + 18.46\ T + 7.0\ \mathrm{GHSER_{Al}} + 3.0\ \mathrm{GHSER_{Cu}}$$
$$+ 6.0\ \mathrm{GHSER_{Mg}}$$

Phase Laves–$C14$

$$L^{0,\mathrm{Laves}-C14}_{\mathrm{Cu,Mg:Al}} = 13011.35$$

$$L^{0,\mathrm{Laves}-C14}_{\mathrm{Cu:Al,Mg}} = 8000$$

$$L^{0,\mathrm{Laves}-C14}_{\mathrm{Al,Mg:Cu}} = 15000$$

$$L^{0,\mathrm{Laves}-C14}_{\mathrm{Al:Cu,Mg}} = 6599.45$$

$$L^{0,\mathrm{Laves}-C14}_{\mathrm{Al,Cu:Mg}} = -224000 + 2.44\ T$$

Phase Laves–$C15$

$$L^{0,\mathrm{Laves}-C15}_{\mathrm{Cu,Mg:Al}} = 13011.35$$

$$L^{0,\mathrm{Laves}-C15}_{\mathrm{Cu:Al,Mg}} = 8000$$

$$L^{0,\mathrm{Laves}-C15}_{\mathrm{Al,Mg:Cu}} = 15000$$

$$L^{0,\mathrm{Laves}-C15}_{\mathrm{Al:Cu,Mg}} = 6599.45$$

$$L^{0,\mathrm{Laves}-C15}_{\mathrm{Al,Cu:Mg}} = -180000 - 1.615\ T$$

Phase Laves–$C36$

$$L^{0,\mathrm{Laves}-C36}_{\mathrm{Cu,Mg:Al}} = 13011.35$$

$$L^{0,\mathrm{Laves}-C36}_{\mathrm{Cu:Al,Mg}} = 8000$$

$$L^{0,\mathrm{Laves}-C36}_{\mathrm{Al,Mg:Cu}} = 15000$$

$$L^{0,\mathrm{Laves}-C36}_{\mathrm{Al:Cu,Mg}} = 6599.45$$

$$L^{0,\mathrm{Laves}-C36}_{\mathrm{Al,Cu:Mg}} = -227442 + 14.61\ T$$

Phase S–Phase

$$G^{\circ}(T) - 2.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Cu{:}Mg)} = -63200 + 4.13\ T + 2.0\ \mathrm{GHSER}_{\mathrm{Al}} + \mathrm{GHSER}_{\mathrm{Cu}} + \mathrm{GHSER}_{\mathrm{Mg}}$$

Phase V–Phase

$G^\circ(T) - 5.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 6.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K})$
$- 2.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Cu{:}Mg)} =$
$- 274527.45 + 13.0\ T + 5.0\ \mathrm{GHSER_{Al}} + 6.0\ \mathrm{GHSER_{Cu}} + 2.0\ \mathrm{GHSER_{Mg}}$

Phase τ

$G^\circ(T) - 7.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 48.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K})$
$- 26.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Al{:}Cu{:}Al)} =$
$- 23000 + 440\ T + 7.0\ \mathrm{GHSER_{Al}} + 48.0\ \mathrm{GHSER_{Cu}}$
$+ 26.0\ \mathrm{GHSER_{Mg}}$
$G^\circ(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 48.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K})$
$- 32.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Mg{:}Cu{:}Al)} =$
$- 220000 + 440\ T + \mathrm{GHSER_{Al}} + 48.0\ \mathrm{GHSER_{Cu}}$
$+ 32.0\ \mathrm{GHSER_{Mg}}$

$L^{0,\tau}_{\mathrm{Mg:Al:Al,Cu:Al}} = - 4649190 + 2261.86\ T$

$L^{0,\tau}_{\mathrm{Mg:Mg:Al,Cu:Al}} = - 4649190 + 2261.86\ T$

$L^{0,\tau}_{\mathrm{Mg:Mg:Cu,Mg:Al}} = - 220000$

Table I – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sublattices	Comments
Al-Cu-Mg	(Al)	Cu	$cF4$ $Fm\bar{3}m$	M 4	
	(Cu)	Cu	$cF4$ $Fm\bar{3}m$	M 4	
	(Mg)	Mg	$hP2$ $P6_3/mmc$	M 2	
	Laves-$C14$	$MgZn_2$	$hP12$ $P6_3/mmc$	Cu 2 Cu 6 Mg 4	
	Laves-$C15$	Cu_2Mg	$cF24$ $Fd\bar{3}m$	Mg_1 8 Cu_2 16	
	Laves-$C36$	$MgNi_2$	$hP24$ $P6_3/mmc$	Cu_1 6 Cu_2 6 Mg_1 3 Mg_2 3	
	$Al_{11}Cu_{11}Mg_4$	Mg_2Zn_{11}	$cP39$ $Pm\bar{3}$		V-phase
	$Al_7Cu_3Mg_6$		$cI96$ $Pm\bar{3}$		Q-phase
	Al_2CuMg	BRe_3	$oC16$ $Cmcm$	Cu 4 Mg 4 Al 8	S-phase
	$(Al_xCu_{1-x})_{49}Mg_{32}$	$Mg_{32}(Al,Zn)_{49}$	$cI163$	Al_1 1 Cu_1 1 Mg 6 Al_2 6 Al_3 8 Cu_2 12	

System Al–Cu–Si

Ternary Solution Phases:

Liquid, fcc–*A*1, bcc–*A*2, hcp–*A*3

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc–*A*2 : Substitutional, Redlich-Kister
fcc–*A*1 : Substitutional, Redlich-Kister
hcp–*A*3 : Substitutional, Redlich-Kister

Assessor and Date:

T. Bühler, RWTH, Aachen, Germany, (1997).

Comments:

No coefficients for the ternary solution phases.
No ternary compounds.

Table I – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices
Al-Cu-Mg	(Al)	Cu	*cF4* $Fm\bar{3}m$	M 4
	(Cu)	Cu	*cF4* $Fm\bar{3}m$	M 4
	(Si)	diamond	*cF8* $Fd\bar{3}m$	M 8

System Al–Fe–Mn

Ternary Solution Phases:

Liquid, fcc-$A1$, Al_8Mn_5-$D8_{10}$

Quasi-binary phases:

$Al_{13}Fe_4$, Al_2Fe, Al_5Fe_2, Al_6Mn,Al_4Mn, $Al_{12}Mn$

Modelling:

Liquid : Substitutional, Redlich-Kister
Al_5Fe4 : Substitutional, Redlich-Kister
fcc-$A1$: Substitutional, Redlich-Kister
Al_8Mn_5-$D8_{10}$: Sublattice model, $(Al)_{12}(Mn)_4(Al,Fe,Mn)_{10}$
Al_2Fe : Quasi-binary, $(Al)_2(Fe,Mn)$
Al_5Fe_2 : Quasi-binary, $(Al)_5(Fe,Mn)_2$
$Al_{13}Fe_4$: Quasi-binary, $(Al)_{.6275}(Fe,Mn)_{.235}(Al,\square)_{.1375}$
Al_4Mn : Quasi-binary, $(Al)_4(Fe,Mn)$
Al_6Mn : Quasi-binary, $(Al)_6(Fe,Mn)$
$Al_{12}Mn$: Quasi-binary, $(Al)_{12}Mn$

Comments:

The data below are valid in the composition range $x_{Mn} < 0.25$ ($wt\%_{Mn} < 40.0$) and $x_{Fe} < 0.25$ ($wt\%_{Fe} < 40.0$)
No ternary interaction coefficients for the liquid phase. Interactions between Fe and Mn in $Al_{12}Mn$,Al_2Fe and Al_5Fe_2 assumed to be ideal.

Assessor and Date:

Å. Jansson, and T.G. Chart (August 1997)

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase fcc-$A1$

$$L^{0,fcc-A1}_{Al,Fe,Mn:\square} = 0.000$$

$$=$$

$$L^{1,fcc-A1}_{Al,Fe,Mn:\square} = -63652$$

$$=$$

$$L^{2,fcc-A1}_{Al,Fe,Mn:\square} = -26753$$

Phase $\mathrm{Al_{13}Fe_4}$

$$\begin{aligned} L^{0,\mathrm{Al_{13}Fe_4}}_{\mathrm{Al:Fe,Mn:Al}} &= -11987 + 6\ T \\ &= \\ L^{0,\mathrm{Al_{13}Fe_4}}_{\mathrm{Al:Fe,Mn:\square}} &= -11987 + 6\ T \end{aligned}$$

Phase $\mathrm{Al_4Mn}$

$$L^{0,\mathrm{Al_4Mn}}_{\mathrm{Al:Fe,Mn}} = -10000$$

Phase $\mathrm{Al_6Mn}$

$$L^{0,\mathrm{Al_6Mn}}_{\mathrm{Al:Fe,Mn}} = -32753 + 21\ T$$

Phase $\mathrm{Al_8Mn_5}$–$D8_{10}$

$$\begin{aligned} &G^\circ(T) - 12.0\ H^{\mathrm{o,fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 10.0\ H^{\mathrm{o,bcc}-A2,\mathrm{para}}_{\mathrm{Fe}}(298.15\mathrm{K}) \\ &- 4.0\ H^{\mathrm{o,cbcc}-A12,\mathrm{para}}_{\mathrm{Mn}}(298.15\ \mathrm{K}) = \\ &\qquad - 632544.85 + 12.0\ \mathrm{GHSER_{Al}} + 10.0\ \mathrm{GHSER_{Fe}} \\ &\qquad + 4.0\ \mathrm{GHSER_{Mn}} \end{aligned}$$

$$L^{0,\mathrm{Al_8Mn_5}-D8_{10}}_{\mathrm{Al:Mn:Al,Fe}} = -457832.778$$

$$L^{0,\mathrm{Al_8Mn_5}-D8_{10}}_{\mathrm{Al:Mn:Fe,Mn}} = -11169.158$$

Table I - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-Fe-Mn	(Al)	Cu	*cF*4 $Fm\bar{3}m$	M 4	
	(Fe)	Cu	*cF*4 $Fm\bar{3}m$	M 4	
	(Fe)	W	*cI*2 $Im\bar{3}m$	M 2	
	α-Mn	α-Mn	*c*58 $I\bar{4}3m$		cbcc-*A*1
	β-Mn	β-Mn	*cP*20 $P4_132$		cub-*A*13
	AlFe	CsCl	*cP*2 $Pm\bar{3}m$	M_1 1 M_2 1	
	$AlFe_3$	BiF_3	*cF*16 $Fm\bar{3}m$	Al 4 Fe_1 4 Fe_2 8	not considered
	Al_2Fe	Al_2Fe	*aP*18 $P1$		
	Al_3Fe		*mC*102 $C2/m$		designated by $Al_{13}Fe_4$
	Al_5Fe_2		*oC** *Cmcm*		
	Al_4Mn	Al_4Mn	*oP*60 *Pnnn*		
	Al_6Mn	Al_6Mn	*oC*28		
	$Al_{12}Mn$	$Al_{12}W$	*cI*26 $Im\bar{3}$		not quoted in [90Mas] metast.
	Al_8Mn_5	Al_8Cr_5	*hR*26 $R3m$		Al_8Mn_5-$D8_8$

System Al–Fe–Si

Ternary Solution Phases:

Liquid, fcc-*A*1, bcc-*A*2, bcc-*B*2

Quasi-binary phases:

AlFeSi-α, AlFeSi-β, AlFeSi-γ, AlFeSi-γ, $Al_{13}Fe_4$

Modelling:

Liquid : Substitutional, Redlich-Kister
Al_5Fe_4 : Substitutional, Redlich-Kister
fcc-*A*1 : Substitutional, Redlich-Kister
bcc-*A*2 : Substitutional, Redlich-Kister
bcc-*B*2 : Sublattice model, $(Al,Fe,Si)_{0.5}(Al,Fe,Si)_{0.5}(\square)_3$
$Al_{13}Fe_4$: Quasi-binary, $(Al)_{.6275}(Fe)_{.235}(Al,Si,\square)_{.1375}$
AlFeSi-α : Quasi-binary, $(Al)_{.6612}(Fe)_{.19}(Si)_{.0496}(Al,Si)_{.0992}$
AlFeSi-β : Stoichiometric, $(Al)_{14}(Fe)_3(Si)_3$
AlFeSi-δ : Stoichiometric, $(Al)_{.55}(Fe)_{.15}(Si)_{.3}$
AlFeSi-γ : Stoichiometric, $(Al)_3(Fe)(Si)$
AlFeSi-τ_1 : Stoichiometric, $(Al)_2(Fe)_2(Si)$
AlFeSi-τ_3 : Stoichiometric, $(Al)_2(Fe)(Si)$

Comments:

No ternary interaction coefficients for the substitutional solutions.

Assessor and Date:

P. Kolby, 1997.

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase $Al_{13}Fe_4$

$$\begin{aligned} G^\circ(T) &- 0.6275\ H_{Al}^{\circ,fcc-A1}(298.15\ K) - 0.235\ H_{Fe}^{\circ,bcc-A2,para}(298.15\ K) \\ &- 0.1375\ H_{Si}^{\circ,diamond}(298.15\ K) = G(Al:Fe:Si) = \\ &- 22013.336 + 0.6275\ GHSER_{Al} + 0.235\ GHSER_{Fe} + 0.1375\ GHSER_{Si} \end{aligned}$$

Phase AlFeSi–α

$G^{\circ}(T) - 0.7604\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - 0.19\ H_{\mathrm{Fe}}^{\circ,\mathrm{bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K})$
$- 0.0496\ H_{\mathrm{Si}}^{\circ,\mathrm{diamond}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Fe{:}Si{:}Al)} =$
$- 24920.609 + 5.4894\ \mathrm{T} + 0.7604\ \mathrm{GHSER}_{\mathrm{Al}} + 0.19\ \mathrm{GHSER}_{\mathrm{Fe}} + 0.0496$
$\mathrm{GHSER}_{\mathrm{Si}}$
$G^{\circ}(T) - 0.6612\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - 0.19\ H_{\mathrm{Fe}}^{\circ,\mathrm{bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K})$
$- 0.1488\ H_{\mathrm{Si}}^{\circ,\mathrm{diamond}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Fe{:}Si{:}Si)} =$
$- 25340.922 + 5.4894\ \mathrm{T} + 0.6612\ \mathrm{GHSER}_{\mathrm{Al}} + 0.19\ \mathrm{GHSER}_{\mathrm{Fe}}$
$+ 0.1488\ \mathrm{GHSER}_{\mathrm{Si}}$

Phase AlFeSi–β

$G^{\circ}(T) - 14.0\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Fe}}^{\circ,\mathrm{bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K})$
$- 3.0\ H_{\mathrm{Si}}^{\circ,\mathrm{diamond}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Fe{:}Si)} =$
$- 391310.9 + 55.84756\ \mathrm{T} + 14.0\ \mathrm{GHSER}_{\mathrm{Al}} + 3.0\ \mathrm{GHSER}_{\mathrm{Fe}}$
$+ 3.0\ \mathrm{GHSER}_{\mathrm{Si}}$

Phase AlFeSi–δ

$G^{\circ}(T) - 0.55\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - 0.15\ H_{\mathrm{Fe}}^{\circ,\mathrm{bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K})$
$- 0.3\ H_{\mathrm{Si}}^{\circ,\mathrm{diamond}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Fe{:}Si)} =$
$- 14431.105 - 2.90062\ \mathrm{T} + 0.55\ \mathrm{GHSER}_{\mathrm{Al}} + 0.15\ \mathrm{GHSER}_{\mathrm{Fe}}$
$+ 0.3\ \mathrm{GHSER}_{\mathrm{Si}}$

Phase AlFeSi–γ

$G^{\circ}(T) - 3.0\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Fe}}^{\circ,\mathrm{bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K})$
$- H_{\mathrm{Si}}^{\circ,\mathrm{diamond}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Fe{:}Si)} =$
$- 116929.6 + 8.399833\ \mathrm{T} + 3.0\ \mathrm{GHSER}_{\mathrm{Al}} + \mathrm{GHSER}_{\mathrm{Fe}} + \mathrm{GHSER}_{\mathrm{Si}}$

Phase AlFeSi–τ_1

$G^{\circ}(T) - 2.0\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Fe}}^{\circ,\mathrm{bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K})$
$- H_{\mathrm{Si}}^{\circ,\mathrm{diamond}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Fe{:}Si)} =$
$- 153000 + 2.0\ \mathrm{GHSER}_{\mathrm{Al}} + 2.0\ \mathrm{GHSER}_{\mathrm{Fe}} + \mathrm{GHSER}_{\mathrm{Si}}$

Phase AlFeSi–τ_3

$G^{\circ}(T) - 2.0\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - H_{\mathrm{Fe}}^{\circ,\mathrm{bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K})$
$- H_{\mathrm{Si}}^{\circ,\mathrm{diamond}}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Fe{:}Si)} =$
$- 99325.65 + 2.0\ \mathrm{GHSER}_{\mathrm{Al}} + \mathrm{GHSER}_{\mathrm{Fe}} + \mathrm{GHSER}_{\mathrm{Si}}$

Table I - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-Fe-Si	(Al)	Cu	*cF4* $Fm\bar{3}m$	M 4	
	(Fe)	Cu	*cF4* $Fm\bar{3}m$	M 4	
	(Fe)	W	*cI2* $Im\bar{3}m$	M 2	
	(Si)	diamond	*cF8* $Fd3m$		
	Al_3Fe		*mC102* $C2/m$		designated by $Al_{13}Fe_4$
Al-Fe-Si	AlFeSi-α	Fe_2Al_7Si	*hP246*		*hP246* and $Fe_2Al_{7.4}Si$ in [92Pet]
	AlFeSi-β	$Fe_2Al_9Si_2$	m^{**}		
	AlFeSi-γ		c^{**}		
	AlFeSi-δ	$PdGa_5$	*tI24*		$FeAl_4Si_2$ in [91Vil] $FeAl_4Si_3$ in [92Pet]
	AlFeSi-τ_1				$Fe_3Al_3Si_2$
	AlFeSi-τ_3				$Fe_5Al_9Si_5$

System Al–Li–Mg

Ternary Solution Phases:

Liquid, fcc-$A1$, bcc-$A2$, hcp-$A3$

Ternary Compounds:

AlLi, AlLiMg-τ, AlMg-β, $Al_{12}Mg_{17}$

Modelling:

Liquid	:	Substitutional, Redlich-Kister
bcc-$A2$	:	Substitutional, Redlich-Kister
fcc-$A1$	:	Substitutional, Redlich-Kister
hcp-$A3$	:	Substitutional, Redlich-Kister
AlLi	:	Sublattice model, (Al,Li,Mg)(Li,Mg,□)
AlLiMg-τ	:	Stoichiometric, $(Al)_{0.53}(Li)_{0.33}(Mg)_{0.14}$
AlMg-β	:	Sublattice model, $(Al)_{0.615}(Li,Mg)_{0.385}$
$Al_{12}Mg_{17}$	:	Sublattice model, $(Li,Mg)_{24}(Al,Li,Mg)_{10}(Al,Mg)_{24}$

Assessor and Date:

N. Saunders, (1994).

Comments:

The data below are comptatible with Version I of the Al-Mg system.

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase Liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Al,Li,Mg}} = -20000$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Al,Li,Mg}} = -15000$$

$$L^{2,\mathrm{liquid}}_{\mathrm{Al,Li,Mg}} = -20000$$

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Al,Li,Mg:\square}} = -71200.0 + 50.0\ T$$

Phase fcc–$A1$

$$L^{0,\mathrm{fcc}-A1}_{\mathrm{Al,Li,Mg:\square}} = -63650.0 + 50.0\ T$$

Phase hcp–$A3$

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Al,Li,Mg:\square}} = 1.0\mathrm{E}\text{-}4$$

$$L^{1,\mathrm{hcp}-A3}_{\mathrm{Al,Li,Mg:\square}} = 1.0\mathrm{E}\text{-}4$$

$$L^{2,\mathrm{hcp}-A3}_{\mathrm{Al,Li,Mg:\square}} = -80000 + 50.0\ T$$

Phase AlLi

$$L^{0,\mathrm{AlLi}}_{\mathrm{Al,Mg:Li}} = 3300.0 - 2.0\ T$$

$$L^{0,\mathrm{AlLi}}_{\mathrm{Al,Mg:Li,Mg}} = -43460.0 + 60.0\ T$$

$$L^{0,\mathrm{AlLi}}_{\mathrm{Al:Li,Mg}} = -25000.0 + 10.0\ T$$

Phase AlMg–β

$$L^{0,\mathrm{AlMg}-\beta}_{\mathrm{Al:Li,Mg}} = -4250$$

Phase AlLiMg–τ

$$G^\circ(T) - 0.53\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 0.33\ H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Li}}(298.15\ \mathrm{K})$$
$$- 0.14\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Al:Li:Mg)} =$$
$$- 15500 + 23.93\ \mathrm{T} - 3.0\ T\cdot \ln T + 0.53\ \mathrm{GHSER_{Al}}$$
$$+ 0.33\ \mathrm{GHSER_{Li}} + 0.14\ \mathrm{GHSER_{Mg}}$$

Phase $\mathrm{Al_{12}Mg_{17}}$

$$G^\circ(T) - 24.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 10.0\ H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Li}}(298.15\ \mathrm{K})$$
$$- 24.0\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Mg:Li:Al)} =$$
$$- 610000 + 125\ T + 24.0\ \mathrm{GHSER_{Al}} + 10.0\ \mathrm{GHSER_{Li}}$$
$$+ 24.0\ \mathrm{GHSER_{Mg}}$$

$$G^\circ(T) - 24.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 24.0\ H^{\circ,\mathrm{bcc}-A2}_{\mathrm{Li}}(298.15\ \mathrm{K})$$
$$- 10.0\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K}) = \mathrm{G(Li:Mg:Al)} =$$
$$- 625000 + 269\ T + 24.0\ \mathrm{GHSER_{Al}} + 24.0\ \mathrm{GHSER_{Li}}$$
$$+ 10.0\ \mathrm{GHSER_{Mg}}$$

$$G^{\circ}(T) - 24.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 10.0\ H_{\mathrm{Li}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K})$$
$$- 24.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Li{:}Al{:}Mg)} =$$
$$1.0\mathrm{E}{-4} + 24.0\ \mathrm{GHSER_{Al}} + 10.0\ \mathrm{GHSER_{Li}} + 24.0\ \mathrm{GHSER_{Mg}}$$

$$L^{0,\mathrm{Al_{12}Mg_{17}}}_{\mathrm{Li,Mg:Al:Al}} = -220000$$

$$L^{0,\mathrm{Al_{12}Mg_{17}}}_{\mathrm{Mg:Al,Li:Al}} = -50000$$

Table I - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-Li-Mg	(Al)	Cu	$cF4$ $Fm\bar{3}m$	M 4	
	(Li)	W	$cI2$ $Im\bar{3}m$	M 2	
	(Mg)	Mg	$hP2$ $P6_3/mmc$	M 2	
	AlLi	NaTl	$cF16$ $Fd\bar{3}m$	M_1 8 M_2 8	
	AlMg-γ	α-Mn cbcc-$A12$	$cI58$ $I\bar{4}3m$	Al 24 Mg_1 2 Mg_2 8 Mg_3 24	designated as $Al_{12}Mg_{17}$
	Al_3Mg_2	Cd_2Na	$cF112$ $Fd\bar{3}m$		$cF1832$ in [91Vil] designated as AlMg-β
	Al_2LiMg		$c*456$		AlLiMg-τ

System Al–Mg–Mn

Ternary Solution Phases:

Liquid, fcc–*A*1

Ternary Compound:

AlMgMn–T

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc–*A*2 : Substitutional, Redlich-Kister
fcc–*A*1 : Substitutional, Redlich-Kister
AlMgMn–T : Stoichiometric, $(\mathrm{Al})_{18}(\mathrm{Mg})_{3}(\mathrm{Mn})_{2}$

Assessor and Date:

I. Ansara (1994).

Comments:

The data are valid only in the Al-rich corner. Very little information on the phase relationships is known

Thermodynamic properties of the solution and compound phases ($\mathrm{J.mol^{-1}}$)

Phase AlMgMn–T

$$G^{\circ}(T) - 18.0\ H_{\mathrm{Al}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Mg}}^{\circ,\mathrm{hcp}-A3}(298.15\ \mathrm{K})$$
$$- 2.0\ H_{\mathrm{Mn}}^{\circ,\mathrm{cbcc}-A12,\mathrm{para}}(298.15\ \mathrm{K}) = G(\mathrm{Al{:}Mg{:}Mn}) =$$
$$- 206402.0 + 11.85\ T + 18.0\ \mathrm{GHSER_{Al}} + 3.0\ \mathrm{GHSER_{Mg}}$$
$$+ 2.0\ \mathrm{GHSER_{Mn}}$$

Table I - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-Mg-Mn	(Al)	Cu	*cF4* $Fm\bar{3}m$	M 4	
	(Mg)	Mg	*hP2* $P6_3/mmc$	M 2	
	α-Mn	α-Mn	c58 $I\bar{4}3m$		cbcc-*A*1
	β-Mn	β-Mn	*cP20* $P4_132$		cub-*A*13
	γ-Mn	Cu	*cF4* $Fm\bar{3}m$	M 4	
	δ-Mn	W	*cI2* $Im\bar{3}m$	M 2	
	$Al_{18}Mg_3Mn_2$	$Al_{18}Cr_2Mg_3$	*cF*184 $Fd\bar{3}m$		designated as AlMgMn-T

System Al–Mg–Si

Ternary Solution Phases:

Liquid, fcc–*A*1, hcp–*A*3, diamond

Modelling:

Liquid	:	Substitutional, Redlich-Kister
fcc–*A*1	:	Substitutional, Redlich-Kister
hcp–*A*3	:	Substitutional, Redlich-Kister
diamond	:	Substitutional, Redlich-Kister

Assessor and Date:

H. L. Lukas (1996)

Comments:

No ternary compounds or quasi-binary phases

Publication:

H. Feufel, T. Gödecke, H. L. Lukas, and F. Sommer,
J. Alloys Comp. **247**, 31–42 (1997).

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase Liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Al,Mg,Si}} = 4125.86 - 0.51573\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Al,Mg,Si}} = -47961.64 + 5.9952\ T$$

$$L^{2,\mathrm{liquid}}_{\mathrm{Al,Mg,Si}} = 25813.8 - 3.22672\ T$$

Table I - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-Mg-Si	(Al)	Cu	*cF4* $Fm\bar{3}m$	M 4	
	(Mg)	Mg	*hP2* $P6_3/mmc$	M 2	
	(Si)	diamond	*cF8* $Fd3m$		

System Al–Mg–Zn

Ternary Solution Phases:

Liquid, fcc-*A*1, hcp-*A*3, hcp-Zn, τ, φ

Compounds:

AlMg-β, AlMg-γ, Laves-*C*14

Modelling:

Liquid : Substitutional, Redlich-Kister
fcc-*A*1 : Substitutional, Redlich-Kister
hcp-*A*3 : Substitutional, Redlich-Kister
hcp-Zn : Substitutional, Redlich-Kister
AlMg-β : Sublattice model, $(Mg)_{89}(Al,Zn)_{140}$
AlMg-γ : Sublattice model, $(Al,Mg,Zn)_{12}(Al,Mg,Zn)_{12}(Mg)_{5}$
Laves-*C*14 : Sublattice model, $(Al,Mg,Zn)(Al,Mg,Zn)_{2}$
τ : Sublattice model, $(Mg)_{26}(Al,Mg)_{6}(Al,Mg,Zn)_{48}(Al)$
φ : Sublattice model, $(Mg)_{6}(Al,Zn)_{5}$

Assessor and Date:

P. Liang, H. L. Lukas (1967)

Publication:

P. Liang, T. Tarfa, J. A. Robinson, S. Wagner, P. Ochin, M. G. Harmelin, H. J. Seifert, H. L. Lukas, G. Effenberg, F. Aldinger

Thermochimica Acta, **314**, 1-2, 87-110 (1998).

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase Liquid

$L^{0,\mathrm{liquid}}_{\mathrm{Al,Mg,Zn}} = -11475 + 11\ T$

$L^{1,\mathrm{liquid}}_{\mathrm{Al,Mg,Zn}} = -11475 + 11\ T$

$L^{2,\mathrm{liquid}}_{\mathrm{Al,Mg,Zn}} = -11475 + 11\ T$

Phase hcp–$A3$

$L^{0,\mathrm{hcp}-A3}_{\mathrm{Al,Mg,Zn}} = 1.0\mathrm{E}{-4}$

$L^{1,\mathrm{hcp}-A3}_{\mathrm{Al,Mg,Zn}} = 1.0\mathrm{E}{-4}$

$L^{2,\mathrm{hcp}-A3}_{\mathrm{Al,Mg,Zn}} = 1.0\mathrm{E}{-4}$

Phase hcp–Zn

$L^{0,\mathrm{hcp-Zn}}_{\mathrm{Al,Mg,Zn}} = 1.0\mathrm{E}{-4}$

$L^{1,\mathrm{hcp-Zn}}_{\mathrm{Al,Mg,Zn}} = 1.0\mathrm{E}{-4}$

$L^{2,\mathrm{hcp-Zn}}_{\mathrm{Al,Mg,Zn}} = 1.0\mathrm{E}{-4}$

Phase Laves–$C14$

$L^{0,\mathrm{Laves}-C14}_{\mathrm{Mg,Zn:Al}} = 35000$

$L^{0,\mathrm{Laves}-C14}_{\mathrm{Zn:Al,Mg}} = 15000$

$L^{0,\mathrm{Laves}-C14}_{\mathrm{Al,Zn:Mg}} = -7500 - 18\ T$

$L^{0,\mathrm{Laves}-C14}_{\mathrm{Al:Mg,Zn}} = 8000$

$L^{0,\mathrm{Laves}-C14}_{\mathrm{Al,Mg:Zn}} = 8000$

Phase AlMg–β

$L^{0,\mathrm{AlMg}-\beta}_{\mathrm{Al,Mg,Zn}} = -1717500 + 343.5\ T$

Phase AlMg–γ

$$L^{0,\mathrm{AlMg}-\gamma}_{\mathrm{Mg:Mg:Al:Zn}} = -116000 + 58\ T$$

$$L^{0,\mathrm{AlMg}-\gamma}_{\mathrm{Mg:Zn:Al:Mg}} = 113100\text{-}14.5\ T$$

Phase φ

$$L^{0,\varphi}_{\mathrm{Mg:Mg:Al,Zn}} = -\ 23100 + 11\ T$$

Phase τ

$$G^{\circ}(T) - 7.0\ H^{\mathrm{o,fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 26.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K})$$
$$-\ 48.0\ H^{\mathrm{o,hcp-Zn}}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Al{:}Zn{:}Al)} =$$
$$-\ 832680 + 162\ T + 7.0\ \mathrm{GHSER_{Al}} + 26.0\ \mathrm{GHSER_{Mg}}$$
$$+\ 48.0\ \mathrm{GHSER_{Zn}}$$
$$G^{\circ}(T) - H^{\mathrm{o,fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 32.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K})$$
$$-\ 48.0\ H^{\mathrm{o,hcp-Zn}}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Mg{:}Mg{:}Zn{:}Al)} =$$
$$-\ 811620 + 162\ T + \mathrm{GHSER_{Al}} + 32.0\ \mathrm{GHSER_{Mg}} + 48.0\ \mathrm{GHSER_{Zn}}$$

$$L^{0,\tau}_{\mathrm{Mg:Al:Al,Zn:Al}} = -\ 16200 + 243\ T$$

$$L^{0,\tau}_{\mathrm{Mg:Mg:Al,Zn:Al}} = -\ 105300 + 243\ T$$

$$L^{0,\tau}_{\mathrm{Mg:Al:Mg,Zn:Al}} = 243000 + 81\ T$$

$$L^{0,\tau}_{\mathrm{Mg:Mg:Mg,Zn:Al}} = 243000 + 81\ T$$

Table I – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub–lattices	Comments
Al-Cu-Mg	(Al)	Cu	$cF4$ $Fm\bar{3}m$	M 4	
	(Mg)	Mg	$hP2$ $P6_3/mmc$	M 2	
	Laves-$C14$	$MgZn_2$	$hP12$ $P6_3/mmc$	Cu 2 Cu 6 Mg 4	
	Al_3Mg_2	Cd_2Na	$cF112$ $Fd\bar{3}m$		$cF1832$ in [91Vil] designated as AlMg-β
	AlMg-γ	α–Mn	$cI58$ $I\bar{4}3m$	Al 24 Mg_1 2	designated as $Al_{12}Mg_{17}$
	Φ		o*		
	τ	$Mg_{32}(Al,Zn)_{49}$	$cI162$ $Im\bar{3}$		

System Al–Mn–Si

Ternary Solution Phases:

Liquid, fcc-$A1$, Al_8Mn_5-$D8_{10}$

Quasi-binary phases:

AlMnSi-α, AlMnSi-β

Compounds:

AlMnSi-δ

Modelling:

Liquid : Substitutional, Redlich–Kister
fcc-$A1$: Substitutional, Redlich–Kister
Al_8Mn_5-$D8_{10}$: Sublattice model, $(Al,Si)_{12}(Mn)_4(Al,Mn)_{10}$
AlMnSi-α : Quasi-binary, $(Al)_{16}(Mn)_4(Si)(Al,Si)_2$
AlMnSi-β : Quasi-binary, $(Al)_{15}(Si)(Al,Si)_4(Mn)_6$
AlMnSi-δ : Stoichiometric, $(Al)_2(Mn)(Si)_3$

Comments:

The data below are valid in the composition range $x_{Si} < 0.2$ and $x_{Mn} < 0.05$
The fcc-$A1$ phase is assumed to be ideal

Assessor and Date:

P. Kolby, M.H. Rand, and T.G. Chart, 1997.

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase Liquid

$$L^{0,\mathrm{Liquid}}_{\mathrm{Al,Mn,Si}} = -37000$$

Phase Al_8Mn_5–$D8_{10}$

$$G^{\circ}(T) - 10.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 4.0\ H^{\circ,\mathrm{cbcc}-A12,\mathrm{para}}_{\mathrm{Mn}}(298.15\ \mathrm{K}) - 12.0\ H^{\circ,\mathrm{diamond}}_{\mathrm{Si}}(298.15\ \mathrm{K}) = 10.0\ \mathrm{GHSER_{Al}} + 4.0\ \mathrm{GHSER_{Mn}} + 12.0\ \mathrm{GHSER_{Si}}$$

Phase AlMnSi-α

$$G^{\circ}(T) - 18.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 4.0\ H_{\mathrm{Mn}}^{\mathrm{o,cbcc-}A12\mathrm{,para}}(298.15\ \mathrm{K}) - H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = - 755772 + 3544.43\ T - 573.95\ T \cdot \ln T - 0.114419\ T^2 + 9.70013\mathrm{E}\text{-}06\ T^3 + 3716760\ T^{-1}$$

$$G^{\circ}(T) - 16.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 4.0\ H_{\mathrm{Mn}}^{\mathrm{o,cbcc-}A12\mathrm{,para}}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = - 698911 + 2958.7\ T - 493.78\ T \cdot \ln T - 0.17905\ T^2 + 1.87237\mathrm{E}\text{-}05\ T^3 + 1822810\ T^{-1}$$

$$L_{\mathrm{Al:Mn:Si:Al,Si}}^{0,\mathrm{AlMnSi-}\alpha} = 0.0001$$

Phase AlMnSi-β

$$G^{\circ}(T) - 19.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 6.0\ H_{\mathrm{Mn}}^{\mathrm{o,cbcc-}A12\mathrm{,para}}(298.15\ \mathrm{K}) - H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = - 880648 + 3451.04\ T - 572.75\ T \cdot \ln T - 0.201935\ T^2 + 2.0\mathrm{E}\text{-}05\ T^3 + 2184750\ T^{-1}$$

$$G^{\circ}(T) - 15.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 6.0\ H_{\mathrm{Mn}}^{\mathrm{o,cbcc-}A12\mathrm{,para}}(298.15\ \mathrm{K}) - 5.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = - 779980 + 3451.04\ T - 593.657\ T \cdot \ln T - 0.16164\ T^2 + 1.35092\mathrm{E}\text{-}05\ T^3 + 2946120\ T^{-1}$$

$$L_{\mathrm{Al:Si:Al,Si:Mn}}^{0,\mathrm{AlMnSi-}\beta} = 0.0001$$

Phase AlMnSi-δ

$$G^{\circ}(T) - 2.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Mn}}^{\mathrm{o,cbcc-}A12\mathrm{,para}}(298.15\ \mathrm{K}) - H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = - 70000 - 2\ T + 2.0\ \mathrm{GHSER}_{\mathrm{Al}} + 3.0\ \mathrm{GHSER}_{\mathrm{Mn}} + \mathrm{GHSER}_{\mathrm{Si}}$$

Table I - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-Mn-Si	(Al)	Cu	$cF4$ $Fm\bar{3}m$	M 4	
	(Mg)	Mg	$hP2$ $P6_3/mmc$	M 2	
	α-Mn	α-Mn	c58 $I\bar{4}3m$		cbcc-$A1$
	β-Mn	β-Mn	$cP20$ $P4_132$		cub-$A13$
	γ-Mn	Cu	$cF4$ $Fm\bar{3}m$	M 4	
	δ-Mn	W	$cI2$ $Im\bar{3}m$	M 2	
	(Si)	diamond	$cF8$ $Fd\bar{3}m$		
	AlMnSi-α	Al_9Mn_2Si	$cP138$ $Pm\bar{3}$		
	AlMnSi-β	$Al_{10}Mn_3$	$hP26$ $P6_3/mmc$		
	AlMnSi-δ		$hP100$		quoted in [93Pet]
	Al_8Mn_5-$D8_{10}$	Al_8Cr_5	$hR26$ $R\bar{3}m$		

System Al–Mo–Ti

Solution Phases:

Liquid, bcc-$A2$, fcc-$A1$, bcc-$B2$, hcp-$A3$

Ternary Compounds:

AlM-$D0_{19}$, AlM-$D0_{22}$, AlTi-$L1_0$

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-$A2$: Substitutional, Redlich-Kister
fcc-$A1$: Substitutional, Redlich-Kister
hcp-$A3$: Substitutional, Redlich-Kister
bcc-$B2$: Sublattice model, $(\mathrm{Al,Mo,Ti})_{0.5}(\mathrm{Al,Mo,Ti})_{0.5}(\square)_3$
The thermodynamic description of the bcc-B2 takes into account the ordering reaction bcc-$A2$ $\rightleftharpoons$ bcc-$B2$.
Two descriptions are given:
one using equations 23 and 27,
the other using equations 23 and 28.
For the latter, the parameters are given in a frame.
AlM-$D0_{19}$: Sublattice model, $(\mathrm{Al,Mo,Ti})_3(\mathrm{Al,Mo,Ti})(\square)_{0.5}$
AlM-$D0_{22}$: Sublattice model, $(\mathrm{Al,Mo,Ti})_3(\mathrm{Al,Mo,Ti})$
AlTi-$L1_0$: Sublattice model, $(\mathrm{Al,Mo,Ti})(\mathrm{Al,Mo,Ti})$

Assessor and Date:

N. Saunders, 1996

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase AlM–$D0_{19}$

$$L^{0,\mathrm{AlM}-D0_{19}}_{\mathrm{Mo:Al,Ti:\square}} = 10656 - 1.332\ T$$

$$L^{0,\mathrm{AlM}-D0_{19}}_{\mathrm{Al,Ti:Mo:\square}} = 32000 - 4\ T$$

Phase AlM–$D0_{22}$

$$L^{0,\text{AlM}-D0_{22}}_{\text{Al:Mo,Ti}} = -212000 + 120\ T$$

Phase AlTi–$L1_0$

$$L^{0,\text{AlTi}-L1_0}_{\text{Mo,Ti:Al}} = L^{0,\text{AlTi}-L1_0}_{\text{Al:Mo,Ti}} = -13000$$

$$L^{1,\text{AlTi}-L1_0}_{\text{Mo,Ti:Al}} = L^{1,\text{AlTi}-L1_0}_{\text{Al:Mo,Ti}} = 1.0\text{E-}4$$

$$L^{2,\text{AlTi}-L1_0}_{\text{Mo,Ti:Al}} = L^{2,\text{AlTi}-L1_0}_{\text{Al:Mo,Ti}} = -13000$$

$$L^{0,\text{AlTi}-L1_0}_{\text{Mo:Al,Ti}} = L^{0,\text{AlTi}-L1_0}_{\text{Al,Ti:Mo}} = -15134 - 2.36\ T$$

Phase bcc–$A2$

$$L^{1,\text{bcc}-A2}_{\text{Al,Mo,Ti:}\square} = 0$$

$$L^{2,\text{bcc}-A2}_{\text{Al,Mo,Ti:}\square} = 0$$

$$L^{3,\text{bcc}-A2}_{\text{Al,Mo,Ti:}\square} = 0$$

Phase bcc–$B2$

$$L^{0,\text{bcc}-B2}_{\text{Mo,Ti:Al:}\square} = L^{0,\text{bcc}-B2}_{\text{Al:Mo,Ti:}\square} = -5000$$

$$L^{0,\text{bcc}-B2}_{\text{Mo:Al,Ti:}\square} = L^{0,\text{bcc}-B2}_{\text{Al,Ti:Mo:}\square} = 8750 - 1.25\ T$$

$$L^{0,\text{bcc}-B2}_{\text{Ti:Al,Mo:}\square} = L^{0,\text{bcc}-B2}_{\text{Al,Mo:Ti:}\square} = 14100 - 2\ T$$

Phase bcc–$A2$

$$L^{0,\text{bcc}-A2}_{\text{Al,Mo,Ti:}\square} = 0$$

$$L^{1,\text{bcc}-A2}_{\text{Al,Mo,Ti:}\square} = 0$$

$$L^{2,\text{bcc}-A2}_{\text{Al,Mo,Ti:}\square} = 0$$

Table I - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-Mo-Ti	(Al)	Cu	*cF4* $Fm\bar{3}m$	M 4	
	(Mo)	W	*cI2* $Im\bar{3}m$	M 2	
	bcc-*B2*	CsCl	*cP2* $Pm\bar{3}m$	M_1 1 M_2 1	
	(Ti)	Mg	*hP2* $P6_3/mmc$	M 2	
	(Ti)	W	*cI2* $Im\bar{3}m$	M 2	
	AlTi	AuCu	*tP4* $P4/mmm$	Al 2 Ti_1 1 Ti_2 1	AlTi-$L1_0$
	$AlTi_3$	Ni_3Sn	*hP8* $P6_3/mmc$		AlM-$D0_{19}$
	Al_3Ti	Al_3Ti	*tI8* $I4/mmm$	Al_1 2 Al_2 4 Ti 2	AlM-$D0_{22}$

System Al–N–Ti

Ternary Solution Phases:

Liquid, bcc–$A2$, hcp–$A3$

Ternary Compounds:

$AlNTi_2$, $AlNTi_3$, $Al_2N_2Ti_3$

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc–$A2$: Substitutional, Redlich-Kister
hcp–$A3$: Substitutional, Redlich-Kister
$AlNTi_2$: Stoichiometric, $(Al)(Ti)_2(N)_{0.82}$
$AlNTi_3$: Stoichiometric, $(Al)(Ti)_3(N)_{0.56}$
$Al_2N_2Ti_3$: Stoichiometric, $(Al)_2(Ti)_3(N)_2$

Assessor and Date:

K. Zeng, and R. Schmid-Fetzer, Univ. Clausthal, Germany, (1996).

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Al,Ti:N}} = -\,200000$$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Al,Ti:N,}\square} = -\,200000$$

Phase hcp–$A3$

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Al,Ti:N}} = -\,100000$$

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Al,Ti:N,}\square} = -\,80000$$

$$L^{1,\mathrm{hcp}-A3}_{\mathrm{Al,Ti:N,}\square} = -\,37300 + 100\ T$$

Phase $AlNTi_2$

$$G^{\circ}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 0.82\ H_{0.5\mathrm{N}_2}^{\mathrm{o,gas}}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = -389592 + 104\ \mathrm{T} + \mathrm{GHSER}_{\mathrm{Al}} + 2.0\ \mathrm{GHSER}_{\mathrm{Ti}} + 0.82\ \mathrm{GHSER}_{0.5\mathrm{N}_2}$$

Phase $AlNTi_3$

$$G^{\circ}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 0.56\ H_{0.5\mathrm{N}_2}^{\mathrm{o,gas}}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = -349502.5 + 92.5\ \mathrm{T} + \mathrm{GHSER}_{\mathrm{Al}} + 3.0\ \mathrm{GHSER}_{\mathrm{Ti}} + 0.56\ \mathrm{GHSER}_{0.5\mathrm{N}_2}$$

Phase $Al_2N_2Ti_3$

$$G^{\circ}(T) - 2.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) - 2.0\ H_{0.5\mathrm{N}_2}^{\mathrm{o,gas}}(298.15\ \mathrm{K}) - 3.0\ H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) = 3405331.05 - 5217.37371\ T + 1.75061514\ T^2 + 2.0\ \mathrm{GHSER}_{\mathrm{Al}} + 3.0\ \mathrm{GHSER}_{\mathrm{Ti}} + 2.0\ \mathrm{GHSER}_{0.5\mathrm{N}_2}$$

Table I:a - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices
Al-N-Ti	(Al)	Cu	*cF4* *Fm$\bar{3}$m*	M 4
	(Ti)	Mg	*hP2* *P6$_3$/mmc*	M 2
	(Ti)	W	*cI2* *Im$\bar{3}$m*	M 2
	$AlNTi_2$	$AlCCr_2$	*hP8* *P6$_3$/mmc*	
	$AlNTi_3$	CaO_3Ti	*cP5* *Pm$\bar{3}$m*	M_1 1 M_2 1 Ti 3

Table I:b - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices
	$Al_2N_2Ti_3$	$Al_2N_2Ti_3$	*hP*22 *P*31*c*	Al_1 2 Ti_1 2 Al_2 2 N_1 2 N_2 2 N_3 2 N_4 2 Ti_2 2 Ti_3 2 Ti_4 2 Ti_5 2

System Al–Nb–Ti

Solution Phases:

Liquid, bcc-$A2$, fcc-$A1$, bcc-$B2$, hcp-$A3$

Ternary Compounds:

AlM-$D0_{19}$, AlM-$D0_{22}$, AlTi-$L1_0$, σ,AlNb$_3$-$A15$

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-$A2$: Substitutional, Redlich-Kister
fcc-$A1$: Substitutional, Redlich-Kister
hcp-$A3$: Substitutional, Redlich-Kister
bcc-$B2$: Sublattice model, $(\mathrm{Al,Nb,Ti})_{0.5}(\mathrm{Al,Nb,Ti})_{0.5}(\square)_3$
bcc-$B2$: Sublattice model, $(\mathrm{Al,Mo,Ti})_{0.5}(\mathrm{Al,Mo,Ti})_{0.5}(\square)_3$
The thermodynamic description of the bcc-B2 takes into account the ordering reaction bcc-$A2$ $\rightleftharpoons$ bcc-$B2$.
Two descriptions are given:
one using equations 23 and 27,
the other using equations 23 and 28.
For the latter, the parameters are given in a frame.
AlNb$_3$-$A15$: Sublattice model, $(\mathrm{Al,Nb})(\mathrm{Nb})_3$
AlM-$D0_{19}$: Sublattice model, $(\mathrm{Al,Nb,Ti})_3(\mathrm{Al,Nb,Ti})(\square)_{0.5}$
AlM-$D0_{22}$: Sublattice model, $(\mathrm{Al,Nb,Ti})_3(\mathrm{Al,Nb,Ti})$
AlTi-$L1_0$: Sublattice model, $(\mathrm{Al,Nb,Ti})(\mathrm{Al,Nb,Ti})$
σ : Sublattice model, $(\mathrm{Al})_8(\mathrm{Nb,Ti})_4(\mathrm{Al,Nb,Ti})_{18}$

Assessor and Date:

N. Saunders, 1996

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase AlM–$D0_{22}$

$$L^{0,\mathrm{AlM-}D0_{22}}_{\mathrm{Al:Nb,Ti}} = 20000$$

Phase AlM–$D0_{19}$

$$L^{0,\mathrm{AlM}-D0_{19}}_{\mathrm{Nb:Al,Ti:\square}} = 10656 - 1.333\ T$$

$$L^{0,\mathrm{AlM}-D0_{19}}_{\mathrm{Ti:Al,Nb:\square}} = 4000$$

$$L^{0,\mathrm{AlM}-D0_{19}}_{\mathrm{Al,Ti:Nb:\square}} = 32000 - T$$

$$L^{0,\mathrm{AlM}-D0_{19}}_{\mathrm{Al,Nb:Ti:\square}} = 12000$$

Phase AlTi–$L1_0$

$$L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Al,Nb,Ti:Al}} = -\ 45000$$

$$L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Al:Al,Nb,Ti}} = -\ 45000$$

$$L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Nb,Ti:Al}} = -\ 18076 + 12\ T$$

$$L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Nb:Al,Ti}} = -\ 15134 - 2.36\ T$$

$$L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Ti:Al,Nb}} = -\ 37600$$

$$L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Al,Ti:Nb}} = -\ 15134 - 2.36\ T$$

$$L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Al:Nb,Ti}} = -\ 18076 + 12\ T$$

$$L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Al,Nb:Ti}} = -\ 37600$$

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Al,Nb,Ti:\square}} = 0$$

$$L^{1,\mathrm{bcc}-A2}_{\mathrm{Al,Nb,Ti:\square}} = 0$$

$$L^{2,\mathrm{bcc}-A2}_{\mathrm{Al,Nb,Ti:\square}} = 0$$

Phase bcc–$B2$

$$G^{\bullet}_{\mathrm{Al:Nb:\square}} = -8650 + T$$
$$G^{\bullet}_{\mathrm{Al:Ti:\square}} = -\ 8750 + 1.35\ T$$
$$G^{\bullet}_{\mathrm{Nb:Ti:\square}} = 5500$$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Nb,Ti:Al:}\square} = L^{0,\mathrm{bcc}-B2}_{\mathrm{Al:Nb,Ti:Al:}\square} = -G^{*}_{\mathrm{Nb:Ti:}\square}$$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Nb:Al,Ti:}\square} = L^{0,\mathrm{bcc}-B2}_{\mathrm{Al,Ti:Nb:}\square} = -G^{*}_{\mathrm{Al:Ti:}\square}$$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Ti:Al,Nb:}\square} = L^{0,\mathrm{bcc}-B2}_{\mathrm{Al,Nb:Ti:}\square} = -G^{*}_{\mathrm{Al:Nb:}\square}$$

Phase bcc–*A*2

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Al,Nb,Ti:}\square} = 0$$

$$L^{1,\mathrm{bcc}-A2}_{\mathrm{Al,Nb,Ti:}\square} = 0$$

$$L^{2,\mathrm{bcc}-A2}_{\mathrm{Al,Nb,Ti:}\square} = 0$$

Phase hcp–*A*3

$$L^{0,\mathrm{hcp}-A3}_{\mathrm{Al,Nb,Ti:}\square} = -10\ T$$

Phase σ

$$G^{\circ}(T) - 8.0\ H^{\mathrm{o,fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 18.0\ H^{\mathrm{o,bcc}-A2}_{\mathrm{Nb}}(298.15\ \mathrm{K}) - 4.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Al:Ti:Nb)} = -660000 + 79.5\ T + 8.0\ \mathrm{GHSER_{Al}} + 18.0\ \mathrm{GHSER_{Nb}} + 4.0\ \mathrm{GHSER_{Ti}}$$

$$G^{\circ}(T) - 8.0\ H^{\mathrm{o,fcc}-A1}_{\mathrm{Al}}(298.15\ \mathrm{K}) - 4.0\ H^{\mathrm{o,bcc}-A2}_{\mathrm{Nb}}(298.15\ \mathrm{K}) - 18.0\ H^{\mathrm{o,hcp}-A3}_{\mathrm{Ti}}(298.15\ \mathrm{K}) = \mathrm{G(Al:Nb:Ti)} = -690000 + 148.5\ T + 8.0\ \mathrm{GHSER_{Al}} + 4.0\ \mathrm{GHSER_{Nb}} + 18.0\ \mathrm{GHSER_{Ti}}$$

$$L^{0,\sigma}_{\mathrm{Al:Nb:Al,Ti:}\square} = -1680000 + 510\ T$$

$$L^{0,\sigma}_{\mathrm{Al:Ti:Al,Nb:}\square} = -990000 + 270\ T$$

$$L^{1,\sigma}_{\mathrm{Al:Ti:Al,Nb:}\square} = 420000$$

Table I - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al–Nb–Ti	(Al)	Cu	$cF4$ $Fm\bar{3}m$	M 4	
	(Nb)	W	$cI2$ $Im\bar{3}m$	M 2	
	bcc-$B2$	CsCl	$cP2$ $Pm\bar{3}m$	M_1 1 M_2 1	
	(Ti)	Mg	$hP2$ $P6_3/mmc$	M 2	
	(Ti)	W	$cI2$ $Im\bar{3}m$	M 2	
	AlTi	AuCu	$tP4$ $P4/mmm$	Al 2 Ti_1 1 Ti_2 1	AlTi-$L1_0$
	$AlTi_3$	Ni_3Sn	$hP8$ $P6_3/mmc$		AlM-$D0_{19}$
	Al_3Ti	Al_3Ti	$tI8$ $I4/mmm$	Al_1 2 Al_2 4 Ti 2	AlM-$D0_{22}$
	$AlNb_3$	Cr_3Si	$cP8$ $Pm\bar{3}n$	Al 2 Nb 6	cub-$A15$
	σ	σ CrFe	$tP30$ $P4_2/mnm$		

System Al–Si–Zn

Ternary Solution Phases:

Liquid, fcc-*A*1, hcp-Zn

Modelling:

Liquid : Substitutional, Redlich-Kister
fcc-*A*1 : Substitutional, Redlich-Kister
hcp-Zn : Substitutional, Redlich-Kister

Assessor and Date:

M. Jacobs (1992).

Comments:

No ternary interaction coefficients.
No ternary compounds.

Table I - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices
Al-Si-Zn	(Al)	Cu	*cF4* $Fm\bar{3}m$	M 4
	(Si)	diamond	*cF8* *Fd3m*	
	(Zn)	Mg	*hP2* $P6_3/mmc$	M 2

System Al–Sn–Zn

Ternary Solution Phases:

Liquid, fcc–*A*1, hcp–*A*3, hcp–Zn

Modelling:

Liquid : Substitutional, Redlich-Kister
fcc–*A*1 : Substitutional, Redlich-Kister
hcp–*A*3 : Substitutional, Redlich-Kister
hcp–Zn : Substitutional, Redlich-Kister

Assessor and Date:

H. L. Lukas (1991)

Publication:

N. Chakraborti, G. Effenberg, S. Fries, S. Kuang,
H.-L. Lukas, and G. Petzow,
Vortr. Poster Symp. Materialforsch., 1991,
2nd, 3, 2692-2693 (1991).

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase Liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{Al,Sn,Zn}} = -2777.03 + 0.59427\ T$$

$$L^{1,\mathrm{liquid}}_{\mathrm{Al,Sn,Zn}} = 15225.63 - 3.25821\ T$$

$$L^{2,\mathrm{liquid}}_{\mathrm{Al,Sn,Zn}} = -16198.13 + 3.46632\ T$$

Phase hcp–*A*3

$$L^{0,\mathrm{hcp-}A3}_{\mathrm{Al,Sn,Zn}} = 1.0\mathrm{E}\text{-}4$$

Phase hcp–Zn

$$L^{0,\mathrm{hcp-Zn}}_{\mathrm{Al,Sn,Zn}} = 1.0\mathrm{E}\text{-}4$$

Table I - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices
Al-Sn-Zn	(Al)	Cu	$cF4$ $Fm\bar{3}m$	M 4
	(Sn)	β-Sn	$tI4$ $I4_1/amd$	
	(Zn)	Mg	$hP2$ $P6_3/mmc$	M 2

System Al–Sn–Zr

Ternary Solution Phases:

Liquid, bcc–$A2$, bct–$A5$, fcc–$A1$, hcp–$A3$

Compound:

$AlSn_2Zr_5$

Modelling:

Liquid : Substitutional, Redlich-Kister
bct–$A5$: Substitutional, Redlich-Kister
fcc–$A1$: Substitutional, Redlich-Kister
hcp–$A3$: Substitutional, Redlich-Kister
$AlSn_2Zr_5$: Stoichiometric, $(Al)(Sn)_2(Zr)_5$

Assessor and Date:

J. Korb, and K. Hack, GTT, Germany (1997)

Thermodynamic properties of the compound phase (J.mol^{-1})

Phase $AlSn_2Zr_5$

$$G^\circ(T) - H_{Al}^{o,fcc-A1}(298.15\ K) - 2.0\ H_{Sn}^{o,bct-A5}(298.15\ K) - 5.0\ H_{Zr}^{o,hcp--A3}(298.15\ K) = - 58824.4 + 896.225\ T - 177.0982\ T \cdot \ln T - 0.0411\ T^2 - 8.4073E\text{-}6\ T^3 + 261079\ T^{-1}$$

Table I - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol	Sub-lattices	Comments
Al-Sn-Zr	(Al)	Cu	*cF4* $Fm\bar{3}m$		
	(Sn)	β-Sn	*tI4* $I4_1/amd$		
	(Zr)	Mg	*hP2* $P6_3/mmc$	M 2	
	(Zr)	W	*cI2* $Im\bar{3}m$	M 4	
	$AlSn_2Zr_5$				not quoted in [91Vil] nor in [90Mas]

System Al–Ta–Ti

Solution Phases:

Liquid, bcc-*A*2, fcc-*A*1, bcc-*B*2, hcp-*A*3

Ternary Compounds:

AlM-$D0_{19}$, AlM-$D0_{22}$, AlTi-$L1_0$, σ

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-*A*2 : Substitutional, Redlich-Kister
fcc-*A*1 : Substitutional, Redlich-Kister
hcp-*A*3 : Substitutional, Redlich-Kister
bcc-*B*2 : Sublattice model, $(\mathrm{Al,Ta,Ti})_{0.5}(\mathrm{Al,Ta,Ti})_{0.5}(\square)_3$
The thermodynamic description of the bcc-B2 takes into account the ordering reaction bcc-*A*2 ⇌ bcc-*B*2.
Two descriptions are given:
one using equations 23 and 27,
the other using equations 23 and 28.
For the latter, the parameters are given in a frame.
AlM-$D0_{19}$: Sublattice model, $(\mathrm{Al,Ta,Ti})_3(\mathrm{Al,Ta,Ti})(\square)_{0.5}$
AlM-$D0_{22}$: Sublattice model, $(\mathrm{Al,Ta,Ti})_3(\mathrm{Al,Ta,Ti})$
AlTi-$L1_0$: Sublattice model, $(\mathrm{Al,Ta,Ti})(\mathrm{Al,Ta,Ti})$
σ : Sublattice model, $(\mathrm{Al})_8(\mathrm{Ta,Ti})_4(\mathrm{Al,Ta,Ti})_{18}$

Assessor and Date:

N. Saunders, 1996

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase hcp-*A*3

$$L^{0,\mathrm{hcp}-B3}_{\mathrm{Al,Ta,Ti}:\square} = -40000$$

Phase AlTi–$L1_0$

$$L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Ta,Ti:Al}} = L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Al:Ta,Ti}} = -\ 11000$$

$$L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Ta:Al,Ti}} = L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Al,Ti:Ta}} = -\ 15134 - 2.36\ T$$

Phase AlM–$D0_{19}$

$$L^{0,\mathrm{AlM}-D0_{19}}_{\mathrm{Ta,Ti:Al:}\Box} = -\ 24000$$

$$L^{0,\mathrm{AlM}-D0_{19}}_{\mathrm{Ta:Al,Ti:}\Box} = 10656 - 1.332\ T$$

$$L^{0,\mathrm{AlM}-D0_{19}}_{\mathrm{Ti:Al,Ta:}\Box} = 8000$$

$$L^{0,\mathrm{AlM}-D0_{19}}_{\mathrm{Al,Ti:Ta:}\Box} = 32000 - T$$

$$L^{0,\mathrm{AlM}-D0_{19}}_{\mathrm{Al:Ta,Ti:}\Box} = 2128$$

$$L^{0,\mathrm{AlM}-D0_{19}}_{\mathrm{Al,Ta:Ti:}\Box} = 20000$$

Phase AlM–$D0_{22}$

$$L^{0,\mathrm{AlM}-D0_{22}}_{\mathrm{Al:Ta,Ti}} = 20000$$

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Al,Ta,Ti:Box}} = -\ 10000$$

Phase bcc–$B2$

$G^{*}_{\mathrm{Al:Ta}} = -\ 8250 + T$
$G^{*}_{\mathrm{Al:Ti}} = -8750 + 1.25\ T$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Ti:Al,Ta:}\Box} = L^{0,\mathrm{bcc}-B2}_{\mathrm{Al,Ta:Ti:}\Box} = -\ G^{*}_{\mathrm{Al:Ta}}$$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Ta:Al,Ti:}\Box} = L^{0,\mathrm{bcc}-B2}_{\mathrm{Al,Ti:Ta:}\Box} = -\ G^{*}_{\mathrm{Al:Ti}}$$

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Al,Mo,Ti:}\Box} = -\ 10000$$

$$L^{1,\mathrm{bcc}-A2}_{\mathrm{Al,Mo,Ti:}\Box} = -\ 10000$$

$$L^{2,\mathrm{bcc}-A2}_{\mathrm{Al,Mo,Ti:}\Box} = -\ 10000$$

Phase σ

$$G^{\circ}(T) - 8.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 18.0\ H_{\mathrm{Ta}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) - 4.0\ H_{\mathrm{Ti}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Ti{:}Ta)} =$$

$$-\ 672000 + 105\ T + 8.0\ \mathrm{GHSER_{Al}} + 18.0\ \mathrm{GHSER_{Ta}} + 4.0\ \mathrm{GHSER_{Ti}}$$

$$G^{\circ}(T) - 8.0\ H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 4.0\ H_{\mathrm{Ta}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) - 18.0\ H_{\mathrm{Ti}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) = \mathrm{G(Al{:}Ta{:}Ti)} =$$

$$-\ 720000 + 153.9\ T + 8.0\ \mathrm{GHSER_{Al}} + 4.0\ \mathrm{GHSER_{Ta}} + 18.0\ \mathrm{GHSER_{Ti}}$$

$$L^{0,\sigma}_{\mathrm{Al:Ta:Al,Ti:\square}} = -\ 1680000 + 510\ T$$

$$L^{0,\sigma}_{\mathrm{Al:Ti:Al,Ta:\square}} = -\ 1230000 + 450\ T$$

$$L^{1,\sigma}_{\mathrm{Al:Ti:Al,Ta:\square}} = 1.0\mathrm{E}\text{-}4$$

$$L^{2,\sigma}_{\mathrm{Al:Ti:Al,Ta:\square}} = 300000$$

Table I - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al–Ta–Ti	(Al)	Cu	*cF4* $Fm\bar{3}m$	M 4	
	(Ta)	W	*cI2* $Im\bar{3}m$	M 2	
	bcc-$B2$	CsCl	*cP2* $Pm\bar{3}m$	$\mathrm{M_1}$ 1 $\mathrm{M_2}$ 1	
	(Ti)	Mg	*hP2* $P6_3/mmc$	M 2	
	(Ti)	W	*cI2* $Im\bar{3}m$	M 2	
	AlTi	AuCu	*tP4* $P4/mmm$	Al 2 $\mathrm{Ti_1}$ 1 $\mathrm{Ti_2}$ 1	AlTi-$L1_0$
	$\mathrm{AlTi_3}$	$\mathrm{Ni_3Sn}$	*hP8* $P6_3/mmc$		AlM-$D0_{19}$
	$\mathrm{Al_3Ti}$	$\mathrm{Al_3Ti}$	*tI8* $I4/mmm$	$\mathrm{Al_1}$ 2 $\mathrm{Al_2}$ 4 Ti 2	AlM-$D0_{22}$
	σ	σ CrFe	*tP30* $P4_2/mnm$		

System Al–Ti–W

Solution Phases:

Liquid, bcc–$A2$, fcc–$A1$, bcc–$B2$, hcp–$A3$

Ternary Compounds:

AlM-$D0_{19}$, AlTi-$L1_0$

Modelling:

Liquid	:	Substitutional, Redlich-Kister
bcc–$A2$	:	Substitutional, Redlich-Kister
fcc–$A1$	:	Substitutional, Redlich-Kister
hcp-$A3$	:	Substitutional, Redlich-Kister
bcc-$B2$	:	Sublattice model, $(\mathrm{Al,Ti,W})_{0.5}(\mathrm{Al,Ti,W})_{0.5}(\square)_3$ The thermodynamic description of the bcc-B2 takes into account the ordering reaction bcc–$A2$ ⇌ bcc–$B2$. Two descriptions are given: one using equations 23 and 27, the other using equations 23 and 28. For the latter, the parameters are given in a frame.
AlM-$D0_{19}$	:	Sublattice model, $(\mathrm{Al,Ti,W})_3(\mathrm{Al,Ti,W})(\square)_{0.5}$
AlTi-$L1_0$	:	Sublattice model, (Al,Ti,W)(Al,Ti,W)

Assessor and Date:

N. Saunders, 1996

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase AlM–$D0_{19}$

$$L^{0,\mathrm{AlM}-D0_{19}}_{\mathrm{Ti,W:Al:\square}} = 73212$$

$$L^{0,\mathrm{AlM}-D0_{19}}_{\mathrm{Ti:Al,W:\square}} = -2000$$

$$L^{0,\mathrm{AlM}-D0_{19}}_{\mathrm{Al,Ti:W:\square}} = 8000$$

$$L^{0,\mathrm{AlM}-D0_{19}}_{\mathrm{Al:Ti,W:\square}} = 8136$$

Phase AlTi–$L1_0$

$$L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Ti,W:Al}} = L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Al:Ti,W}} = 16914$$

$$L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{W:Al,Ti}} = L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Al,Ti:W}} = -\,15134 - 2.36\ T$$

$$L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Ti:Al,W}} = L^{0,\mathrm{AlTi}-L1_0}_{\mathrm{Al,W:Ti}} = -\,3000$$

Phase bcc–$A2$

$$L^{1,\mathrm{bcc}-A2}_{\mathrm{Al,Ti,W:\square}} = 0$$

$$L^{2,\mathrm{bcc}-A2}_{\mathrm{Al,Ti,W:\square}} = 0$$

$$L^{3,\mathrm{bcc}-A2}_{\mathrm{Al,Ti,W,Ti:\square}} = 0$$

Phase bcc–$B2$

$$G^{*}_{\mathrm{Al:Ti:\square}} = -\,8750 + 1.25\ T$$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{W:Al,Ti:\square}} = L^{0,\mathrm{bcc}-B2}_{\mathrm{Al,Ti:W:\square}} = -\,G^{*}_{\mathrm{Al:Ti:\square}}$$

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Al,Ti:W:\square}} = 0$$

$$L^{1,\mathrm{bcc}-A2}_{\mathrm{Al,Ti:W:\square}} = 0$$

$$L^{2,\mathrm{bcc}-A2}_{\mathrm{Al,Ti:W:\square}} = 0$$

Table I - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Al-Ti-W	(Al)	Cu	*cF4* $Fm\bar{3}m$	M 4	
	(W)	W	*cI2* $Im\bar{3}m$	M 2	
	bcc-*B*2	CsCl	*cP2* $Pm\bar{3}m$	M_1 1 M_2 1	
	(Ti)	Mg	*hP2* $P6_3/mmc$	M 2	
	(Ti)	W	*cI2* $Im\bar{3}m$	M 2	
	AlTi	AuCu	*tP4* $P4/mmm$	Al 2 Ti_1 1 Ti_2 1	AlTi-$L1_0$
	$AlTi_3$	Ni_3Sn	*hP8* $P6_3/mmc$		AlM-$D0_{19}$

System B–Hf–Ti

Ternary Solution Phases:

Liquid, bcc-$A2$, hcp-$A3$

Quasi-binary phases:

B_2M, B_4M_3, BM

Modelling:

Liquid	:	Substitutional, Redlich-Kister
bcc-$A2$	:	Sublattice model $(Hf,Ti)(B,\square)_3$
hcp-$A3$	:	Sublattice model $(Hf,Ti)(B,\square)_{0.5}$
B_2M	:	Quasi-binary, $(B)_2(Hf,Ti)$
B_4M_3	:	Quasi-binary, $(B)_4(Hf,Ti)_3$
BM	:	Quasi-binary, (B)(Hf,Ti)

Comments:

No ternary compounds

Assessor and Date:

H. Bittermann, (1997)

Publication:

H. Bittermann, and P. Rogl, J. Phase Equil., **18**, 24-47 (1997).

Thermodynamic properties of the solution and compound phases ($J.mol^{-1}$)

Phase Liquid

$$L^{0,\mathrm{liquid}}_{\mathrm{B,Hf,Ti}} = 41733.1$$

$$L^{0,\mathrm{liquid}}_{\mathrm{B,Hf,Ti}} = 125.375\ T$$

$$L^{0,\mathrm{liquid}}_{\mathrm{B,Hf,Ti}} = 93.6697\ T$$

Phase B_2M

$$L^{0,B_2M}_{B:Hf,Ti} = 7223.32 + 1.75379\ T$$

Phase B_4M_3

$$L^{0,B_4M_3}_{B:Hf,Ti} = 115124 - 49.5166\ T$$

Phase BM

$$L^{0,BM}_{B:Hf,Ti} = 19396.7 - 6.57772\ T$$

Table I - Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices
B-Hf-Ti	(B)	β-rhombo-B		
	(Hf)	Mg	*hP2* $P6_3/mmc$	M 2
	(Hf)	W	*cI2* $Im\bar{3}m$	M 2
	(Ti)	Mg	*hP2* $P6_3/mmc$	M 2
	(Ti)	W	*cI2* $Im\bar{3}m$	M 2
	BM	BFe	*oP8* *Pnma*	B 4 Ti 4
	B_2M	AlB_2	*hP3* *P6/mmm*	B 2 Ti 1
	B_4M_3	B_4Ta_3	*oI14* *Immm*	

System Cu–Mg–Y

Ternary Solution Phases:

Liquid, fcc–*A*1, bcc–*A*2, hcp–*A*3

Modelling:

Liquid : Substitutional, Redlich–Kister
fcc–*A*1 : Substitutional, Redlich–Kister
hcp–*A*3 : Substitutional, Redlich–Kister

Assessor and Date:

T. Bühler, RWTH, Aachen, Germany, (1997).

Comments:

No coefficents for the ternary solution phases.
No ternary compounds.

Table I – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices
Cu–Mg–Si	(Cu)	Cu	*cF4* $Fm\bar{3}m$	M 4
	(Mg)	Mg	*hP2* $P6_3/mmc$	M 2
	(Y)	W	*cI2* $Im\bar{3}m$	M 4
	(Y)	Mg	*hP2* $P6_3/mmc$	M 2

System Cu–Mg–Si

Ternary Solution Phases:

(stable) Liquid, fcc-*A*1, bcc-*A*2, hcp-*A*3
(metastable) hcp-Zn

Ternary Compounds:

CuMgSi-σ, CuMgSi-τ, Laves-*C*15

Modelling:

Liquid : Substitutional, Redlich-Kister
bcc-*A*2 : Substitutional, Redlich-Kister
fcc-*A*1 : Substitutional, Redlich-Kister
hcp-*A*3 : Substitutional, Redlich-Kister
hcp-Zn : Substitutional, Redlich-Kister
CuMgSi-σ : Stoichiometric, $(\mathrm{Cu})_{16}(\mathrm{Mg})_{6}(\mathrm{Si})_{7}$
CuMgSi-τ : Stoichiometric, $(\mathrm{Cu})_{3}(\mathrm{Mg})_{2}(\mathrm{Si})$
Laves-*C*15 : Sublattice model, $(\mathrm{Cu,Mg,Si})_{2}(\mathrm{Cu,Mg,Si})$

Assessor and Date:

T. Bühler, RWTH, Aachen, Germany, (1997).

Thermodynamic properties of the solution and compound phases (J.mol^{-1})

Phase CuMgSi-σ

$$G^{\circ}(T) - 16.0\ H_{\mathrm{Cu}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) - 6.0\ H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K})$$
$$- 7.0\ H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Mg{:}Si)} =$$
$$- 559636 + 110.94\ T + 16.0\ \mathrm{GHSER_{Cu}} + 6.0\ \mathrm{GHSER_{Mg}}$$
$$+ 7.0\ \mathrm{GHSER_{Si}}$$

Phase CuMgSi–τ

$$G^{\circ}(T) - 3.0\ H_{\mathrm{Cu}}^{\circ,\mathrm{fcc}-A1}(298.15\ \mathrm{K}) - 2.0\ H_{\mathrm{Mg}}^{\circ,\mathrm{hcp}-A3}(298.15\ \mathrm{K}) - H_{\mathrm{Si}}^{\circ,\mathrm{diamond}}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Mg{:}Si)} = -141720 + 20.26\ T + 3.0\,\mathrm{GHSER_{Cu}} + 2.0\ \mathrm{GHSER_{Mg}} + \mathrm{GHSER_{Si}}$$

Phase Liquid

$L^{0,\mathrm{liquid}}_{\mathrm{Cu,Mg,Si}} = 1\mathrm{E}\text{-}04$

$L^{1,\mathrm{liquid}}_{\mathrm{Cu,Mg,Si}} = -141736$

$L^{2,\mathrm{liquid}}_{\mathrm{Cu,Mg,Si}} = 1\mathrm{E}\text{-}04$

Phase hcp–Zn

$L^{0,\mathrm{hcp-Zn}}_{\mathrm{Cu,Mg,Si:\square}} = 50000$

$L^{1,\mathrm{hcp-Zn}}_{\mathrm{Cu,Mg,Si:\square}} = 50000$

$L^{2,\mathrm{hcp-Zn}}_{\mathrm{Cu,Mg,Si:\square}} = 50000$

Phase Laves–$C15$

$L^{0,\mathrm{Laves}-C15}_{\mathrm{Mg,Si:Cu}} = 15000$

$L^{0,\mathrm{Laves}-C15}_{\mathrm{Si:Cu,Mg}} = 6599.45$

$L^{0,\mathrm{Laves}-C15}_{\mathrm{Cu,Si:Mg}} = -193131 + 20.69\ T$

$L^{0,\mathrm{Laves}-C15}_{\mathrm{Cu:Mg,Si}} = 8000$

$L^{0,\mathrm{Laves}-C15}_{\mathrm{Cu,Mg:Si}} = 13011.35$

Table I:a – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Cu-Mg-Si	(Cu)	Cu	*cF4* $Fm\bar{3}m$	M 4	
	(Mg)	Mg	*hP2* $P6_3/mmc$	M 2	
	(Si)	diamond	*cF8* $Fd\bar{3}m$	M 8	

Table I:b – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
	Cu_2Mg	Cu_2Mg	*cF24* $Fd\bar{3}m$	Cu 16 Mg 8	Laves-C15
	$Cu_{16}Mg_9Si_7$	$Mn_{23}Th_6$	*cF*112 $Fm\bar{3}m$	Si_1 4 Si_1 24 Mg 24 Cu_1 32 Cu_2 32	CuMgSi-σ
	Cu_3Mg_2Si	$MgZn_2$	*hP*12 $P6_3/mmc$	Si 2 Mg 4 Cu 6	CuMgSi-τ

System Cu–Mg–Zn

Ternary Solution Phases:

Liquid, fcc-*A*1, bcc-*A*2, bcc-*B*2, hcp-*A*3, hcp-Zn

Compounds:

Laves-*C*14, Laves-*C*15, Laves-*C*36, CuZn-γ, MgZn, Mg_2Zn_3, Mg_2Zn_{11}

Modelling:

Liquid : Substitutional, Redlich-Kister
fcc-*A*1 : Substitutional, Redlich-Kister
hcp-*A*3 : Substitutional, Redlich-Kister
hcp-Zn : Substitutional, Redlich-Kister
bcc-*B*2 : Sublattice model, $(Cu,Mg,Zn)_{0.5}(Cu,Mg,Zn)_{0.5}$
Two descriptions of the bcc-*A*2:bcc-*B*2 order-disorder transformation are given: one which includes the parameters of the order and disordered phases in a single description (equation 21 and 22 in the thermodynamic modelling chapter), and a second one where the order and disorder contributions are expressed by equation 23. For the second case, the parameters are in a frame.
hcp-Zn : Substitutional, Redlich-Kister-Muggianu
CuZn-γ : Sublattice model, $(Cu,Zn)_2(Cu,Zn)_2(Cu)_3(Mg,Zn)_6$
Laves-*C*14 : Sublattice model, $(Cu,Mg,Zn)_2(Cu,Mg,Zn)$
Laves-*C*15 : Sublattice model, $(Cu,Mg,Zn)_2(Cu,Mg,Zn)$
Laves-*C*36 : Sublattice model, $(Cu,Mg,Zn)_2(Cu,Mg,Zn)$
MgZn : Sublattice model, $(Mg)_{12}(Cu,Zn)_{13}$
Mg_2Zn_3 : Sublattice model, $(Mg)_2(Cu,Zn)_3$
Mg_2Zn_{11} : Sublattice model, $(Mg)_2(Cu,Zn)_{11}$

Assessor and Date:

P. Liang, H. L. Lukas (1997)

Publication:

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Thermodynamic properties of the solution and compound phases ($\mathrm{J.mol^{-1}}$)

Phase bcc–$B2$

$G^{\bullet}_{\mathrm{Cu:Mg}} = 0.0$
$L^{0}_{\mathrm{Cu,Mg}} = -\ 2500$
$G^{\bullet}_{\mathrm{Cu:Zn}} = 0.0$
$L^{0}_{\mathrm{Cu,Zn}} = -\ 12898.97+3.26598\ T$
$L^{1}_{\mathrm{Cu,Zn}} = 945.265 - 0.80679\ T$
$L^{2}_{\mathrm{Cu,Zn}} = 1921.485 - 1.86969\ T$
$G^{\bullet}_{\mathrm{Mg:Zn}} = 0.0$
$L^{0}_{\mathrm{Mg,Zn}} = -\ 2500$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Cu,Mg:Zn:\square}} = L^{0,\mathrm{bcc}-B2}_{\mathrm{Zn:Cu,Mg:\square}} = -\ G^{\bullet}_{\mathrm{Cu:Mg}} + L^{0}_{\mathrm{Cu,Mg}} - L^{1}_{\mathrm{Cu,Zn}} + 0.5\ \ L^{2}_{\mathrm{Cu,Zn}}$$

$$L^{1,\mathrm{bcc}-B2}_{\mathrm{Cu,Mg:Zn:\square}} = L^{1,\mathrm{bcc}-B2}_{\mathrm{Zn:Cu,Mg:\square}} = -\ 0.5\ \ L^{2}_{\mathrm{Cu,Zn}}$$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Cu,Zn:Mg:\square}} = L^{0,\mathrm{bcc}-B2}_{\mathrm{Mg:Cu,Zn:\square}} = -\ G^{\bullet}_{\mathrm{Cu:Zn}} + L^{0}_{\mathrm{Cu,Zn}}$$

$$L^{1,\mathrm{bcc}-B2}_{\mathrm{Cu,Zn:Mg:\square}} = L^{1,\mathrm{bcc}-B2}_{\mathrm{Mg:Cu,Zn:\square}} = L^{1}_{\mathrm{Cu,Zn}}$$

$$L^{2,\mathrm{bcc}-B2}_{\mathrm{Cu,Zn:Mg:\square}} = L^{2,\mathrm{bcc}-B2}_{\mathrm{Mg:Cu,Zn:\square}} = L^{2}_{\mathrm{Cu,Zn}}$$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Mg,Zn:Cu:\square}} = L^{0,\mathrm{bcc}-B2}_{\mathrm{Cu:Mg,Zn:\square}} = -\ G^{\bullet}_{\mathrm{Mg:Zn}} + L^{0}_{\mathrm{Mg,Zn}} + L^{1}{}_{\mathrm{Cu,Zn}} + 0.5\ \ L^{2}{}_{\mathrm{Cu,Zn}}$$

$$L^{1,\mathrm{bcc}-B2}_{\mathrm{Mg,Zn:Cu:\square}} = L^{1,\mathrm{bcc}-B2}_{\mathrm{Cu:Mg,Zn:\square}} = 0.5\ \ L^{2}_{\mathrm{Cu,Zn}}$$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Mg,Zn:Cu,Zn:\square}} = L^{0,\mathrm{bcc}-B2}_{\mathrm{Cu,Zn:Mg,Zn:\square}} = -\ 5\ \ L^{2}_{\mathrm{Cu,Zn}}$$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Mg,Zn:Cu,Mg:\square}} = L^{0,\mathrm{bcc}-B2}_{\mathrm{Cu,Mg:Mg,Zn:\square}} = -\ 2\ \ L^{2}_{\mathrm{Cu,Zn}}$$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Cu,Zn:Cu,Mg:\square}} = L^{0,\mathrm{bcc}-B2}_{\mathrm{Cu,Mg:Cu,Zn:\square}} = -\ 5\ \ L^{2}_{\mathrm{Cu,Zn}}$$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Cu,Mg,Zn:Cu:\square}} = L^{0,\mathrm{bcc}-B2}_{\mathrm{Cu:Cu,Mg,Zn:\square}} = 1.5\ \ L^{2}_{\mathrm{Cu,Zn}}$$

$$L^{0,\mathrm{bcc}-B2}_{\mathrm{Cu,Mg,Zn:Zn:\square}} = L^{0,\mathrm{bcc}-B2}_{\mathrm{Zn:Cu,Mg,Zn:\square}} = 1.5\ \ L^{2}_{\mathrm{Cu,Zn}}$$

Phase bcc–$A2$

$$L^{0,\mathrm{bcc}-A2}_{\mathrm{Cu,Mg,Zn:\square}} = 0$$

$$L^{1,\mathrm{bcc}-A2}_{\mathrm{Cu,Mg,Zn:\square}} = 0$$

$$L^{2,\mathrm{bcc}-A2}_{\mathrm{Cu,Mg,Zn:\square}} = 0$$

Phase $\mathrm{Mg_2Zn_{11}}$

$$L^{0,\mathrm{Mg_2Zn_{11}}}_{\mathrm{Mg:Cu,Zn}} = -351000$$

Phase Laves–$C14$

$$L^{0,\mathrm{Laves}-C14}_{\mathrm{Mg,Zn:Cu}} = 35000.00$$

$$L^{0,\mathrm{Laves}-C14}_{\mathrm{Cu:Mg,Zn}} = 35000.00$$

$$L^{0,\mathrm{Laves}-C14}_{\mathrm{Zn:Cu,Mg}} = 6599.45$$

$$L^{0,\mathrm{Laves}-C14}_{\mathrm{Cu,Mg:Zn}} = 13011.35$$

$$L^{0,\mathrm{Laves}-C14}_{\mathrm{Cu,Zn:Mg}} = -75305.48$$

Phase Laves–$C15$

$$L^{0,\mathrm{Laves}-C15}_{\mathrm{Cu,Mg:Zn}} = 13011.35$$

$$L^{0,\mathrm{Laves}-C15}_{\mathrm{Zn:Cu,Mg}} = 6599.45$$

$$L^{0,\mathrm{Laves}-C15}_{\mathrm{Mg,Zn:Cu}} = 35000.00$$

$$L^{0,\mathrm{Laves}-C15}_{\mathrm{Cu:Mg,Zn}} = 8000.00$$

$$L^{0,\mathrm{Laves}-C15}_{\mathrm{Cu,Zn:Mg}} = -78824.62$$

$$L^{0,\mathrm{Laves}-C15}_{\mathrm{Mg:Cu,Zn}} = 25529.06$$

Phase Laves–$C36$

$L^{0,\mathrm{Laves}-C36}_{\mathrm{Mg,Zn:Cu}} = 35000.00$

$L^{0,\mathrm{Laves}-C36}_{\mathrm{Cu:Mg,Zn}} = 8000.00$

$L^{0,\mathrm{Laves}-C36}_{\mathrm{Zn:Cu,Mg}} = 6599.45$

$L^{0,\mathrm{Laves}-C36}_{\mathrm{Cu,Mg:Zn}} = 13011.35$

$L^{0,\mathrm{Laves}-C36}_{\mathrm{Cu,Zn:Mg}} = -\ 90226.26$

Phase $\mathrm{Mg_2Zn_3}$

$L^{0,\mathrm{Mg_2Zn_3}}_{\mathrm{Mg:Cu,Zn}} = -\ 100000$

Phase MgZn

$L^{0,\mathrm{MgZn}}_{\mathrm{Mg:Cu,Zn}} = -\ 575000$

Phase CuZn–γ

$\mathrm{K4} = -\ 11552.71 - 1.67824\ T$
$\mathrm{K5} = 15732.3 - 10.26575\ T$
$\mathrm{K6} = 37289.2 - 13.05259\ T$
$\mathrm{K7} = 9000.0 - 1.50000\ T$
$13\ \mathrm{K4} + 2\ \mathrm{K5} + 2\ \mathrm{K6} + 6\ \mathrm{K7} = 9857.77 - 77.4538\ T$
$13\ \mathrm{K4} + 6\ \mathrm{K7} = -\ 96185.23 - 30.81712\ T$
$13\ \mathrm{K4} + 2\ \mathrm{K6} + 6\ \mathrm{K7} = -\ 21606.83 - 56.9223\ T$

$G^\circ(T) - 5.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - 6.0\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K})$
$-\ 2.0\ H^{\circ,\mathrm{hcp}-\mathrm{Zn}}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Zn{:}Cu{:}Cu{:}Mg)} =$
$13.0\ \mathrm{K4} + 2.0\ \mathrm{K5} + 2.0\ \mathrm{K6} + 6\ \mathrm{K7} + 5.0\ \mathrm{GHSER_{Cu}}$
$+\ 6.0\ \mathrm{GHSER_{Mg}} + 2.0\ \mathrm{GHSER_{Zn}}$

$G^\circ(T) - 5.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - 6.0\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K})$
$-\ 2.0\ H^{\circ,\mathrm{hcp}-\mathrm{Zn}}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Zn{:}Cu{:}Mg)} =$
$13.0\ \mathrm{K4} + 6.0\ \mathrm{K7} + 5.0\ \mathrm{GHSER_{Cu}} + 6.0\ \mathrm{GHSER_{Mg}}$
$+\ 2.0\ \mathrm{GHSER_{Zn}}$

$G^\circ(T) - 3.0\ H^{\circ,\mathrm{fcc}-A1}_{\mathrm{Cu}}(298.15\ \mathrm{K}) - 6.0\ H^{\circ,\mathrm{hcp}-A3}_{\mathrm{Mg}}(298.15\ \mathrm{K})$
$-\ 4.0\ H^{\circ,\mathrm{hcp}-\mathrm{Zn}}_{\mathrm{Zn}}(298.15\ \mathrm{K}) = \mathrm{G(Cu{:}Zn{:}Cu{:}Mg)} =$
$13.0\ \mathrm{K4} + 2.0\ \mathrm{K6} + 6.0\ \mathrm{K7} + 3.0\ \mathrm{GHSER_{Cu}} + 6.0\ \mathrm{GHSER_{Mg}}$
$+\ 4.0\ \mathrm{GHSER_{Zn}}$

Table I – Crystal Structure and Phase Description.

System	Phase	Prototype	Pearson Symbol Space Group	Sub-lattices	Comments
Cu-Mg-Zn	(Cu)	Cu	*cF4* $Fm\bar{3}m$	M 4	
	(Mg)	Mg	*hP2* $P6_3/mmc$	M 2	
	(Zn)	Mg	*hP2* $P6_3/mmc$	M 2	
	$CuMg_2$	$CuMg_2$	*oF48* *Fddd*	Cu 16 Mg1 16 Mg2 16	
	Cu_2Mg	Cu_2Mg	*cF24* $Fd\bar{3}m$	Cu 16 Mg 8	Laves-*C*15
	Laves-*C*36	$MgNi_2$	*hP*24 $P6_3/mmc$	Cr_1 6 Cr_2 6 Zr_1 3 Zr_2 3	Laves-*C*36
	Laves-C14	$MgZn_2$	*hP*12 $P6_3/mmc$	Cr 2 Cr 6 Zr 4	Laves-*C*14
	γ	Cu_5Zn_8	*cI52* $I\bar{4}3m$	Cu_1 8 Cu_2 12 Zn_1 8 Zn_2 24	Cu_5Zn
	Mg_2Zn_{11}	Mg_2Zn_{11}	*cP39* $Pm\bar{3}$		
	MgZn				
	Mg_2Zn_3		*mC110* *B2/m*		

APPENDICES

APPENDIX I: THERMODYNAMIC PROPERTIES OF THE ELEMENTS ($J.mol^{-1}$)

NOTE: The Gibbs Energies of Formation at T are relative to the Enthalpy of the Pure Elements in their Reference Phase at 298.15 K [1]

ALUMINIUM

Aluminium fcc–$A1$

$$\mathrm{GHSER}_{\mathrm{Al}} = G_{\mathrm{Al}}^{\mathrm{fcc}-A1}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) =$$

$$\begin{array}{lll}
298.15 < T < 700.00 & : & -7976.15 + 137.093038\ T - 24.3671976\ T\cdot \ln T \\
 & & - 1.884662\mathrm{E}{-3}\ T^{2} - 0.877664\mathrm{E}{-6}\ T^{32} \\
 & & + 74092\ T^{-1} \\
700.00 < T < 933.47 & : & -11276.24 + 223.048446\ T - 38.5844296\ T\cdot \ln T \\
 & & + 18.531982\mathrm{E}{-3}\ T^{2} - 5.764227\mathrm{E}{-6}\ T^{3} \\
 & & + 74092\ T^{-1} \\
933.47 < T < 2900.00 & : & -11278.378 + 188.684153\ T - 31.748192\ T\cdot \ln T \\
 & & - 1230.524\mathrm{E}25\ T^{-9}
\end{array}$$

Aluminium bcc–$A2$

$$\mathrm{GBCC}_{\mathrm{Al}} = G_{\mathrm{Al}}^{\mathrm{bcc}-A2}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) =$$

$298.15 < T < 2900.00$: $10083.00 - 4.813\ T + \mathrm{GHSER}_{\mathrm{Al}}$

Aluminium cbcc–$A12$

$$G_{\mathrm{Al}}^{\mathrm{cbcc-A12}}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) =$$

$298.15 < T < 2900.00$: $10083.40 - 4.813\ T + \mathrm{GHSER}_{\mathrm{Al}}$

Aluminium bcc–B2

$$G_{\mathrm{Al:Al}}^{\mathrm{bcc}-B2}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) =$$

$298.15 < T < 2900.00$: $\mathrm{GBCC}_{\mathrm{Al}}$

Aluminium bct–$A5$

$$G_{\mathrm{Al}}^{\mathrm{bct}-A5}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1} =$$

$298.15 < T < 2900.00$: $10083.0 - 4.813\ T + \mathrm{GHSER}_{\mathrm{Al}}$

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[1] Scientific Group Thermodata Europe (S.G.T.E.) Data for Pure Elements, A.T. Dinsdale, CALPHAD, 15, 4, 317 - 425 (1991).

Aluminium cub–$A13$

$G_{\mathrm{Al}}^{\mathrm{cub}-A13}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1} =$

$298.15 < T < 2900.00 \; : \; 10920.44 - 4.8116\ T + \mathrm{GHSER}_{\mathrm{Al}}$

Aluminium diamond

$G_{\mathrm{Al}}^{\mathrm{diamond}}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) =$

$298.15 < T < 2900.00 \; : \; 30.0\ T + \mathrm{GHSER}_{\mathrm{Al}}$

Aluminium hcp–$A3$

$\mathrm{GHCP}_{\mathrm{Al}} = G_{\mathrm{Al}}^{\mathrm{hcp}-A3}(\mathrm{T}) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) =$

$298.15 < T < 2900.00 \; : \; 5481.0 - 1.8\ T + \mathrm{GHSER}_{\mathrm{Al}}$

Aluminium hcp–Zn

$G_{\mathrm{Al}}^{\mathrm{hcp-Zn}}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00 \; : \; 5482 - 1.8\ T + \mathrm{GHSER}_{Al}$

Aluminium liquid

$\mathrm{GLIQ}_{\mathrm{Al}} = G_{\mathrm{Al}}^{\mathrm{liquid}}(T) - H_{\mathrm{Al}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) =$

$298.15 < T < 933.47 \; : \; + 11005.029 - 11.841867\ T + 7.934\mathrm{E}{-20}\ T^{7} + \mathrm{GHSER}_{\mathrm{Al}}$

$933.47 < T < 2900.00 \; : \; + 10482.382 - 11.253974\ T + 1.231\mathrm{E}{+28}\ T^{-9} + \mathrm{GHSER}_{\mathrm{Al}}$

BORON

Boron β–rhombo–B

$\mathrm{GHSER}_{\mathrm{B}} = G_{\mathrm{B}}^{\beta-\mathrm{rhombo-B}}(T) - H_{\mathrm{B}}^{\mathrm{o},\beta-\mathrm{rhombo-B}}(298.15\ \mathrm{K}) =$

$298.15 < T < 1100.00 \; : \; - 7735.284 + 107.111864\ T - 15.6641\ T \cdot \ln T - 0.006864515\ T^{2} + 6.18878\mathrm{E}{-07}\ T^{3} + 370843\ T^{-1}$

$1100.00 < T < 2348.00 \; : \; - 16649.474 + 184.801744\ T - 26.6047\ T \cdot \ln T - 7.9809\mathrm{E}{-04}\ T^{2} - 2.556\mathrm{E}{-08}\ T^{3} + 1748270\ T^{-1}$

$2348.00 < T < 3000.00 \; : \; - 36667.582 + 231.336244\ T - 31.5957527\ T \cdot \ln T - 0.00159488\ T^{2} + 1.34719\mathrm{E}{-07}\ T^{3} + 11205883\ T^{-1}$

$3000.00 < T < 6000.00 \; : \; - 21530.653 + 222.396264\ T - 31.4\ T \cdot \ln T$

$\mathrm{GBCC_B} = G_{\mathrm{B}}^{\mathrm{bcc}-A2}(T) - H_{\mathrm{B}}^{\mathrm{o},\beta-\mathrm{rhombo-B}}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $50208.0 - 13.472\ T + \mathrm{GHSER_B}$

Boron diamond

$G_{\mathrm{B}}^{\mathrm{diamond}}(T) - H_{\mathrm{B}}^{\mathrm{o},\beta-\mathrm{rhombo-B}} =$

$298.15 < T < 6000.00$: $20 + \mathrm{GHSER_B}$

Boron fcc–*A*1

$\mathrm{GFCC_B} = G_{\mathrm{B}}^{\mathrm{fcc}-A1}(\mathrm{T}) - H_{\mathrm{B}}^{\mathrm{o},\beta-\mathrm{rhombo-B}}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $43514.0 - 12.217\ T + \mathrm{GHSER_B}$

Boron hcp–*A*3

$\mathrm{GHCP_B} = G_{\mathrm{B}}^{\mathrm{hcp}-A3}(T) - H_{\mathrm{B}}^{\mathrm{o},\beta-\mathrm{rhombo-B}}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $50208.0 - 9.706\ T + \mathrm{GHSER_B}$

Boron liquid

$\mathrm{GLIQ_B} = G_{\mathrm{B}}^{\mathrm{liquid}}(T) - H_{\mathrm{B}}^{\mathrm{o},\beta-\mathrm{rhombo-B}}(298.15\ \mathrm{K}) =$

$298.15 < T < 500.00$: $40723.275 + 86.843839\ T - 15.6641\ T\cdot \ln T$
$- 0.006864515\ T^2 + 6.18878\mathrm{E}{-07}\ T^3$
$+ 370843\ T^{-1}$
$500.00 < T < 2348.00$: $41119.703 + 82.101722\ T - 14.9827763\ T\cdot \ln T$
$- 0.007095669\ T^2 + 5.07347\mathrm{E}{-07}\ T^3$
$+ 335484\ T^{-1}$
$2348.00 < T < 6000.00$: $+ 28842.012 + 200.94731\ T - 31.4\ T\cdot \ln T$

CARBON

Carbon graphite

$\mathrm{GHSER_C} = G_{\mathrm{C}}^{\mathrm{graphite}}(T) - H_{\mathrm{C}}^{\mathrm{o,graphite}}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $- 17368.441 + 170.73\ T - 24.3\ T\cdot \ln T$
$- 4.723\mathrm{E}{-04}\ T^2 + 2562600\ T^{-1} - 2.643\mathrm{E}{+08}\ T^{-2}$
$+ 1.2\mathrm{E}{+10}\ T^{-3}$

Carbon diamond

$G_{\mathrm{C}}^{\mathrm{diamond}}(T) - H_{\mathrm{C}}^{\mathrm{o,graphite}}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $- 16359.441 + 175.61\ T - 24.31\ T\cdot \ln T$
$- 4.723\mathrm{E}{-04}\ T^2 + 2698000\ T^{-1} - 2.61\mathrm{E}{+08}\ T^{-2}$
$+ 1.11\mathrm{E}{+10}\ T^{-3}$

Carbon liquid

$\mathrm{GLIQ_C} = G_{\mathrm{C}}^{\mathrm{liquid}}(T) - H_{\mathrm{C}}^{\mathrm{o,graphite}}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $117369 - 24.63\ T + \mathrm{GHSER_C}$

CERIUM

Cerium fcc–$A1$

$\mathrm{GHSER_{Ce}} = G_{\mathrm{Ce}}^{\mathrm{fcc}-A1}(T) - H_{\mathrm{Ce}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) =$

$298.15 < T < 1000.00$: $-7160.519 + 84.23022\ T - 22.3664\ T \cdot \ln T$

$- 0.0067103\ T^2 - 3.20773\mathrm{E}\text{-}07\ T^3 - 18117\ T^{-1}$

$1000.00 < T < 2000.00$: $- 79678.506 + 659.4604\ T - 101.32248\ T \cdot \ln T$

$+ 0.026046487\ T^2 - 1.9302976\mathrm{E}\text{-}06\ T^3 + 11531707\ T^{-1}$

$2000.00 < T < 4000.00$: $- 14198.639 + 190.370192\ T - 37.6978\ T \cdot \ln T$

Cerium bcc–$A2$

$\mathrm{GBCC_{Ce}} = G_{\mathrm{Ce}}^{\mathrm{bcc}-A2}(T) - H_{\mathrm{Ce}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) =$

$298.15 < T < 1000.00$: $- 1354.69 - 5.21501\ T - 7.7305867\ T \cdot \ln T$

$- 0.029098402\ T^2 + 4.784299\mathrm{E}\text{-}06\ T^3 - 196303\ T^{-1}$

$1000.00 < T < 1072.00$: $- 12101.106 + 187.449688\ T - 37.6142\ T \cdot \ln T$

$1072.00 < T < 6000.00$: $- 11950.375 + 186.333811\ T - 37.4627992\ T \cdot \ln T$

$- 5.7145\mathrm{E}\text{-}05\ T^2 + 2.348\mathrm{E}\text{-}09\ T^3 - 25897\ T^{-11}$

Cerium dhcp

$G_{\mathrm{Ce}}^{\mathrm{dhcp}}(T) - H_{\mathrm{Ce}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) =$

$298.15 < T < 4000.00$: $- 190.0 + 0.56886\ T + \mathrm{GHSER_{Ce}}$

Cerium hcp–$A3$

$\mathrm{GHCP_{Ce}} = G_{\mathrm{Ce}}^{\mathrm{hcp}-A3}(T) - H_{\mathrm{Ce}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) =$

$298.15 < T < 4000.00$: $50000 + \mathrm{GHSER_{Ce}}$

Cerium liquid

$\mathrm{GLIQ_{Ce}} = G_{\mathrm{Ce}}^{\mathrm{liquid}}(T) - H_{\mathrm{Ce}}^{\mathrm{o,fcc}-A1}(298.15\ \mathrm{K}) =$

$298.15 < T < 1000.00$: $4117.865 - 11.423898\ T - 7.5383948\ T \cdot \ln T$

$- 0.02936407\ T^2 + 4.827734\mathrm{E}\text{-}06\ T^3 - 198834\ T^{-1}$

$1000.00 < T < 4000.00$: $- 6730.605 + 183.023193\ T - 37.6978\ T \cdot \ln T$

CHROMIUM

Chromium bcc–$A2$(paramagnetic)

$\mathrm{GHSER_{Cr}} = G_{\mathrm{Cr}}^{\mathrm{bcc}-A2,\mathrm{para}}(T) - H_{\mathrm{Cr}}^{\mathrm{o,bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) =$

$298.15 < T < 2180.00$: $-8856.94 + 157.48\ T - 26.908\ T\cdot \ln T + 1.89435\mathrm{E}{-3}\ T^2 - 1.47721\mathrm{E}{-6}\ T^3 + 139250\ T^{-1}$

$2180.00 < T < 6000.00$: $-34869.344 + 344.18\ T - 50\ T\cdot \ln T - 2885.26\mathrm{E}29\ T^{-9}$

Chromium cbcc–$A12$

$G_{\mathrm{Cr}}^{\mathrm{cbcc-A12,para}}(T) - H_{\mathrm{Cr}}^{\mathrm{o,bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $11087.0 + 2.7196\ T + \mathrm{GHSER_{Cr}}$

Chromium cub–$A13$

$G_{\mathrm{Cr}}^{\mathrm{cub}-A13}(T) - H_{\mathrm{Cr}}^{\mathrm{o,bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $15899.0 + 0.6276\ T + \mathrm{GHSER_{Cr}}$

Chromium fcc–$A1$(paramagnetic)

$\mathrm{GFCC_{Cr}} = G_{\mathrm{Cr}}^{\mathrm{fcc}-A1}(T) - H_{\mathrm{Cr}}^{\mathrm{o,bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $7284.0 + 0.163\ T + \mathrm{GHSER_{Cr}} +$

Chromium hcp–$A3$(paramagnetic)

$\mathrm{GHCP_{Cr}} = G_{\mathrm{Cr}}^{\mathrm{hcp}-A3}(T) - H_{\mathrm{Cr}}^{\mathrm{o,bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $4438.00 + \mathrm{GHSER_{Cr}} +$

Chromium liquid

$\mathrm{GLIQ_{Cr}} = G_{\mathrm{Cr}}^{\mathrm{liquid}}(T) - H_{\mathrm{Cr}}^{\mathrm{o,bcc}-A2,\mathrm{para}}(298.15\ \mathrm{K}) =$

$298.15 < T < 2180.00$: $24339.955 - 11.420225\ T + 2.37615\mathrm{E}{-21}\ T^7 + \mathrm{GHSER_{Cr}}$

$2180.00 < T < 6000.00$: $18409.36 - 8.563683\ T + 2.88526\mathrm{E}{+32}\ T^{-9} + \mathrm{GHSER_{Cr}}$

Chromium Laves–$C14$

$G_{\mathrm{Cr:Cr}}^{\mathrm{Cr,Laves-C14}} - 3.0\ H_{\mathrm{Cr}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $15000.0 + 3.0\ \mathrm{GHSER_{Cr}}$

Chromium Laves–$C15$

$G_{\mathrm{Cr:Cr}}^{\mathrm{Cr,Laves-C15}} - 3.0\ H_{\mathrm{Cr}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $15000.0 + 3.0\ \mathrm{GHSER_{Cr}}$

Chromium Laves–$C36$

$G_{\mathrm{Cr:Cr}}^{\mathrm{Cr,Laves-C36}} - 3.0\ H_{\mathrm{Cr}}^{\mathrm{o,bcc-}A2}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00 : 15000.0 + 3.0\ \mathrm{GHSER_{Cr}}$

COPPER

Copper fcc–$A1$

$\mathrm{GHSER_{Cu}} = G_{\mathrm{Cu}}^{\mathrm{fcc-}A1}(T) - H_{\mathrm{Cu}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) =$

$298.15 < T < 1357.77 : -7770.458 + 130.485235\ T - 24.112392\ T\cdot \ln T$
$- 2.65684\mathrm{E}{-3}\ T^2 + 0.129223\mathrm{E}{-6}\ T^3 + 52478\ T^{-1}$

$1357.77 < T < 3200.00 : -13542.026 + 183.803828\ T - 31.38\ T\cdot \ln T$
$+ 364.167\mathrm{E}27\ T^{-9}$

Copper bcc–$A2$

$\mathrm{GBCC_{Cu}} = G_{\mathrm{Cu}}^{\mathrm{bcc-}A2}(T) - H_{\mathrm{Cu}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) =$

$298.15 < T < 3200.00 : 4017.00 - 1.255\ T + \mathrm{GHSER_{Cu}}$

Copper hcp–$A3$

$\mathrm{GHCP_{Cu}} = G_{\mathrm{Cu}}^{\mathrm{hcp-}A3}(T) - H_{\mathrm{Cu}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) =$

$298.15 < T < 3200.00 : 600.0 + 0.2\ T + \mathrm{GHSER_{Cu}}$

Copper liquid

$\mathrm{GLIQ_{Cu}} = G_{\mathrm{Cu}}^{\mathrm{liquid}}(T) - H_{\mathrm{Cu}}^{\mathrm{o,fcc-}A1}(298.15\ \mathrm{K}) =$

$298.15 < T < 1357.77 : 12964.736 - 9.511904\ T - 5.849\mathrm{E}{-21}\ T^7$
$+ \mathrm{GHSER_{Cu}}$

$1357.77 < T < 3200.00 : 13495.481 - 9.922344\ T - 3.642\mathrm{E}{+29}\ T^9$
$+ \mathrm{GHSER_{Cu}}$

IRON

Iron bcc–$A2$(paramagnetic)

$\mathrm{GHSER_{Fe}} = G_{\mathrm{Fe}}^{\mathrm{bcc-}A2\mathrm{,para}}(T) - H_{\mathrm{Fe}}^{\mathrm{o,bcc-}A2\mathrm{,para}}(298.15\ \mathrm{K}) =$

$298.15 < T < 1811.00 : 1225.7 + 124.134\ T - 23.5143\ T\cdot \ln T$
$- 4.39752\mathrm{E}{-3}\ T^2 - 0.058927\mathrm{E}{-6}\ T^3 + 77359\ T^{-1}$

$1811.00 < T < 6000.00$: $-25383.581 + 299.31255\ T - 46\ T\cdot \ln T$
$+ 2296.03\text{E}28\ T^{-9}$

Iron cbcc-A12

$G_{\text{Fe}}^{\text{cbcc}-A12}(T) - H_{\text{Fe}}^{\text{o,bcc}-A2,\text{para}}(298.15\ \text{K}) =$

$298.15 < T < 6000.00$: $+ 4745 + \text{GHSER}_{\text{Fe}}$

Iron cub-A13

$G_{\text{Fe}}^{\text{cub}-A13}(T) - H_{\text{Fe}}^{\text{o,bcc}-A2,\text{para}}(298.15\ \text{K}) =$

$298.15 < T < 6000.00$: $3745 + \text{GHSER}_{\text{Fe}}$

Iron fcc-A1(paramagnetic)

$\text{GFCC}_{\text{Fe}} = G_{\text{Fe}}^{\text{fcc}-A1}(T) - H_{\text{Fe}}^{\text{o,bcc}-A2,\text{para}}(298.15\ \text{K}) =$

$298.15 < T < 1811.00$: $-1462.4 + 8.8282\ T - 1.15\ T\cdot \ln T$
$+ 0.00064\ T^2 + \text{GHSER}_{\text{Fe}}$

$1811.00 < T < 6000.00$: $-713.815 + 0.94001\ T$
$+ 0.49251\ T^{-9} + \text{GHSER}_{\text{Fe}}$

Iron hcp-A3

$\text{GHCP}_{\text{Fe}} = G_{\text{Fe}}^{\text{hcp}-A3}(T) - H_{\text{Fe}}^{\text{o,bcc}-A2,\text{para}}(298.15\ \text{K}) =$

$298.15 < T < 1811.00$: $-3705.78 + 12.591\ T - 1.15\ T\cdot \ln T$
$+ 6.4\text{E}{-04}\ T^2 + \text{GHSER}_{\text{Fe}}$

$1811.00 < T < 6000.00$: $-3957.199 + 5.24951\ T + 4.9251\text{E}{+30}\ T^{-9}$
$+ \text{GHSER}_{\text{Fe}}$

Iron liquid

$\text{GLIQ}_{\text{Fe}} = G_{\text{Fe}}^{\text{liquid}}(T) - H_{\text{Fe}}^{\text{o,bcc}-A2,\text{para}}(298.15\ \text{K}) =$

$298.15 < T < 1811.00$: $+ 12040.17 - 6.55843\ T - 3.67516\text{E}{-21}\ T^7$
$+ \text{GHSER}_{\text{Fe}}$

$1811.00 < T <$: $+ 14544.751 - 8.01055\ T - 2.29603\text{E}{+31}\ T^{-9}$
6000.00 $+ \text{GHSER}_{\text{Fe}}$

HAFNIUM

Hafnium hcp-A3

$\text{GHSER}_{\text{Hf}} = G_{\text{Hf}}^{\text{hcp}-\text{A}3}(T) - H_{\text{Hf}}^{\text{o,hcp}-A3}(298.15\ \text{K}) =$

$298.15 < T < 2506.00$: $-6987.297 + 110.744026\ T - 22.7075\ T\cdot \ln T$
$- 0.004146145\ T^2 - 4.77\text{E}{-10}\ T^3 - 22590\ T^{-1}$

$2506.00 < T < 6000.00$: $-1446776.33 + 6193.60999\ T - 787.536383\ T\cdot \ln T + 0.1735215\ T^2 - 7.575759\text{E-}06\ T^3 + 5.01742495\text{E+}08\ T^{-1}$

Hafnium bcc–*A*2

$\text{GBCC}_{\text{Hf}} = G_{\text{Hf}}^{\text{bcc-}A2}(T) - H_{\text{Hf}}^{\text{o,hcp-}A3}(298.15\ \text{K}) =$

$298.15 < T < 2506.00$: $5370.703 + 103.836026\ T - 22.8995\ T\cdot \ln T - 0.004206605\ T^2 + 8.71923\text{E-}07\ T^3 - 22590\ T^{-1} - 1.446\text{E-}10\ T^4$

$2506.00 < T < 6000.00$: $+1912456.77 - 8624.20573\ T + 1087.61412\ T\cdot \ln T - 0.286857065\ T^2 + 1.3427829\text{E-}05\ T^3 - 6.10085091\text{E+}08\ T^{-1}$

Hafnium fcc–*A*1

$\text{GFCC}_{\text{Hf}} = G_{\text{Hf}}^{\text{fcc-}A1}(T) - H_{\text{Hf}}^{\text{o,hcp-}A3}(298.15\ \text{K}) =$

$298.15 < T < 6000.00$: $10000 - 2.2\ T + \text{GHSER}_{\text{Hf}}$

Hafnium liquid

$\text{GLIQ}_{\text{Hf}} = G_{\text{Hf}}^{\text{liquid}}(T) - H_{\text{Hf}}^{\text{o,hcp-}A3}(298.15\ \text{K}) =$

$298.15 < T < 1000.00$: $20414.959 + 99.790933\ T - 22.7075\ T\cdot \ln T - 0.004146145\ T^2 - 4.77\text{E-}10\ T^3 - 22590\ T^{-1}$

$1000.00 < T < 2506.00$: $49731.499 - 149.91739\ T + 12.116812\ T\cdot \ln T - 0.021262021\ T^2 + 1.376466\text{E-}06\ T^3 - 4449699\ T^{-1}$

$2506.00 < T < 6000.00$: $-4247.217 + 265.470523\ T - 44\ T\cdot \ln T$

LITHIUM

Lithium bcc–*A*2

$\text{GHSER}_{\text{Li}} = G_{\text{Li}}^{\text{bcc-}A2}(T) - H_{\text{Li}}^{\text{o,bcc-}A2}(298.15\ \text{K}) =$

$200.00 < T < 453.60$: $-10583.817 + 217.637482\ T - 38.940488\ T\cdot \ln T + 35.466931\text{E-}3\ T^2 - 19.869816\text{E-}6\ T^3 + 159994\ T^{-1}$

$453.60 < T < 500.00$: $-559579.123 + 10547.879893\ T - 1702.8886493\ T\cdot \ln T + 2258.329444\text{E-}3\ T^2 - 571.066077\text{E-}6\ T^3 + 33885874\ T^{-1}$

$500.00 < T < 3000.00$: $-9062.994 + 179.278285\ T - 31.2283718\ T\cdot \ln T + 2.633221\text{E-}3\ T^2 - 0.438058\text{E-}6\ T^3 - 102387\ T^{-1}$

Lithium fcc–$A1$

$\mathrm{GFCC_{Li}} = G_{\mathrm{Li}}^{\mathrm{fcc}-A1}(T) - H_{\mathrm{Li}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$

$200.00 < T < 3000.00$: $-108 + 1.3\ T + \mathrm{GHSER_{Li}}$

Lithium hcp–$A3$

$\mathrm{GHCP_{Li}} = G_{\mathrm{Li}}^{\mathrm{hcp}-A3}(T) - H_{\mathrm{Li}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$

$200.00 < T < 3000.00$: $-154 + 2\ T + \mathrm{GHSER_{Li}}$

Lithium liquid

$\mathrm{GLIQ_{Li}} = G_{\mathrm{Li}}^{\mathrm{liquid}}(T) - H_{\mathrm{Li}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$

$200.00 < T < 250.00$: $-7883.612 + 211.841861\ T - 38.940488\ T\cdot \ln T$
$+ 35.466931\mathrm{E}{-3}\ T^2 - 19.869816\mathrm{E}{-6}\ T^3$
$+ 159994\ T^{-1}$

$250.00 < T < 453.60$: $12015.027 - 362.187078\ T + 61.6104424\ T\cdot \ln T$
$- 182.426463\mathrm{E}{-3}\ T^2 + 63.955671\mathrm{E}{-6}\ T^3$
$- 559968\ T^{-1}$

$453.60 < T < 3000.00$: $-6057.31 + 172.652183\ T - 31.2283718\ T\cdot \ln T$
$+ 2.633221\mathrm{E}{-3}\ T^2 - 0.438058\mathrm{E}{-6}\ T^3$
$- 102387\ T^{-1}$

MAGNESIUM

Magnesium hcp–$A3$

$\mathrm{GHSER_{Mg}} = G_{\mathrm{Mg}}^{\mathrm{hcp}-A3}(T) - H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) =$

$298.15 < T < 923.00$: $-8367.34 + 143.675547\ T - 26.1849782\ T\cdot \ln T$
$+ 0.4858\mathrm{E}{-3}\ T^2 - 1.393669\mathrm{E}{-6}\ T^3 + 78950\ T^{-1}$

$923.00 < T < 3000.00$: $-14130.185 + 204.716215\ T - 34.3088\ T\cdot \ln T$
$+ 1038.192\mathrm{E}25\ T^{-9}$

Magnesium bcc–$A2$

$\mathrm{GBCC_{Mg}} = G_{\mathrm{Mg}}^{\mathrm{bcc}-A2}(T) - H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) =$

$298.15 < T < 3000.00$: $3100.00 - 2.1\ T + \mathrm{GHSER}_{Mg}$

Magnesium cbcc–$A12$

$G_{\mathrm{Mg}}^{\mathrm{cbcc-A12}}(T) - H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) =$

$298.15 < T < 3000.00$: $4602.4 - 3.011\ T + \mathrm{GHSER_{Mg}}$

Magnesium cub–$A13$

$G_{\mathrm{Mg}}^{\mathrm{cub}-A13}(T) - H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) =$

$298.15 < T < 3000.00$: $5000.0 - 3.0\ T + \mathrm{GHSER}_{\mathrm{Mg}}$

Magnesium fcc–$A1$

$\mathrm{GFCC}_{\mathrm{Mg}} = G_{\mathrm{Mg}}^{\mathrm{fcc}-A1}(T) - H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) =$

$298.15 < T < 3000.00$: $2600 - 0.90\ T + \mathrm{GHSER}_{\mathrm{Mg}}$

Magnesium liquid

$\mathrm{GLIQ}_{\mathrm{Mg}} = G_{\mathrm{Mg}}^{\mathrm{liquid}}(T) - H_{\mathrm{Mg}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) =$

$298.15 < T < 923.00$: $8202.243 - 8.83693\ T + \mathrm{GHSER}_{\mathrm{Mg}} - 8.0176\mathrm{E}{-20}\ T^{7}$
$+ \mathrm{GHSER}_{\mathrm{Mg}}$
$923.00 < T < 3000.00$: $8690.316 - 9.392158\ T - 1.038192\mathrm{E}{+28}\ T^{-9}$
$+ \mathrm{GHSER}_{\mathrm{Mg}}$

MANGANESE

Manganese cbcc–$A12$(paramagnetic)

$\mathrm{GHSER}_{\mathrm{Mn}} = G_{\mathrm{Mn}}^{\mathrm{cbcc-A12,para}}(T) - H_{\mathrm{Mn}}^{\mathrm{o,cbcc-A12,para}}(298.15\ \mathrm{K}) =$

$298.15 < T < 1519.00$: $- 8115.28 + 130.059\ T - 23.4582\ T \cdot \ln T$
$- 7.34768\mathrm{E}{-3}\ T^{2} + 69827\ T^{-1}$
$1519.00 < T < 3000.00$: $- 28733.41 + 312.2648\ T - 48\ T \cdot \ln T$
$+ 1656.847\mathrm{E}{+27}\ T^{-9}$

Manganese bcc–$A2$(paramagnetic)

$\mathrm{GBCC}_{\mathrm{Mn}} = G_{\mathrm{Mn}}^{\mathrm{bcc}-A2,\mathrm{para}}(T) - H_{\mathrm{Mn}}^{\mathrm{o,cbcc-A12,para}}(298.15\ \mathrm{K}) =$

$298.15 < T < 1519.00$: $- 3235.3 + 127.85\ T - 23.7\ T \cdot \ln T$
$- 7.44271\mathrm{E}{-3}\ T^{2} + 60000\ T^{-1}$
$1519.00 < T < 3000.00$: $- 23188.83 + 307.7043\ T - 48\ T \cdot \ln T$
$+ 1265.152\mathrm{E}27\ T^{-9}$

Manganese fcc–$A1$(paramagnetic)

$\mathrm{GFCC}_{\mathrm{Mn}} = G_{\mathrm{Mn}}^{\mathrm{fcc}-A1,\mathrm{para}}(T) - H_{\mathrm{Mn}}^{\mathrm{o,cbcc-A12,para}}(298.15\ \mathrm{K}) =$

$298.15 < T < 1519.00$: $-3439.3 + 131.884\ T - 24.5177\ T \cdot \ln T$
$- 6\mathrm{E}{-3}\ T^{2} + 69600\ T^{-1}$
$298.15 < T < 1519.00$: $- 26070.1 + 309.6664\ T - 48\ T \cdot \ln T$
$+ 386.196\mathrm{E}28\ T^{-9}$

Manganese Laves–$C15$

$G_{\mathrm{Mn:Mn}}^{\mathrm{Laves}-C15} - 3.0\ H_{\mathrm{Mn}}^{\mathrm{o,cbcc-A12,para}}(298.15\ \mathrm{K}) =$

$298.15 < T < 3000.00$: $3000.0 + 3.0\ \mathrm{GHSER}_{\mathrm{Mn}}$

Manganese cub–$A13$

$G_{\text{Mn}}^{\text{cub}-A13}(T) - H_{\text{Mn}}^{\text{o,ccbcc}-\text{A12,para}}(298.15\text{ K}) =$

$298.15 \quad < T < \quad 1519.00 \quad : \quad + 2314.88 + 5.936\ T - 1.4203\ T\cdot \ln T$
$\quad + 1.51409\text{E-}03\ T^2 + 442.0\ T^{-1} + \text{GHSER}_{\text{Mn}}$

$1519.00 \quad\quad 3000.00 \quad : \quad + 442.65 - 0.9715\ T + 2.3107229\text{E+}30\ T^{-9}$
$\quad + \text{GHSER}_{\text{Mn}}$

Manganese hcp–$A3$(paramagnetic)

$\text{GHCP}_{\text{Mn}} = G_{\text{Mn}}^{\text{hcp}-A3\text{,para}}(T) - H_{\text{Mn}}^{\text{o,cbcc}-\text{A12,para}}(298.15\text{ K}) =$

$298.15 \quad < T < \quad 1519.00 \quad : \quad - 4439.3 + 133.007\ T - 24.5177\ T\cdot \ln T$
$\quad - 6\text{E-}3\ T^2 + 69600\ T^{-1}$

$1519.00 \quad < T < \quad 6000.00 \quad : \quad - 27070.1 + 310.7894\ T - 48\ T\cdot \ln T$
$\quad +386.196\text{E}28\ T^{-9}$

Manganese liquid

$\text{GLIQ}_{\text{Mn}} = G_{\text{Mn}}^{\text{liquid}}(T) - H_{\text{Mn}}^{\text{o,cbcc}-\text{A12,para}}(298.15\text{ K}) =$

$298.15 \quad < T < \quad 1519.00 \quad : \quad 17859.91 - 12.6208\ T - 4.41929\text{E-}21\ T^7$
$\quad + \text{GHSER}_{\text{Mn}}$

$1519.00 \quad < T < \quad 3000.00 \quad : \quad 18739.51 - 13.2288\ T - 1.656847\text{E+}30\ T^{-9}$
$\quad + \text{GHSER}_{\text{Mn}}$

MOLYBDENUM

Molybdenum bcc–$A2$

$\text{GHSER}_{\text{Mo}} = G_{\text{Mo}}^{\text{bcc}-\text{A2}}(T) - H_{\text{Mo}}^{\text{o,bcc}-A2}(298.15\text{ K}) =$

$298.15 \quad < T < \quad 2896.00 \quad : \quad - 7746.302 + 131.9197\ T - 23.56414\ T\cdot \ln T$
$\quad - 0.003443396\ T^2 + 5.66283\text{E-}07\ T^3 + 65812\ T^{-1}$
$\quad - 1.30927\text{E-}10\ T^4$

$2896.00 \quad < T < \quad 5000.00 \quad : \quad - 30556.41 + 283.559746\ T - 42.63829\ T\cdot \ln T$
$\quad - 4.849315\text{E+}33\ T^{-9}$

Molybdenum fcc–$A1$

$\text{GFCC}_{\text{Mo}} = G_{\text{Mo}}^{\text{fcc}-A1}(T) - H_{\text{Mo}}^{\text{o,bcc}-A2}(298.15\text{ K}) =$

$298.15 \quad < T < \quad 2896.00 \quad : \quad 7453.698 + 132.5497\ T - 23.56414\ T\cdot \ln T$
$\quad - 0.003443396\ T^2 + 5.66283\text{E-}07\ T^3 + 65812\ T^{-1}$
$\quad - 1.30927\text{E-}10\ T^4$

$2896.00 \quad < T < \quad 5000.00 \quad : \quad - 15356.41 + 284.189746\ T - 42.63829\ T\cdot \ln T$
$\quad - 4.849315\text{E+}33\ T^{-9}$

Molybdenum hcp–$A3$

$\mathrm{GHCP}_{\mathrm{Mo}} = G_{\mathrm{Mo}}^{\mathrm{hcp}-A3}(T) - H_{\mathrm{Mo}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$

$298.15 < T < 5000.00$: $11550 + \mathrm{GHSER}_{\mathrm{Mo}}$

Molybdenum liquid

$\mathrm{GLIQ}_{\mathrm{Mo}} = G_{\mathrm{Mo}}^{\mathrm{liquid}}(T) - H_{\mathrm{Mo}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$

$298.15 < T < 2896.00$: $34085.045 + 117.224788\ T - 23.56414\ T\cdot \ln T$
$- 0.003443396\ T^2 + 5.66283\mathrm{E}{-}07\ T^3 + 65812\ T^{-1}$
$- 1.30927\mathrm{E}{-}10\ T^4 + 4.24519\mathrm{E}{-}22\ T^7$
$2896.00 < T < 5000.00$: $3538.963 + 271.6697\ T - 42.63829\ T\cdot \ln T$

NITROGEN

Nitrogen gas

$\mathrm{GHSER}_{\mathrm{N}} = G_{\mathrm{N}}^{\mathrm{gas}}(T) - H_{0.5\mathrm{N}_2}^{\mathrm{o}}(298.15\ \mathrm{K}) =$

$298.15 < T < 950.00$: $- 3750.675 - 9.45425\ T - 12.7819\ T\cdot \ln T$
$- 0.00176686\ T^2 + 2.681\mathrm{E}{-}09\ T^3 - 32374\ T^{-1}$
$950.00 < T < 3350.00$: $- 7358.85 + 17.2003\ T - 16.3699\ T\cdot \ln T$
$- 6.5107\mathrm{E}{-}04\ T^2$
$+ 3.0097\mathrm{E}{-}08\ T^3 + 563070\ T^{-1}$
$3350.00 < T < 6000.00$: $- 16392.8 + 50.26\ T - 20.4695\ T\cdot \ln T$
$+ 2.39754\mathrm{E}{-}04\ T^2 - 8.333\mathrm{E}{-}09\ T^3 + 4596375\ T^{-1}$

Nitrogen liquid

$\mathrm{GLIQ}_{\mathrm{N}} = G_{\mathrm{N}}^{\mathrm{liquid}}(T) - H_{0.5\mathrm{N}_2}^{\mathrm{o}}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $29950 + 59.02\ T + \mathrm{GHSER}_{\mathrm{N}}$

NEODYMIUM

Neodymium dhcp

$\mathrm{GHSER}_{\mathrm{Nd}} = G_{\mathrm{Nd}}^{\mathrm{dhcp}} - H_{\mathrm{Nd}}^{\mathrm{o,dhcp}}(298.15\ \mathrm{K}) =$

$298.15 < T < 900.00$: $- 8402.93 + 111.10239\ T - 27.0858\ T\cdot \ln T$
$+ 5.56125\mathrm{E}{-}04\ T^2 - 2.6923\mathrm{E}{-}06\ T^3 + 34887\ T^{-1}$
$900.00 < T < 1128.00$: $- 6984.083 + 83.662617\ T - 22.7536\ T\cdot \ln T$
$- 0.00420402\ T^2 - 1.802\mathrm{E}{-}06\ T^3$
$1128.00 < T < 1799.00$: $- 225610.846 + 1673.04075\ T - 238.182873\ T\cdot \ln T$
$+ 0.078615997\ T^2 - 6.048207\mathrm{E}{-}06\ T^3 + 38810350\ T^{-1}$
$1799.00 < T < 2000.00$: $- 25742.331 + 276.257088\ T - 48.7854\ T\cdot \ln T$

Neodymium bcc–$A2$

$\mathrm{GBCC_{Nd}} = G_{\mathrm{Nd}}^{\mathrm{bcc}-A2} - H_{\mathrm{Nd}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$

$298.15 < T < 400.00$: $- 6965.635 + 110.556109\ T - 27.0858\ T \cdot \ln T$
$+ 5.56125\mathrm{E}{-}04\ T^2 - 2.6923\mathrm{E}{-}06\ T^3 + 34887\ T^{-1}$
$400.00 < T < 1128.00$: $+ 7312.2 - 153.033976\ T + 14.9956777\ T \cdot \ln T$
$- 0.050479\ T^2 + 7.287217\mathrm{E}{-}06\ T^3 - 831810\ T^{-1}$
$1128.00 < T < 1289.00$: $- 18030.266 + 239.677322\ T - 44.5596\ T \cdot \ln T$
$1289.00 < T < 1800.00$: $+ 334513.017 - 2363.9199\ T + 311.409193\ T \cdot \ln T$
$- 0.156030778\ T^2 + 1.2408421\mathrm{E}{-}05\ T^3 - 64319604\ T^{-1}$

Neodymium liquid

$\mathrm{GLIQ_{Nd}} = G_{\mathrm{Nd}}^{\mathrm{bcc}-A2} - H_{\mathrm{Nd}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$

$298.15 < T < 300.00$: $- 3351.187 + 109.517314\ T - 27.0858\ T \cdot \ln T$
$+ 5.56125\mathrm{E}{-}04\ T^2 - 2.6923\mathrm{E}{-}06\ T^3 + 34887\ T^{-1}$
$300.00 < T < 1128.00$: $+ 5350.01 - 86.593963\ T + 5.357301\ T \cdot \ln T$
$- 0.046955463\ T^2 + 6.860782\mathrm{E}{-}06\ T^3 - 374380\ T^{-1}$
$1128.00 < T < 1800.00$: $- 16335.232 + 268.625903\ T - 48.7854\ T \cdot \ln T$

NICKEL

Nickel fcc–$A1$(paramagnetic)

$\mathrm{GHSER_{Ni}} = G_{\mathrm{Ni}}^{\mathrm{fcc}-A1,\mathrm{para}} - H_{Ni}^{\mathrm{o,fcc}-A1,\mathrm{para}}(298.15\ \mathrm{K}) =$

$298.15 < T < 1728.00$: $- 5179.159 + 117.854\ T - 22.096\ T \cdot \ln T$
$- 0.0048407\ T^2$
$1728.00 < T < 3000.00$: $-27840.655 + 279.135\ T - 43.1\ T \cdot \ln T$
$+ 1.12754\mathrm{E}{+}31\ T^{-9}$

Nickel bcc–$A2$(paramagnetic)

$\mathrm{GBCC_{Ni}} = G_{\mathrm{Ni}}^{\mathrm{bcc}-A2} - H_{\mathrm{Ni}}^{\mathrm{o,fcc}-A1,\mathrm{para}}(298.15\ \mathrm{K}) =$

$298.15 < T < 1300.00$: $+ 8715.084 - 3.556\ T + \mathrm{GHSER_{Ni}}$

Nickel hcp–$A3$(paramagnetic)

$\mathrm{GHCP_{Ni}} = G_{\mathrm{Ni}}^{\mathrm{hcp}-A3} - H_{\mathrm{Ni}}^{\mathrm{o,fcc}-A1,\mathrm{para}}(298.15\ \mathrm{K}) =$
$298.15 < T < 3000.00$: $+ 1046 + 1.2552\ T + \mathrm{GHSER_{Ni}}$

Nickel liquid

$\mathrm{GLIQ_{Ni}} = G_{\mathrm{Ni}}^{\mathrm{liquid}} - H_{\mathrm{Ni}}^{\mathrm{o,fcc}-A1,\mathrm{para}}(298.15\ \mathrm{K}) =$
$298.15 < T < 1300.00$: $16414.686 - 9.397\ T - 3.82318\mathrm{E}{-}21\ T^7$
$+ \mathrm{GHSER_{Ni}}$
$1728.00 < T < 3000.00$: $18290.88 - 10.537\ T - 1.127554{+}31\ T^{-9}$
$+ \mathrm{GHSER_{Ni}}$

NIOBIUM

Niobium bcc–$A2$

$\mathrm{GHSER}_{\mathrm{Nb}} = G_{\mathrm{Nb}}^{\mathrm{bcc}-A2}(T) - H_{\mathrm{Nb}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$

$298.15 < T < 2750.00$: $-\,8519.353 + 142.045475\ T - 26.4711\ T \cdot \ln T$
$+\,2.03475\mathrm{E}{-}04\ T^{2} - 3.5012\mathrm{E}{-}07\ T^{3} + 93399\ T^{-1}$

$2750.00 < T < 1000.00$: $-\,37669.3 + 271.720843\ T - 41.77\ T \cdot \ln T$
$+\,1.528238\mathrm{E}{+}32\ T^{-9}$

Niobium fcc–$A1$

$\mathrm{GFCC}_{\mathrm{Nb}} = G_{\mathrm{Nb}}^{\mathrm{fcc}-A1}(T) - H_{\mathrm{Nb}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $13500 + 1.7\ T + \mathrm{GHSER}_{\mathrm{Nb}}$

Niobium hcp–$A3$

$\mathrm{GHCP}_{\mathrm{Nb}} = G_{\mathrm{Nb}}^{\mathrm{hcp}-A3}(T) - H_{\mathrm{Nb}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$

$298.15 < T < 5000.00$: $10000 + 2.4\ T + \mathrm{GHSER}_{\mathrm{Nb}}$

Niobium liquid

$\mathrm{GLIQ}_{\mathrm{Nb}} = G_{\mathrm{Nb}}^{\mathrm{liquid}}(T) - H_{\mathrm{Nb}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$

$298.15 < T < 2750.00$: $29781.555 - 10.816417\ T$
$-\,3.06098\mathrm{E}{-}23\ T^{7}$
$+\,\mathrm{GHSER}_{\mathrm{Nb}}$
$298.15 < T < 2750.00$: $30169.9 - 10.9647\ T - 1.52824\mathrm{E}{+}32\ T^{-9}$
$+\,\mathrm{GHSER}_{\mathrm{Nb}}$

SILICON

Silicon diamond

$\mathrm{GHSER}_{\mathrm{Si}} = G_{\mathrm{Si}}^{\mathrm{diamond}}(T) - H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) =$

$298.15 < T < 1687.00$: $-\,8162.609 + 137.236859\ T - 22.8317533\ T \cdot \ln T$
$-\,1.912904\mathrm{E}{-}3\ T^{2} - 0.003552\mathrm{E}{-}6\ T^{3} + 176667\ T^{-1}$

$1687.00 < T < 3600.00$: $-\,9457.642 + 167.281367\ T - 27.196\ T \cdot \ln T$
$-\,420.369\mathrm{E}28\ T^{-9}$

Silicon bcc–$A2$

$\mathrm{GBCC}_{\mathrm{Si}} = G_{\mathrm{Si}}^{\mathrm{bcc}-A2}(T) - H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) =$

$298.15 < T < 1687.00$: $47000.0 - 22.5\ T + \mathrm{GHSER}_{\mathrm{Si}}$

Silicon cbcc–$A12$

$G_{\mathrm{Si}}^{\mathrm{cbcc-A12}}(T) - H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00 : 50208.0 - 20.377\ T + \mathrm{GHSER}_{\mathrm{Si}}$

Silicon cub–*A*13

$G_{\mathrm{Si}}^{\mathrm{cub-}A13}(T) - H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00 : 47279.0 - 20.377\ T + \mathrm{GHSER}_{\mathrm{Si}}$

Silicon fcc–*A*1

$G_{\mathrm{Si}}^{\mathrm{fcc-}A1}(T) - H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00 : 51000.00 - 21.8\ T + \mathrm{GHSER}_{\mathrm{Si}}$

Silicon hcp–*A*3

$G_{\mathrm{Si}}^{\mathrm{hcp-}A3}(T) - H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00 : 49200 - 20.8\ T + \mathrm{GHSER}_{\mathrm{Si}}$

Silicon liquid

$G_{\mathrm{Si}}^{\mathrm{liquid}}(T) - H_{\mathrm{Si}}^{\mathrm{o,diamond}}(298.15\ \mathrm{K}) =$

$298.15 < T < 1687.00 : 50696.4 - 30.0994\ T + 2.09307\mathrm{E}{-21}\ T^{7}$
$+ \mathrm{GHSER}_{\mathrm{Si}}$
$1687.00 < T < 6000.00 : 49828.2 - 29.5591\ T + 4.20369\mathrm{E}{+30}\ T^{-9}$
$+ \mathrm{GHSER}_{\mathrm{Si}}$

TANTALUM

Tantalum bcc–*A*2

$\mathrm{GHSER}_{\mathrm{Ta}} = G_{\mathrm{Ta}}^{\mathrm{bcc-A2}}(T) - H_{\mathrm{Ta}}^{\mathrm{o,bcc-}A2}(298.15\ \mathrm{K}) =$

$298.15 < T < 1300.00 : - 7285.889 + 119.139858\ T - 23.7592624\ T \cdot \ln T$
$- 0.002623033\ T^{2} + 1.70109\mathrm{E}{-07}\ T^{3} - 3293\ T^{-1}$
$1300.00 < T < 2500.00 : - 22389.955 + 243.88676\ T - 41.137088\ T \cdot \ln T$
$+ 0.006167572\ T^{2} - 6.55136\mathrm{E}{-07}\ T^{3} + 2429586\ T^{-1}$
$2500.00 < T < 3258.00 : + 229382.886 - 722.59722\ T + 78.5244752\ T \cdot \ln T$
$-0.017983376\ T^{2} + 1.95033\mathrm{E}{-07}\ T^{3} - 93813648\ T^{-1}$
$3258.00 < T < 6000.00 : -963392.734 + 2773.7774\ T - 337.227976\ T \cdot \ln T$
$+ 0.039791303\ T^{2} - 9.74251\mathrm{E}{-07}\ T^{3}$
$+ 5.09949511\mathrm{E}{+08}\ T^{-1}$

Tantalum fcc–*A*1

$\mathrm{GFCC}_{\mathrm{Ta}} = G_{\mathrm{Ta}}^{\mathrm{fcc-}A1}(T) - H_{\mathrm{Ta}}^{\mathrm{o,bcc-}A2}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00 : 16000 + 1.7\ T + \mathrm{GHSER}_{\mathrm{Ta}}$

Tantalum hcp–$A3$

$\mathrm{GHCP_{Ta}} = G_{\mathrm{Ta}}^{\mathrm{hcp-A3}}(T) - H_{\mathrm{Ta}}^{\mathrm{o,bcc-}A2}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $12000 + 2.4\ T + \mathrm{GHSER_{Ta}}$

Tantalum liquid

$\mathrm{GLIQ_{Ta}} = G_{\mathrm{Ta}}^{\mathrm{liquid}}(T) - H_{\mathrm{Ta}}^{\mathrm{o,bcc-}A2}(298.15\ \mathrm{K}) =$

$298.15 < T < 1000.00$: $29160.975 - 7.578729\ T + \mathrm{GHSER_{Ta}}$

$1000.00 < T < 1300.00$: $51170.228 - 181.121652\ T + 23.7872147\ T \cdot \ln T - 0.009707033\ T^2 + 4.4449\mathrm{E}{-07}\ T^3 - 3520045\ T^{-1} + \mathrm{GHSER_{Ta}}$

$1300.00 < T < 2500.00$: $66274.294 - 305.868555\ T + 41.1650403\ T \cdot \ln T - 0.018497638\ T^2 + 1.269735\mathrm{E}{-06}\ T^3 - 5952924\ T^{-1} + \mathrm{GHSER_{Ta}}$

$2500.00 < T < 3290.00$: $-185498.547 + 660.615425\ T - 78.4965229\ T \cdot \ln T + 0.00565331\ T^2 + 4.19566\mathrm{E}{-07}\ T^3 + 90290310\ T^{-1} + \mathrm{GHSER_{Ta}}$

$3290.00 < T < 6000.00$: $1036069.47 - 2727.38037\ T + 320.319132\ T \cdot \ln T - 0.043117795\ T^2 + 1.055148\mathrm{E}{-06}\ T^3 - 5.54714342\mathrm{E}{+08}\ T^{-1} + \mathrm{GHSER_{Ta}}$

TIN

Tin bct–$A5$

$\mathrm{GHSER_{Sn}} = G_{\mathrm{Sn}}^{\mathrm{bct-}A5}(T) - H_{\mathrm{Sn}}^{\mathrm{o,bct-}A5}(298.15\ \mathrm{K}) =$

$100.00 < T < 250.00$: $-7958.517 + 122.765451\ T - 25.858\ T \cdot \ln T + 0.51185\mathrm{E}{-3}\ T^2 - 3.192767\mathrm{E}{-6}\ T^3 + 18440\ T^{-1}$

$250.00 < T < 505.078$: $-5855.135 + 65.443315\ T - 15.961\ T \cdot \ln T - 18.8702\mathrm{E}{-3}\ T^2 + 3.121167\mathrm{E}{-6}\ T^3 - 61960\ T^{-1}$

$505.078 < T < 800.00$: $2524.724 + 4.005269\ T - 8.2590486\ T \cdot \ln T - 16.814429\mathrm{E}{-3}\ T^2 + 2.623131\mathrm{E}{-6}\ T^3 - 1081244\ T^{-1} - 123.07\mathrm{E}23\ T^{-9}$

$800.00 < T < 3000.00$: $-8256.959 + 138.99688\ T - 28.4512\ T \cdot \ln T - 123.07\mathrm{E}23\ T^{-9}$

Tin bcc–$A2$

$\mathrm{GBCC_{Sn}} = G_{\mathrm{Sn}}^{\mathrm{bcc-}A2}(T) - H_{\mathrm{Sn}}^{\mathrm{o,bct-}A5}(298.15\ \mathrm{K}) =$

$100.00 < T < 3000.00$: $4400.00 - 6.0\ T + \mathrm{GHSER}_{Sn}$

Tin fcc-$A1$

$\mathrm{GFCC_{Sn}} = G_{\mathrm{Sn}}^{\mathrm{fcc}-A1}(T) - H_{\mathrm{Sn}}^{\mathrm{o,bct}-A5}(298.15\ \mathrm{K}) =$

$100.00 < T < 3000.00$: $5510.0\text{-}8.46\ T + \mathrm{GHSER_{Sn}}$

Tin hcp-$A3$

$\mathrm{GHCP_{Sn}} = G_{\mathrm{Sn}}^{\mathrm{bcc}-A2}(T) - H_{\mathrm{Sn}}^{\mathrm{o,bct}-A5}(298.15\ \mathrm{K}) =$

$100.00\ T < 3000.00$: $3900.00 - 4.4\ T + \mathrm{GHSER_{Sn}}$

Tin liquid

$\mathrm{GLIQ_{Sn}} = G_{\mathrm{Sn}}^{\mathrm{liquid}}(T) - H_{\mathrm{Sn}}^{\mathrm{o,bct}-A5}(298.15\ \mathrm{K}) =$

$100.00 < T < 505.078$: $7103.092 - 14.087767\ T + 1.47031\mathrm{E}{-}18 T^{7} + \mathrm{GHSER_{Sn}}$

$505.078 < T < 3000.00$: $6971.587 - 13.814382\ T + 1.2307\mathrm{E}{+}25\ T^{-9} + \mathrm{GHSER_{Sn}}$

TITANIUM

Titanium hcp-$A3$

$\mathrm{GHSER_{Ti}} = G_{\mathrm{Ti}}^{\mathrm{hcp}-A3}(T) - H_{\mathrm{Ti}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) =$

$298.15 < T < 900.00$: $- 8059.921 + 133.615208\ T - 23.9933\ T \cdot \ln T - 4.777975\mathrm{E}{-}3\ T^{2} + 0.106716\mathrm{E}{-}6\ T^{3} + 72636\ T^{-1}$

$900.00 < T < 1155.00$: $- 7811.815 + 132.988068\ T - 23.9887\ T \cdot \ln T - 4.2033\mathrm{E}{-}3\ T^{2} - 0.090876\mathrm{E}{-}6\ T^{3} + 42680\ T^{-1}$

$1155.00 < T < 1941.00$: $908.837 + 66.976538\ T - 14.9466\ T \cdot \ln T - 8.1465\mathrm{E}{-}3\ T^{2} + 0.202715\mathrm{E}{-}6\ T^{3} - 1477660\ T^{-1}$

$1941.00 < T < 4000.00$: $- 124526.786 + 638.806871\ T - 87.2182461\ T \cdot \ln T + 8.204849\mathrm{E}{-}3\ T^{2} - 0.304747\mathrm{E}{-}6\ T^{3} + 36699805\ T^{-1}$

Titanium bcc-$A2$

$\mathrm{GBCC_{Ti}} = G_{\mathrm{Ti}}^{\mathrm{bcc}-A2}(T) - H_{\mathrm{Ti}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) =$

$298.15 < T < 1155.00$: $- 1272.064 + 134.71418\ T - 25.5768\ T \cdot \ln T - 0.663845\mathrm{E}{-}3\ T^{2} - 0.278803\mathrm{E}{-}6\ T^{3} + 7208\ T^{-1}$

$1155.00 < T < 1941.00$: $6667.385 + 105.366379\ T - 22.3771\ T \cdot \ln T + 1.21707\mathrm{E}{-}3\ T^{2} - 0.84534\mathrm{E}{-}6\ T^{3} - 2002750\ T^{-1}$

$1941.00 < T < 4000.00$: $26483.26 - 182.426471\ T + 19.0900905\ T \cdot \ln T - 22.00832\mathrm{E}{-}3\ T^{2} + 1.228863\mathrm{E}{-}6\ T^{3} + 1400501\ T^{-1}$

Titanium cbcc–$A12$

$G_{\mathrm{Ti}}^{\mathrm{cbcc-A12}}(T) - H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $4602.2 + \mathrm{GHSER_{Ti}}$

Titanium bct–$A5$

$G_{\mathrm{Ti}}^{\mathrm{bct-}A5}(T) - H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $4602.2 + \mathrm{GHSER_{Ti}}$

Titanium cub–$A13$

$G_{\mathrm{Ti}}^{\mathrm{cub-}A13}(T) - H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $7531.2 + \mathrm{GHSER_{Ti}}$

Titanium diamond

$G_{\mathrm{Ti}}^{\mathrm{diamond}}(T) - H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $25000.00 + \mathrm{GHSER_{Ti}}$

Titanium fcc–$A1$

$G_{\mathrm{Ti}}^{\mathrm{fcc-}A1}(T) - H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $6000.0 - 0.1\ T + \mathrm{GHSER_{Ti}}$

Titanium Laves–$C14$

$G_{\mathrm{Ti:Ti}}^{\mathrm{Laves-}C14}(T) - 3.0\ H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $15000.0 + 3.0\ \mathrm{GHSER_{Ti}}$

Titanium Laves–$C15$

$G_{\mathrm{Ti:Ti}}^{\mathrm{Laves-}C14}(T) - 3.0\ H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $15000.0 + 3.0\ \mathrm{GHSER_{Ti}}$

Titanium liquid

$G_{\mathrm{Ti}}^{\mathrm{liquid}}(T) - H_{\mathrm{Ti}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) =$

$298.15 < T < 1300.00$: $+ 12194.415 - 6.980938\ T + \mathrm{GHSER_{Ti}}$

$1300.00 < T < 1941.00$ $+ 368610.36 - 2620.999038\ T + 357.005867\ T \cdot \ln T$
$- 155.262855\mathrm{E}{-03}\ T^2 + 12.254402\mathrm{E}{-06}\ T^3$
$- 65556856\ T^{-1} + \mathrm{GHSER_{Ti}}$

$1941.00 < T < 6000.00$: $+ 104639.72 - 340.070171\ T + 40.9282461\ T \cdot \ln T$
$- 8.204849\mathrm{E}{-03}\ T^2 + 0.304747\mathrm{E}{-06}\ T^3$
$- 36699805\ T^{-1} + \mathrm{GHSER_{Ti}}$

TUNGSTEN

Tungsten bcc–$A2$

$\mathrm{GHSER_W} = G_{\mathrm{W}}^{\mathrm{bcc}-A2}(T) - H_{\mathrm{W}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$

$298.15 < T < 3695.00$: $- 7646.311 + 130.4\ T - 24.1\ T\cdot \ln T$
$- 0.001936\ T^2 + 2.07\mathrm{E}{-07}\ T^3 + 44500\ T^{-1}$
$- 5.33\mathrm{E}{-11}\ T^4$

$3695.00 < T < 6000.00$: $- 82868.801 + 389.362335\ T - 54\ T\cdot \ln T$
$+ 1.528621\mathrm{E}{+33}\ T^{-9}$

Tungsten fcc–$A1$

$\mathrm{GFCC_W} = G_{\mathrm{W}}^{\mathrm{fcc}-A1}(T) - H_{\mathrm{W}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$

$298.15 < T < 3695.00$: $11653.689 + 131.03\ T - 24.1\ T\cdot \ln T$
$- 0.001936\ T^2 + 2.07\mathrm{E}{-07}\ T^3 + 44500\ T^{-1}$
$- 5.33\mathrm{E}{-11}\ T^4$

$3695.00 < T < 6000.00$: $- 63568.801 + 389.992335\ T - 54\ T\cdot \ln T$
$+ 1.528621\mathrm{E}{+33}\ T^{-9}$

Tungsten hcp–$A3$

$\mathrm{GHCP_W} = G_{\mathrm{W}}^{\mathrm{hcp}-\mathrm{A3}}(T) - H_{\mathrm{W}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$

$298.15 < T < 3695.00$: $7103.689 + 130.4\ T - 24.1\ T \cdot \ln T$
$- 0.001936\ T^2 + 2.07\mathrm{E}{-07}\ T^3 + 44500\ T^{-1}$
$- 5.33\mathrm{E}{-11}\ T^4$

$3695.00 < T < 6000.00$: $- 68118.801 + 389.362335\ T - 54\ T\cdot \ln T$
$+ 1.528621\mathrm{E}{+33}\ T^{-9}$

Tungsten liquid

$\mathrm{GLIQ_W} = G_{\mathrm{W}}^{\mathrm{liquid}}(T) - H_{\mathrm{W}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$

$298.15 < T < 3695.00$: $44514.273 + 116.29001\ T - 24.1\ T\cdot \ln T$
$- 0.001936\ T^2 + 2.07\mathrm{E}{-07}\ T^3 + 44500\ T^{-1}$
$- 5.33\mathrm{E}{-11}\ T^4 - 2.713468\mathrm{E}{-24}\ T^7$

$3695.00 < T < 6000.00$: $- 30436.051 + 375.175\ T - 54\ T\cdot \ln T$

VANADIUM

Vanadium bcc–$A2$

$\mathrm{GHSER_V} = G_{\mathrm{V}}^{\mathrm{bcc}-A2}(T) - H_{\mathrm{V}}^{\mathrm{o,bcc}-A2}(298.15\ \mathrm{K}) =$

$298.15 < T < 790.00$: $- 7930.43 + 133.346053\ T - 24.134\ T\cdot \ln T$
$- 3.098\mathrm{E}{-3}\ T^2 + 0.12175\mathrm{E}{-6}\ T^3 + 69460\ T^{-1}$

790.00 $< T <$ 2183.00 : $- 7967.842 + 143.291093\ T - 25.9\ T \cdot \ln T$
$+ 0.0625\mathrm{E}{-3}\ T^2 - 0.68\mathrm{E}{-6}\ T^3$
2183.00 $< T <$ 4000.00 : $- 41689.864 + 321.140783\ T - 47.43\ T \cdot \ln T$
$+ 644.389\mathrm{E}29\ T^{-9}$

Vanadium fcc–$A1$

$\mathrm{GFCC_V} = G_{\mathrm{V}}^{\mathrm{fcc}-A1}(T) - H_{\mathrm{V}}^{\circ,\mathrm{bcc}-A2}(298.15\ \mathrm{K}) =$

298.15 $< T <$ 4000.00 : $7500.0 + 1.7\ T + \mathrm{GHSER_V}$

Vanadium hcp–$A3$

$\mathrm{GHCP_V} = G_{\mathrm{V}}^{\mathrm{hcp}-A3}(T) - H_{\mathrm{V}}^{\circ,\mathrm{bcc}-A2}(298.15\ \mathrm{K}) =$

298.15 $< T <$ 4000.00 : $4000.0 + 2.4\ T + \mathrm{GHSER_V}$

Vanadium liquid

$\mathrm{GLIQ_V} = G_{\mathrm{V}}^{\mathrm{liquid}}(T) - H_{\mathrm{V}}^{\circ,\mathrm{bcc}-A2}(298.15\ \mathrm{K}) =$

298.15 $< T <$ 2183.00 : $20764.117 - 9.455552\ T - 5.19136\mathrm{E}{-22}\ T^7$
$+ \mathrm{GHSER_V}$
2183.00 $< T <$ 6000.00 : $22072.353 - 10.0848\ T - 6.44389\mathrm{E}{+31}\ T^{-9}$
$+ \mathrm{GHSER_V}$

YTTRIUM

Yttrium hcp–$A3$

$\mathrm{GHSER_Y} = G_{\mathrm{Y}}^{\mathrm{hcp}-A3}(T) - H_{\mathrm{Y}}^{\circ,\mathrm{hcp}-A3}(298.15\ \mathrm{K}) =$

298.15 $< T <$ 1500.00 : $- 7347.055 + 117.532124\ T - 23.8685\ T \cdot \ln T$
$- 0.003845475\ T^2 + 1.1125\mathrm{E}{-08}\ T^3 - 16486\ T^{-1}$
1500.00 $< T <$ 1799.00 : $- 15802.62 + 229.831717\ T - 40.2851\ T \cdot \ln T$
$+ 0.0068095\ T^2 - 1.14182\mathrm{E}{-06}\ T^3$
1799.00 $< T <$ 3700.00 : $- 72946.216 + 393.885821\ T - 58.2078433\ T \cdot \ln T$
$+ 0.002436461\ T^2 - 7.2627\mathrm{E}{-08}\ T^3 + 20866567\ T^{-1}$

Yttrium bcc–$A2$

$\mathrm{GBCC_Y} = G_{\mathrm{Y}}^{\mathrm{bcc}-A2}(T) - H_{\mathrm{Y}}^{\circ,\mathrm{hcp}-A3}(298.15\ \mathrm{K}) =$

298.15 $< T <$ 1752.00 : $- 1861.198 + 97.522398\ T - 20.940576\ T \cdot \ln T$
$- 0.007995833\ T^2 + 7.58716\mathrm{E}{-07}\ T^3 - 54349\ T^{-1}$
1752.00 $< T <$ 1799.00 : $- 10207.724 + 195.741984\ T - 35.0201\ T \cdot \ln T$
1799.00 $< T <$ 3700.00 : $+ 104813.954 - 386.167564\ T + 39.8075986\ T \cdot \ln T$

Yttrium liquid

$\mathrm{GLIQ_Y} = G_{\mathrm{Y}}^{\mathrm{liquid}}(T) - H_{\mathrm{Y}}^{\mathrm{o,hcp}-A3}(298.15\ \mathrm{K}) =$

$298.15 < T < 1799.00$: $3934.121 + 59.921688\ T - 14.8146562\ T \cdot \ln T$
$- 0.015623487\ T^2 + 1.442946\mathrm{E}{-06}\ T^3$
$- 140695\ T^{-1}$

$1799.00 < T < 3700.00$: $- 13337.609 + 258.004539\ T - 43.0952\ T \cdot \ln T$
$- 0.019918739\ T^2 + 8.41308\mathrm{E}{-07}\ T^3$
$- 31549963\ T^{-1}$

ZINC

Zinc hcp–Zn

$\mathrm{GHSER_{Zn}} = G_{\mathrm{Zn}}^{\mathrm{hcp}-Zn}(T) - H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) =$

$298.15 < T < 692.68$: $- 7285.787 + 118.470069\ T - 23.701314\ T \cdot \ln T$
$- 1.712034\mathrm{E}{-3}\ T^2 - 1.264963\mathrm{E}{-6}\ T^3$

$692.68 < T < 1700.00$: $- 11070.559 + 172.34566\ T - 31.38\ T \cdot \ln T$
$+ 470.514\mathrm{E}24\ T^{-9}$

Zinc hcp–$A3$

$G_{\mathrm{Zn}}^{\mathrm{hcp}-A3}(T) - H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) =$

$298.15 < T < 1700$: $2970 - 1.57\ T + \mathrm{GHSER}_{Zn}$

Zinc bcc–$A2$

$\mathrm{GBCC_{Zn}} = G_{\mathrm{Zn}}^{\mathrm{bcc}-A2}(T) - H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $2886.96 - 2.5104\ T + \mathrm{GHSER}_{Zn}$

Zinc bct–$A5$

$G_{\mathrm{Zn}}^{\mathrm{bct}-A5}(T) - H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}} =$

$298.15 < T < 6000.00$: $2886.96 - 2.5104\ T + \mathrm{GHSER}_{Zn}$

Zinc fcc–$A1$

$G_{\mathrm{Zn}}^{\mathrm{fcc}-A1}(T) - H_{\mathrm{Zn}}^{\mathrm{o,hcp-Zn}}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $2969.82 - 1.56968\ T + \mathrm{GHSER}_{Zn}$

Zinc liquid

$G^{\rm liquid}_{\rm Zn}(T) - H^{\rm o,hcp-A3}_{\rm Zn}(298.15\ {\rm K}) =$

$298.15 < T < 692.68$: $7157.213 - 10.29299\ T - 3.5896{\rm E}{-}19\ T^{7}$
$+ {\rm GHSER}_{\rm Zn}$

$692.68 < T < 1700.00$: $7450.168 - 10.737066\ T - 4.7051{\rm E}{+}26\ T^{-9}$
$+ {\rm GHSER}_{\rm Zn}$

ZIRCONIUM

Zirconium hcp–$A3$

${\rm GHSER}_{\rm Zr} = G^{\rm T,hcp-A3}_{\rm Zr}(T) - H^{\rm o,hcp-A3}_{\rm Zr}(298.15\ {\rm K}) =$

$298.15 < T < 2128.00$: $-7827.595 + 125.64905\ T - 24.1618\ T\cdot \ln T$
$- 4.37791{\rm E}{-}3\ T^{2} + 34971\ T^{-1}$

$2128.00 < T < 4000.00$: $-26085.921 + 262.724183\ T - 42.144\ T\cdot \ln T$
$- 1342.895{\rm E}28\ T^{-9}$

Zirconium bcc–$A2$

${\rm GBCC}_{\rm Zr} = G^{\rm T,bcc-A2}_{\rm Zr}(T) - H^{\rm o,hcp-A3}_{\rm Zr}(298.15\ {\rm K}) =$

$298.15 < T < 2128.00$: $7302.056 - 0.70335\ T - 1.445606\ T\cdot \ln T$
$+ 4.037826{\rm E}{-}3\ T^{2} - 9.7289735{\rm E}{-}9\ T^{3}$
$- 7.6142894{\rm E}{-}11\ T^{4} - 9737.0\ T^{-1} + {\rm GHSER}_{\rm Zr}$

$2128.00 < T < 4000.00$: $-4620.034 + 1.55998\ T + 1.41035{\rm E}{+}32\ T^{-9}$

Zirconium fcc–$A1$

${\rm GFCC}_{\rm Zr} = G^{\rm fcc-A1}_{\rm Zr}(T) - H^{\rm o,hcp-A3}_{\rm Zr}(298.15\ {\rm K}) =$

$130.00 < T < 4000.00$: $7600.00 - 0.9\ T + {\rm GHSER}_{\rm Zr}$

Zirconium liquid

${\rm GLIQ}_{\rm Zr} = G^{\rm liquid}_{\rm Zr}(T) - H^{\rm o,hcp-A3}_{\rm Zr}(298.15\ {\rm K}) =$

$130.00 < T < 2128.00$: $+ 18147.703 - 9.080762\ T + 1.6275{\rm E}{-}22\ T^{7}$
: $+ {\rm GHSER}_{\rm Zr}$

$2128.00 < T < 4000.00$: $+ 17804.649 - 8.91153\ T + 1.343{\rm E}{+}31\ T^{-9}$
$+ {\rm GHSER}_{\rm Zr}$

Zirconium Laves–$C14$

$G^{\rm Zr,Laves-C14}_{\rm Zr:Zr} - 3.0\ H^{\rm o,hcp-A3}_{\rm Zr}(298.15\ {\rm K}) =$

$298.15 < T < 6000.00$: $15000.0 + 3.0\ {\rm GHSER}_{\rm Zr}$

Zirconium Laves–$C15$

$G_{\mathrm{Zr:Zr}}^{\mathrm{Zr,Laves-C15}} - 3.0\ H_{\mathrm{Zr}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $15000.0 + 3.0\ \mathrm{GHSER_{Zr}}$

Zirconium Laves–$C36$

$G_{\mathrm{Zr:Zr}}^{\mathrm{Zr,Laves-C36}} - 3.0\ H_{\mathrm{Zr}}^{\mathrm{o,hcp-}A3}(298.15\ \mathrm{K}) =$

$298.15 < T < 6000.00$: $15000.0 + 3.0\ \mathrm{GHSER_{Zr}}$

APPENDIX II: MAGNETIC CONTRIBUTION TO THE GIBBS ENERGIES OF THE PURE ELEMENTS (S.I. units) [1]

$$G^{\mathrm{mag}} = R\,T\ \ln\,(\beta^{mag} + 1)\mathrm{g}(\tau)$$

Chromium

Chromium bcc–A2

$T_{\mathrm{N},}$(bcc–A2,Cr) = 311.5 β^{mag}(bcc-A2,Cr) = 0.008

Chromium fcc–A1

$T_{\mathrm{N},}$(fcc–A1,Cr) = 369.667 β^{mag}(fcc-A1,Cr) = 0.82

Chromium hcp–A3

$T_{\mathrm{N},}$(hcp–A3,Cr) = 369.667 β^{mag}(hcp–A3,Cr) = 0.82

Iron

Iron bcc–A2

$T_{\mathrm{c},}$(bcc–A2,Fe) = 1043.0 β^{mag}(bcc-A2,Fe) = 2.22

Iron fcc–A1

$T_{\mathrm{c},}$(fcc–A1,Fe) = 1043.0 β^{mag}(fcc-A1,Fe) = 2.22

Manganese

Manganese cbcc–A12

$T_{\mathrm{N},}$(cbcc–A12,Mn) = 95.0 β^{mag}(cbcc-A12,Mn) = 0.22

Manganese bcc–A2

$T_{\mathrm{N},}$(bcc–A2,Mn) = 580.0 β^{mag}(bcc-A2,Mn) = 0.27

Manganese fcc–A1

$T_{\mathrm{N},}$(fcc–A1,Fe) = 540.0 β^{mag}(fcc-A1,Mn) = 0.62

Manganese hcp–A3

$T_{\mathrm{N},}$(hcp–A3,Fe) = 540.0 β^{mag}(hcp–A3,Mn) = 0.62

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[1] Scientific Group Thermodata Europe (S.G.T.E.) Data for Pure Elements, A.T. Dinsdale, Calphad, 15, 4, 317 - 425 (1991).

Nickel

Nickel bcc–*A*2

$T_{c,}(\text{bcc–}A2,\text{Ni}) = 575.0$ $\beta^{mag}(\text{bcc-A2,Ni}) = 0.85$

Nickel fcc–*A*1

$T_{c,}(\text{fcc–}A1,\text{Ni}) = 633.0$ $\beta^{mag}(\text{fcc-A1,Ni}) = 0.52$

Nickel hcp–*A*3

$T_{c,}(\text{hcp–}A3,\text{Ni}) = 633.0$ $\beta^{mag}(\text{hcp-A3,Ni}) = 0.52$

---

bcc–*A*2

for $\tau = T < T_c$ $g(\tau) = 1 - 0.905299383\ \tau^{-1} - 0.153008346\ \tau^{3}$
$- 0.00680037095\ \tau^{9} - 0.00153008346\ \tau^{15}$

for $\tau = T_c < T$ $g(\tau) = - 0.0641731208\ \tau^{-5} - 0.00203724193\ \tau^{-15}$
$- 4.27820805\text{E-}04\ \tau^{-25}$

cbcc–*A*12

for $\tau = T < T_c$ $g(\tau) = 1 - 0.8603387550\tau^{-1} - 0.17449124\tau^{3}$
$- 0.00775516624\ \tau^{9} - 0.0017449124\ \tau^{15}$

for $\tau = T_c < T$ $g(\tau) = - 0.0426902268\tau^{-5} - 0.0013552453\tau^{-15}$
$- 2.84601512\text{E-}04\tau^{-25}$

fcc-A1

for $\tau = T < T_c$ $g(\tau) = 1 - 0.8603387550\tau^{-1} - 0.17449124\tau^{3}$
$- 0.00775516624\ \tau^{9} - 0.0017449124\ \tau^{15}$

for $\tau = T_c < T$ $g(\tau) = - 0.0426902268\tau^{-5} - 0.0013552453\tau^{-15}$
$- 2.84601512\text{E-}04\tau^{-25}$

hcp–*A*3

for $\tau = \text{T}<\text{T}_c$ $g(\tau) = 1 - 0.8603387550\tau^{-1} - 0.17449124\tau^{3}$
$- 0.00775516624\ \tau^{9} - 0.0017449124\ \tau^{15}$

for $\tau = T_c < T$ $g(\tau) = - 0.0426902268\tau^{-5} - 0.0013552453\tau^{-15}$
$- 2.84601512\text{E-}04\tau^{-25}$

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