正电子概况VIII

正电子技术在材料科学中的应用-半导体

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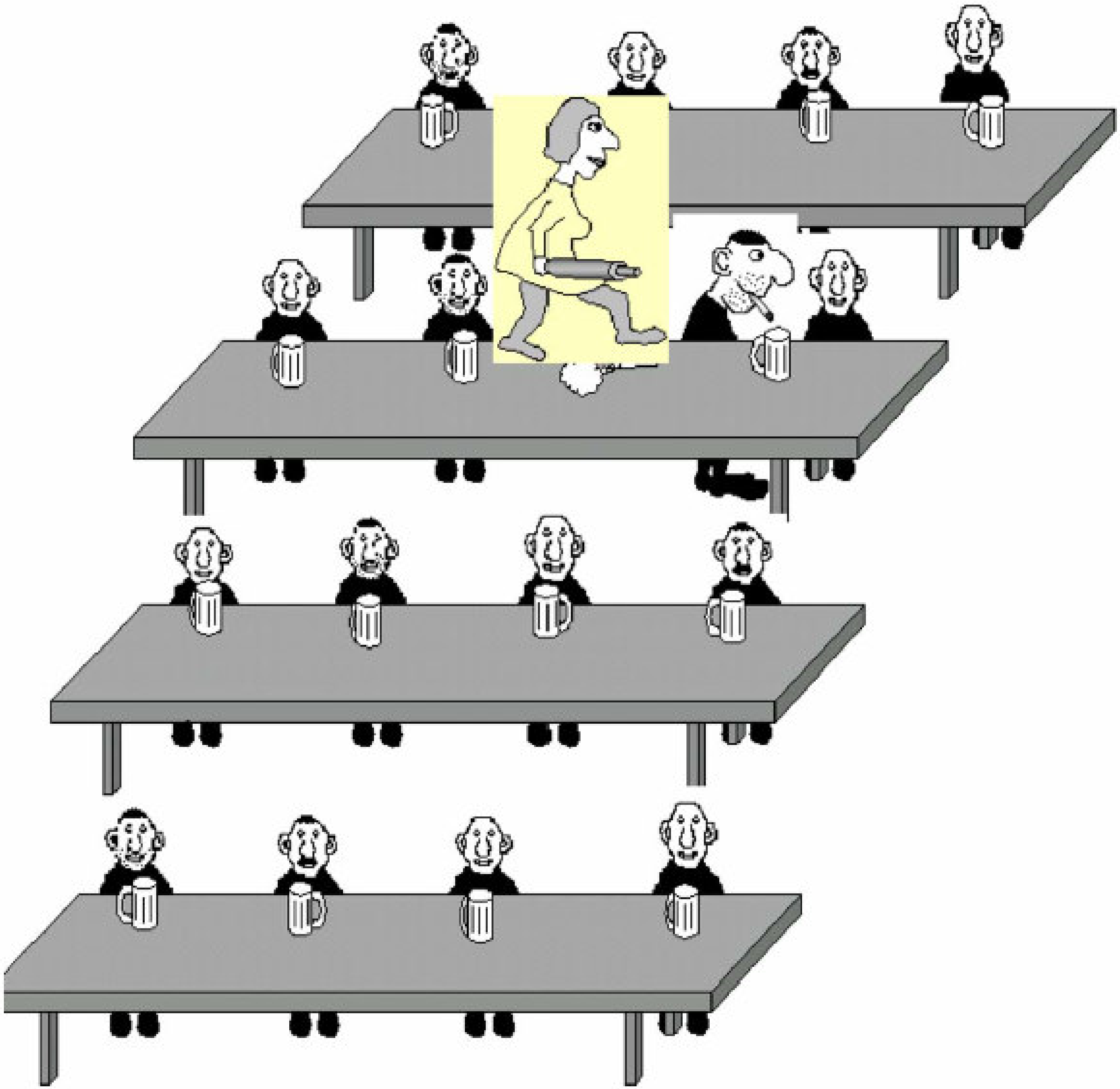
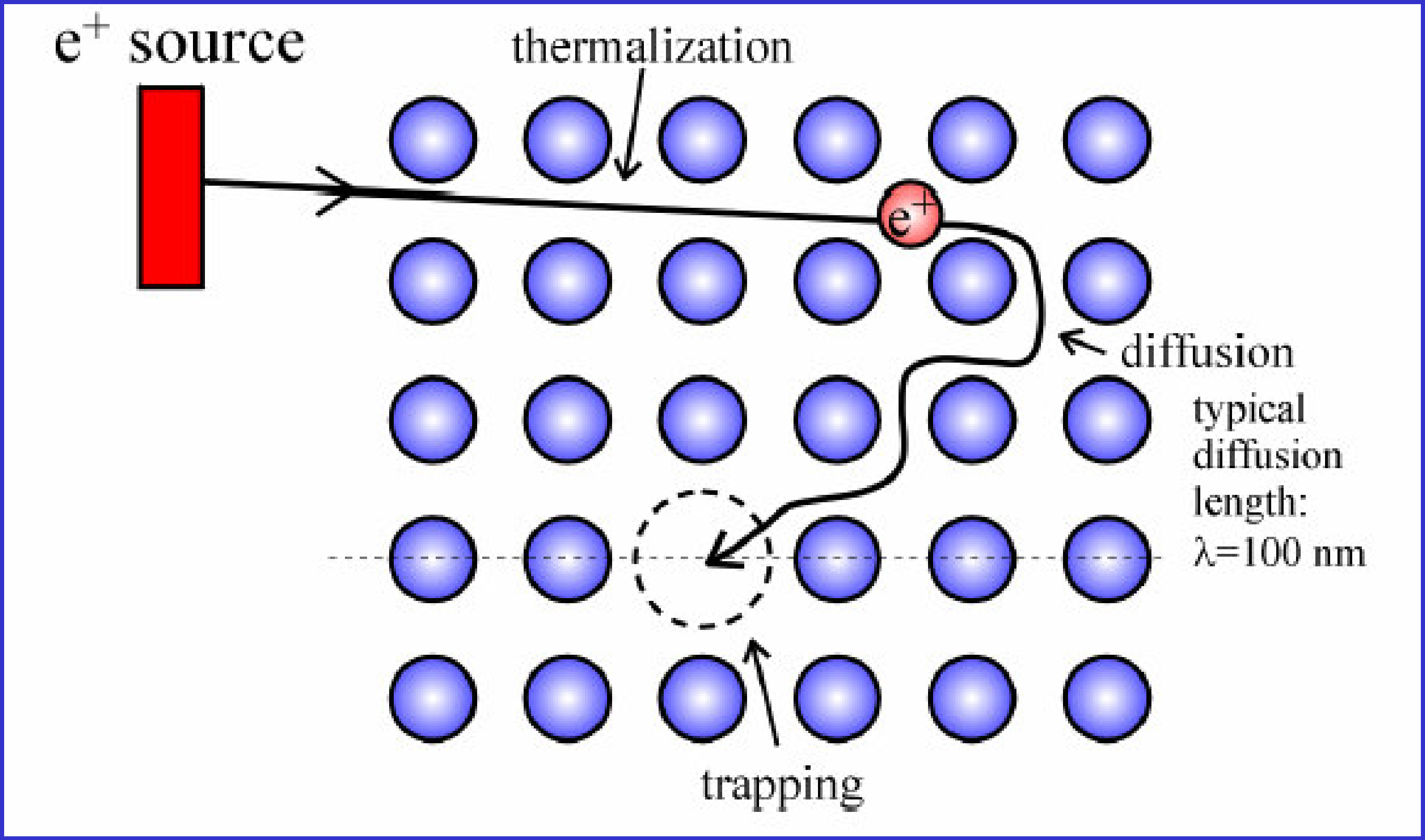


正电子在半导体中的应用



半导体材料

- 第一代半导体材料: **Si, Ge**
- 第二代半导体材料: **III-V** 族化合物（**GaAs, InP** 等**)**
- **II-VI**族化合物等单晶（**CdSe** 等），
- 第三代宽带隙半导体: **IV-IV** 族化合物（**SiC** 等**)** 单晶、微晶、纳米晶和非晶半导体。

Positron Studies of Semiconductor Defects (PSSD)

- **PSSD-2004,第4届, 美国华盛顿州立大学**
- **PSSD-2002,第3届, 日本东北大学**
- **PSSD-1999,第2届, McMaster Univ. 加拿大**
- **PSSD-1994,第1届, Halle, 德国**

PSSD-Topics

1. Basic work such as identification of defects: defect formation, migration, agglomeration and annealing.
2. Momentum distribution studies of defects: coincidence Doppler broadening, angular correlation of annihilation radiation (ACAR).
3. Low-k/High-k dielectric insulating materials in semiconductor devices
4. Theoretical calculations of momentum distributions and positron lifetimes
5. Slow beam studies of surface and near surface regions of semiconductors
6. High resolution positron lifetime studies of semiconductors
7. Semiconductor defects studied by the experimental methods other than positron annihilation
8. Industrial application of positron annihilation to semiconductor devices.

Positron Annihilation in Semiconductors

Defect Studies

R.Krause-Rehberg
H.S.Leipner

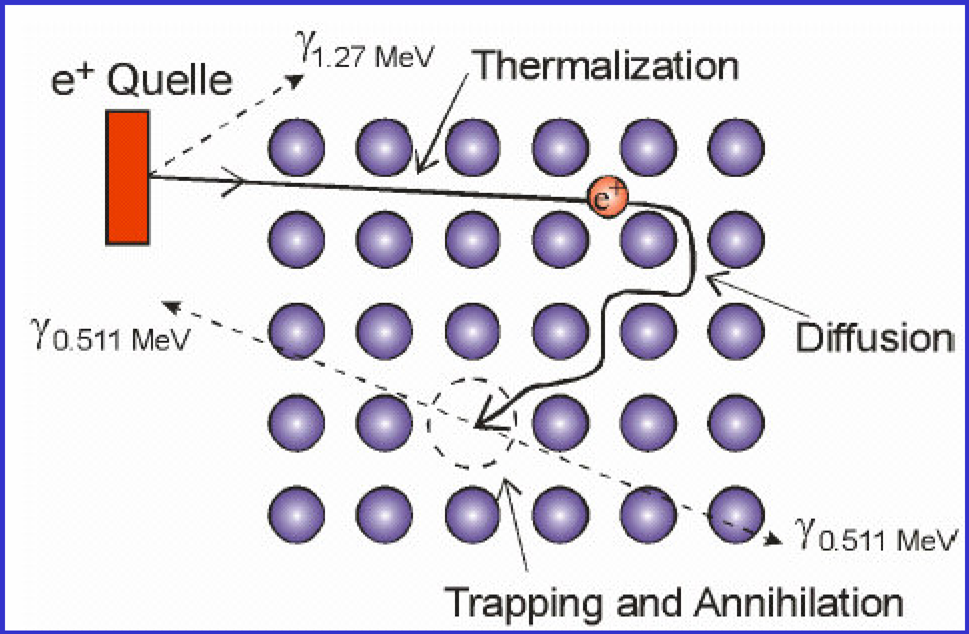
Springer Series in Solid-State Science, 1998

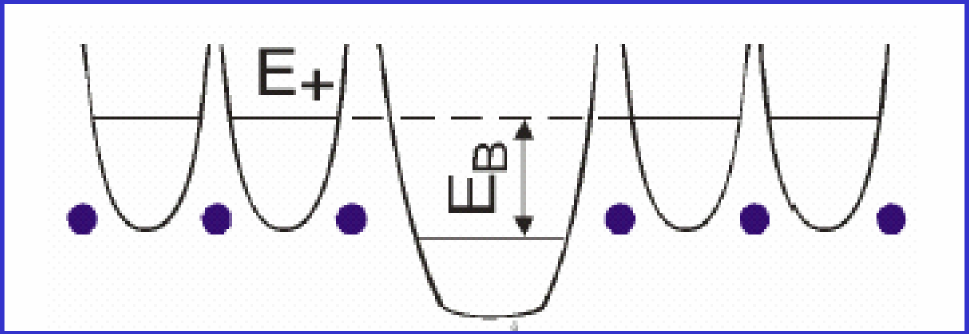
Introduction

- Questions of semiconductor industry
  - Defect types?
  - Defect charge states?
  - Defect concentrations?

- Answers of positron annihilation
  - Vacancy-like defects and defect complexes
    Size of a vacancy (mono-, di-, vacancy cluster)
  - Neutral or negatively charged vacancy-complexes
    Positively charged defects are invisible
  - Sensitivity limits 10^{14}-10^{19} cm^{-3}

Positron in materials

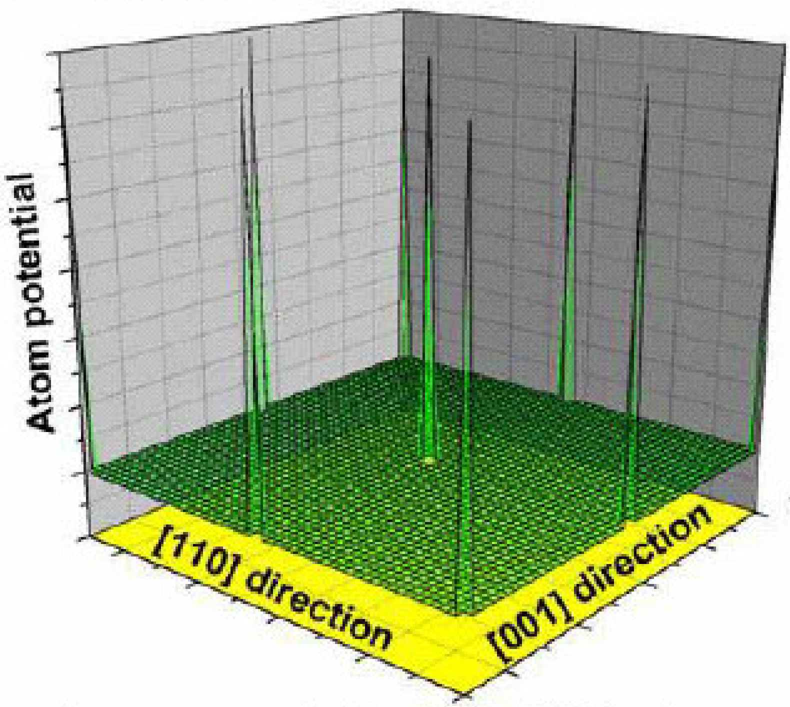




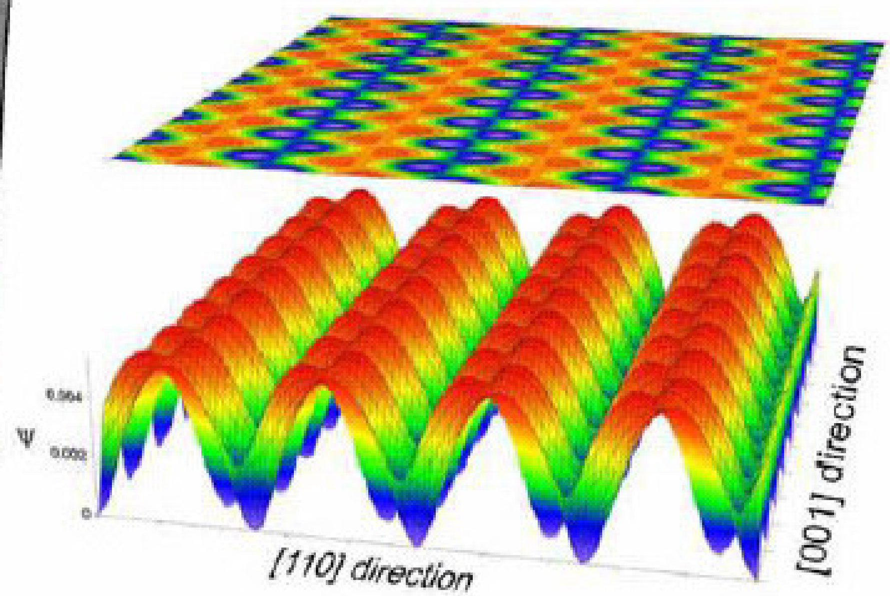
- positron wave-function can be localized in the attractive potential of a defect
- annihilation parameters change in the localized state
- e.g. positron lifetime increases in a vacancy
- lifetime is measured as time difference between 1.27 and 0.51 MeV quanta
- defect identification and quantification possible

Positron trapping - Vacancy

- Perfect lattice



Atom potential in GaAs (110) plane

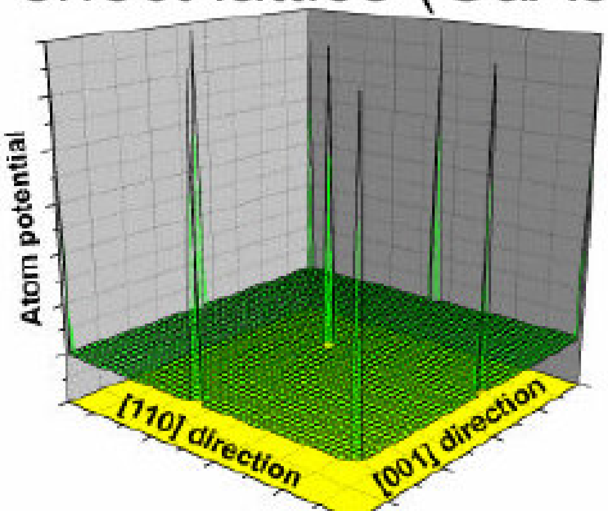


Positron wave function in GaAs (110) plane

- Positrons are repelled by positive atom cores

Positron trapping

- Perfect lattice (GaAs plane [110])

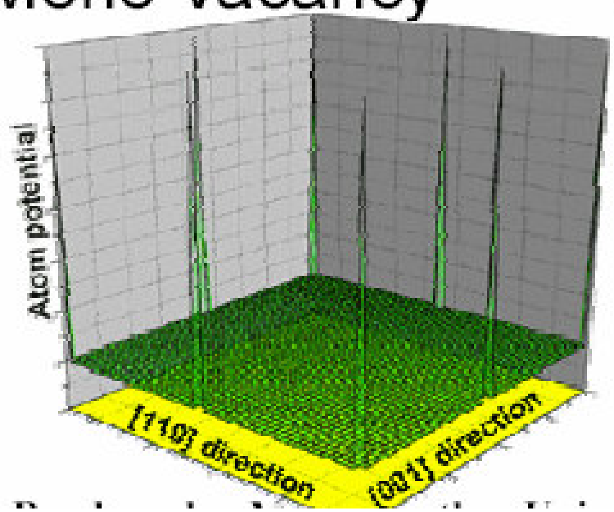


- Positrons are repelled by positive atom cores

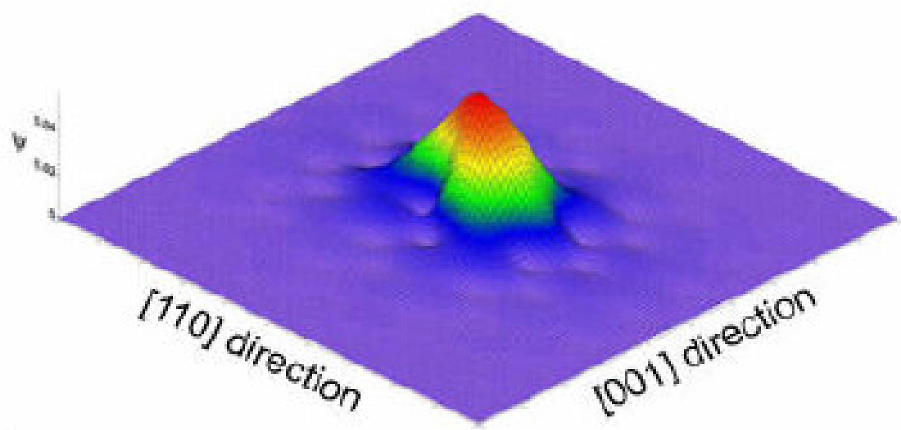
- Vacancy represents a positron trap due to the missing nuclei (potential well for a positron)

Positron Annihilation is sensitive to vacancy-like defects

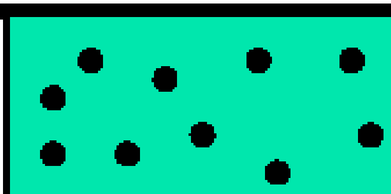
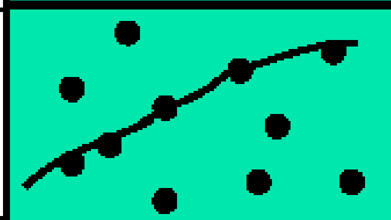
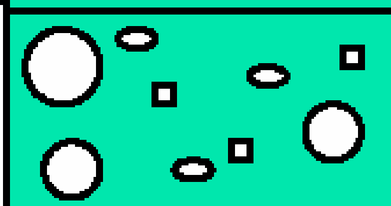
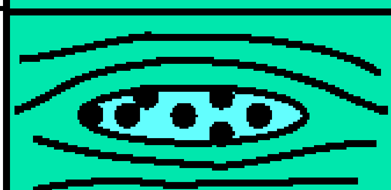
- Mono-vacancy



- Because of reduced electron density positrons live longer in vacancies

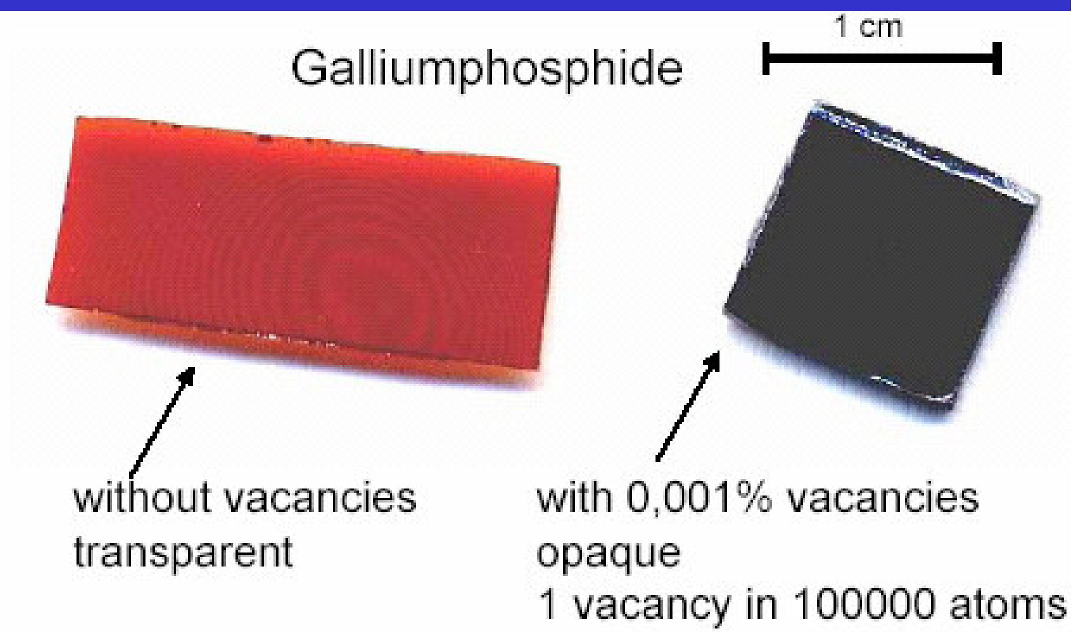


Defects in Materials

Defect Type		Size	Materials
Atomic Vacancies		.1 nm	Metals
Dislocations		1 nm-10 µm	Metals
Voids		.1 nm-1 µm	Composites
Holes		.1 nm-10 µm	Polymers

Point defects determine optical and electronic properties of semiconductors

- Point defects determine electronic and optical properties
- electric conductivity strongly influenced
- Doping of semiconductors (n-, p-Si)



- Point defects are generated by irradiation (e.g. cosmic rays), by plastic deformation or by diffusion, ...
- Metals in high radiation environment -> formation of voids -> embrittlement
- -> Properties of vacancies and other point defects must be known
- Analytical tools are needed to characterize point defects

The Diffusion of Positrons

Diffusion can be described by the time-dependent diffusion equation:

$$\frac{\partial}{\partial t} n_+(\mathbf{r},t) = D_+ \nabla^2 n_+(\mathbf{r},t) - \nabla\left[v_d n_+(\mathbf{r},t)\right] - \lambda_{\text{eff}} n_+(\mathbf{r},t).$$

$n_+(\mathbf{r},t)$ ... positron density

v_d ... drift velocity (electric field)

$\lambda_{\text{eff}} = 1/\tau_b + \kappa(\mathbf{r})$ ... effective annihilation rate

$\kappa = \mu C$

μ ... trapping coefficient

C ... defect density

Mean free path l and positron diffusion length L_+ in semiconductors is mainly determined by acoustic phonon scattering $\Rightarrow D \propto T^{-0.5}$

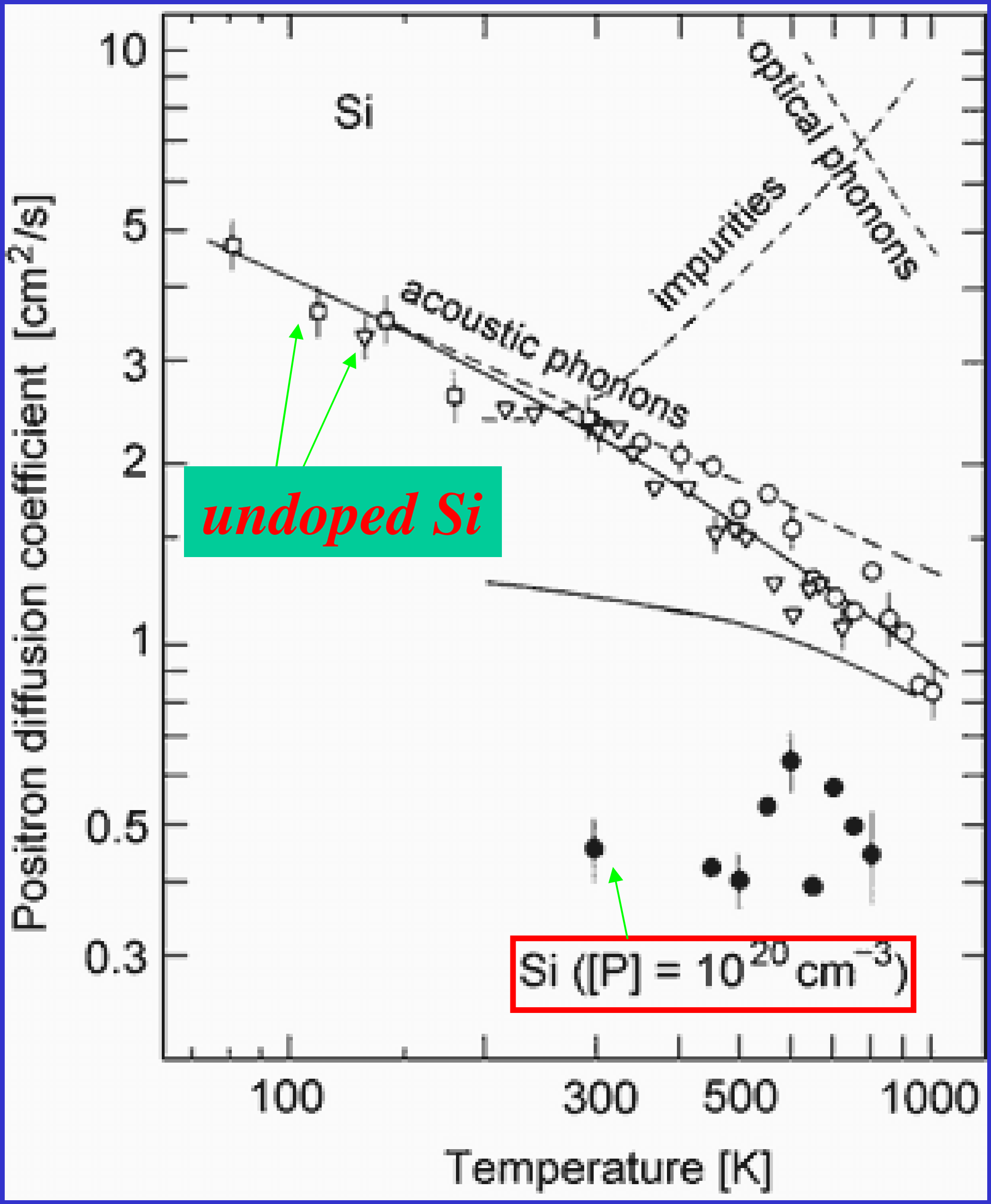
扩散长度

The positron diffusion length L_+ is limited due to the finite lifetime of positrons in the defect-free bulk, τ $_b$,

$$L_+ = \sqrt{\tau_b D_+}, \quad D_+ = \tau_r \frac{k_B T}{m^*}$$

τ $_r$ is the relaxation time for the dominant scattering mechanism. The mean free path <*l*> and the positron diffusion length L_+ of some representative semiconductors at room temperature are presented in Table.

Material	<*l*>[nm]	*L*+[nm]
Si	6.9, 6.6, 8.5	219, 214, 243
GaAs	5.3	198
Ge	5.3	200



Soininen, 1992

Effect diffusion length L_{eff}

1994年, Britton等人发现, 由于晶体缺陷和电场的影响,扩散长度应修正为:

$$L_{eff} = \frac{1}{\sqrt{\frac{\lambda_{eff}}{D_+} + \left(\frac{eE_{drift}}{2k_BT}\right)^2} - \frac{2\left|E_{drift}\right|}{2k_BT}}$$

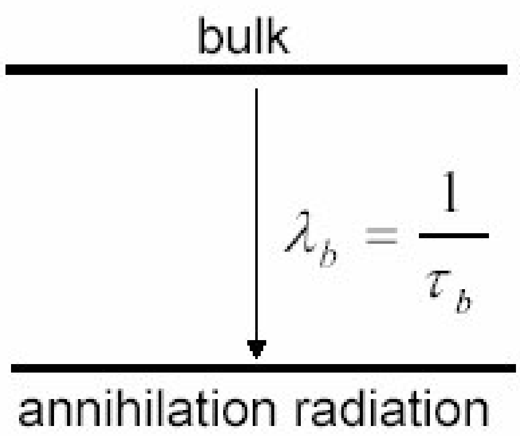
E_{drift} 是电场强度. 有效扩散长度随电场强度的增加而增加.

Trapping

- Vacancies
- Shallow positron traps
- Dislocations
- Voids
- Precipitates
- Surfaces
- Interfaces
- Graned Material
- Positronium formation

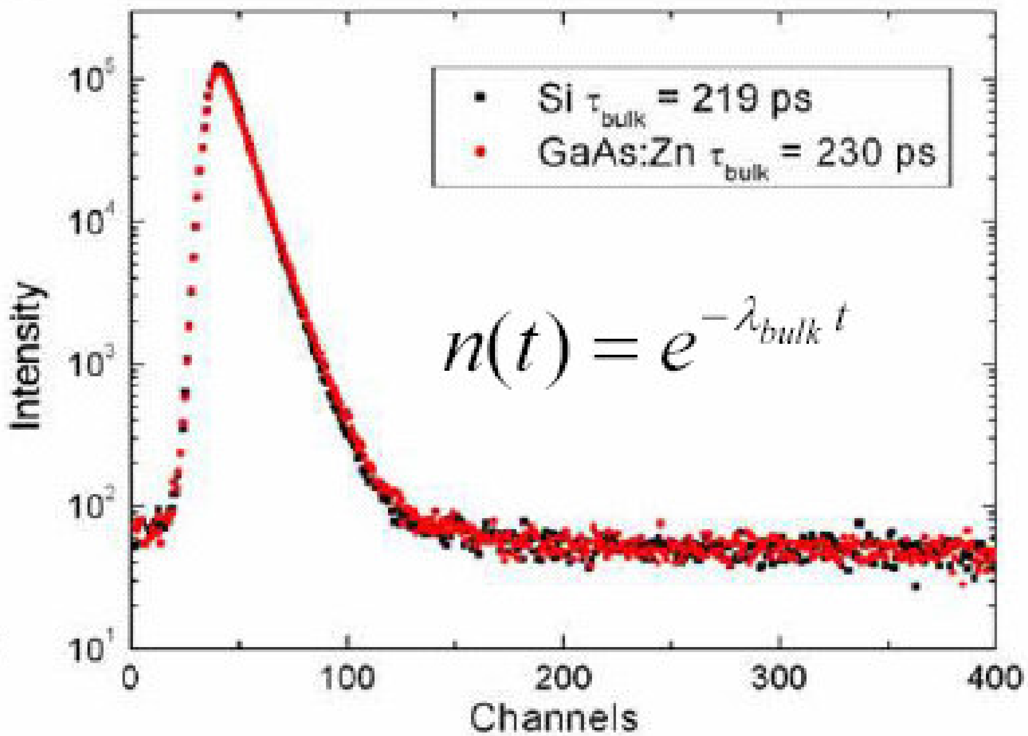
Positron Annihilation Lifetime Spectroscopy

- probability **n(t)** that e^+ is alive at time **t**: $$\frac{dn(t)}{dt} = -\lambda\, n(t) \qquad n(0) = 1$$
  λ - positron annihilation rate
- Positron lifetime spectrum in bulk:
  (no trapping of positrons)

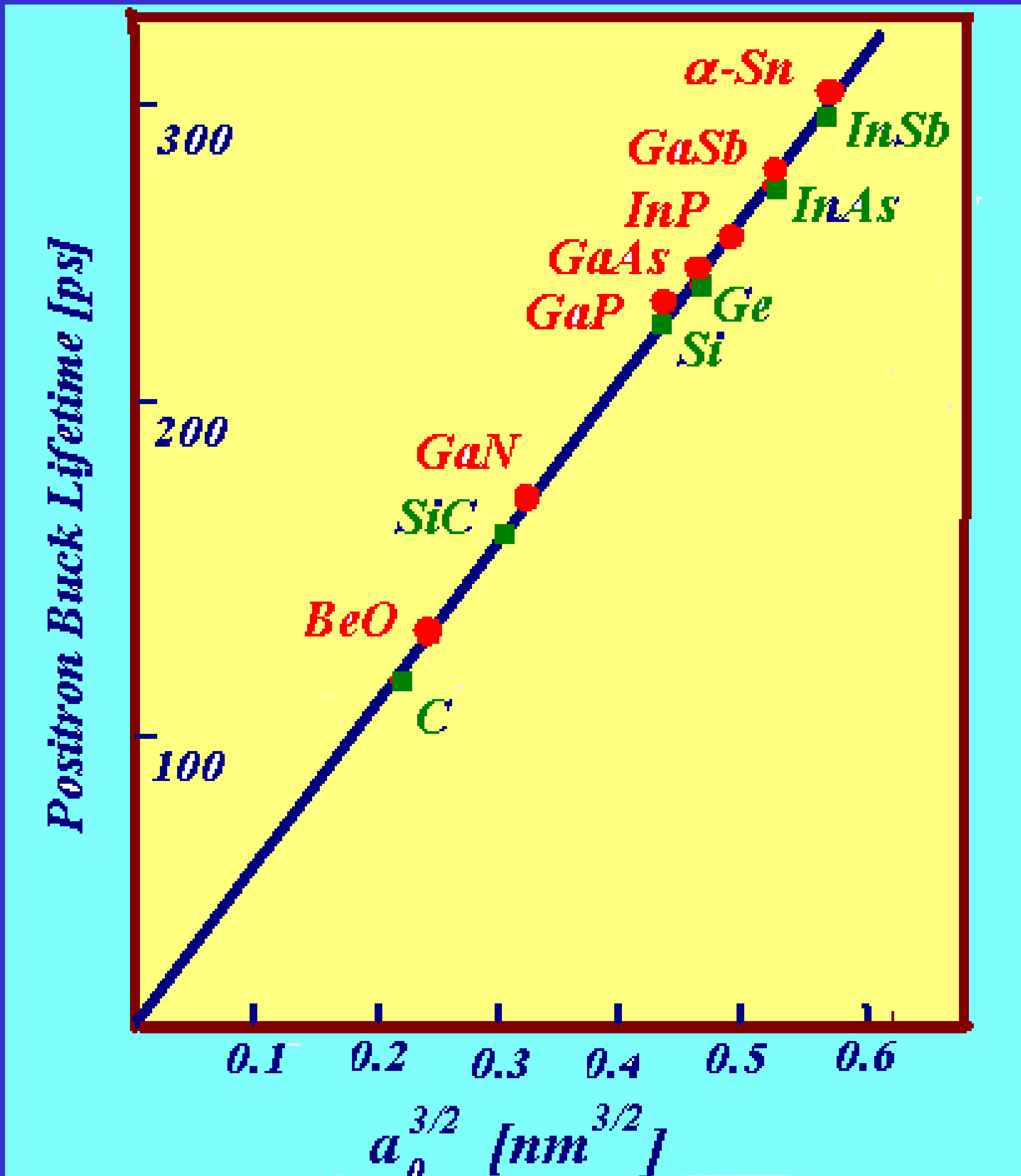


$$\lambda_b = \frac{1}{\tau_b}$$

λ - slope of the exponential decay



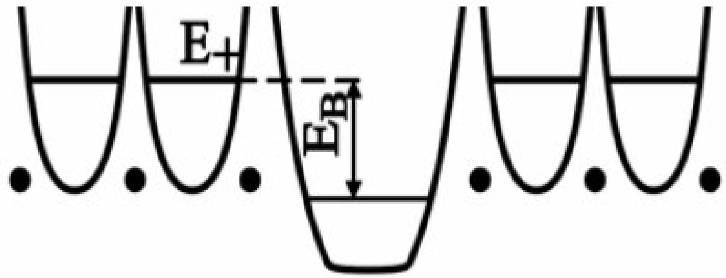
$$n(t) = e^{-\lambda_{bulk} t}$$

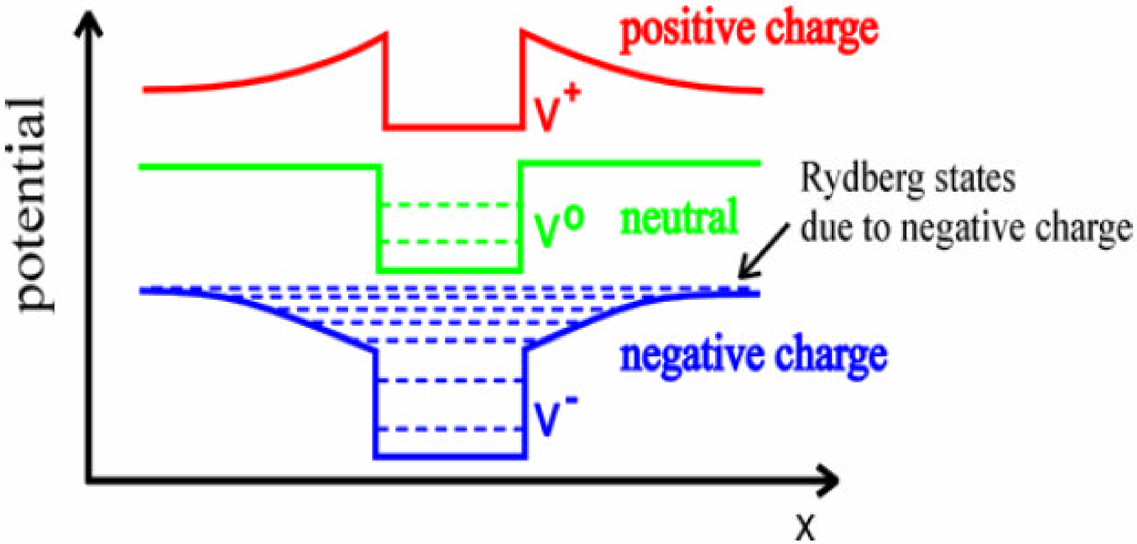


$$\tau_b = C_1 a_0^{3/2},$$
$$(C_1 = 543.8\, ps / nm^{1.5})$$

Siethoff 1998
Phys.stat.sol.(b)205,R3

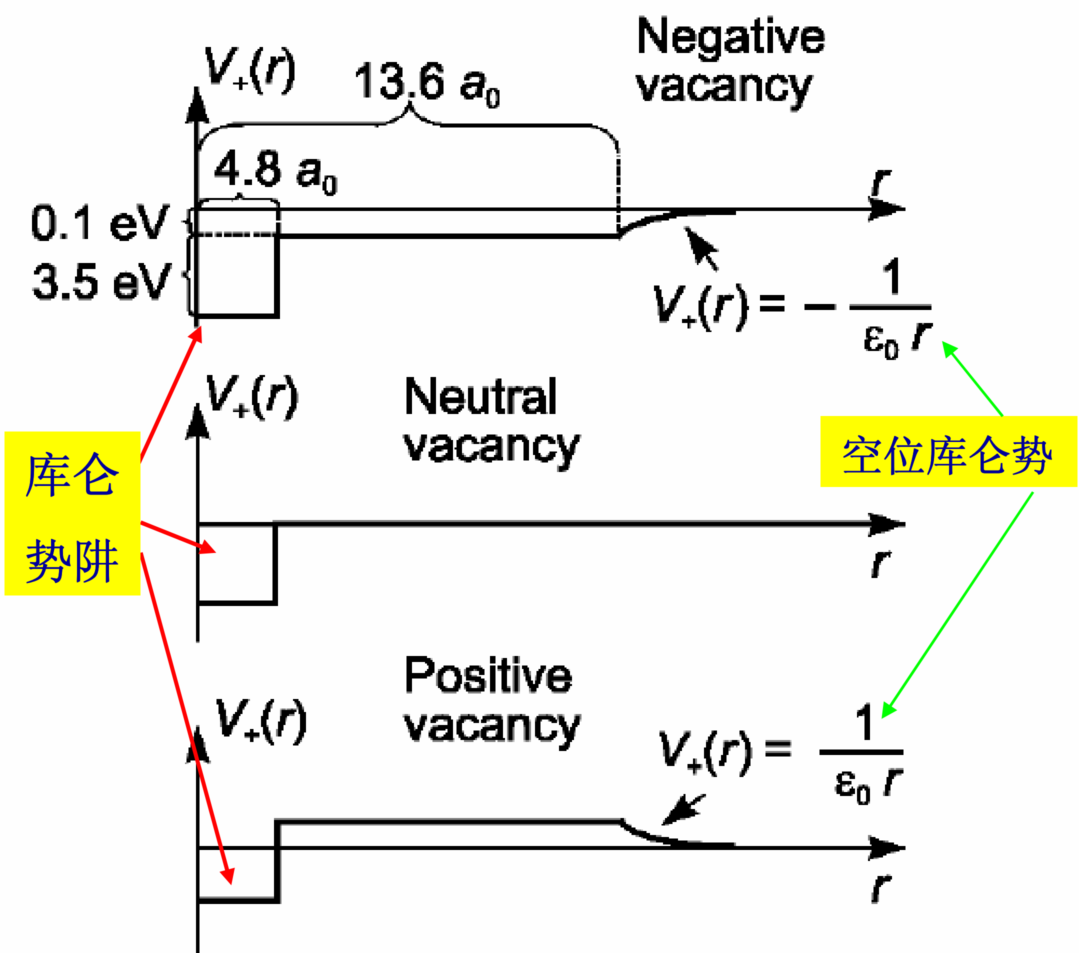
Vacancies in a semiconductor may be charged





- in a metal: charge of a vacancy is effectively screened by free electrons
- they are not available in semiconductors
- thus, long-range Coulomb potential added
- positrons may be attracted or repelled
- trapping coefficient μ is function of charge state

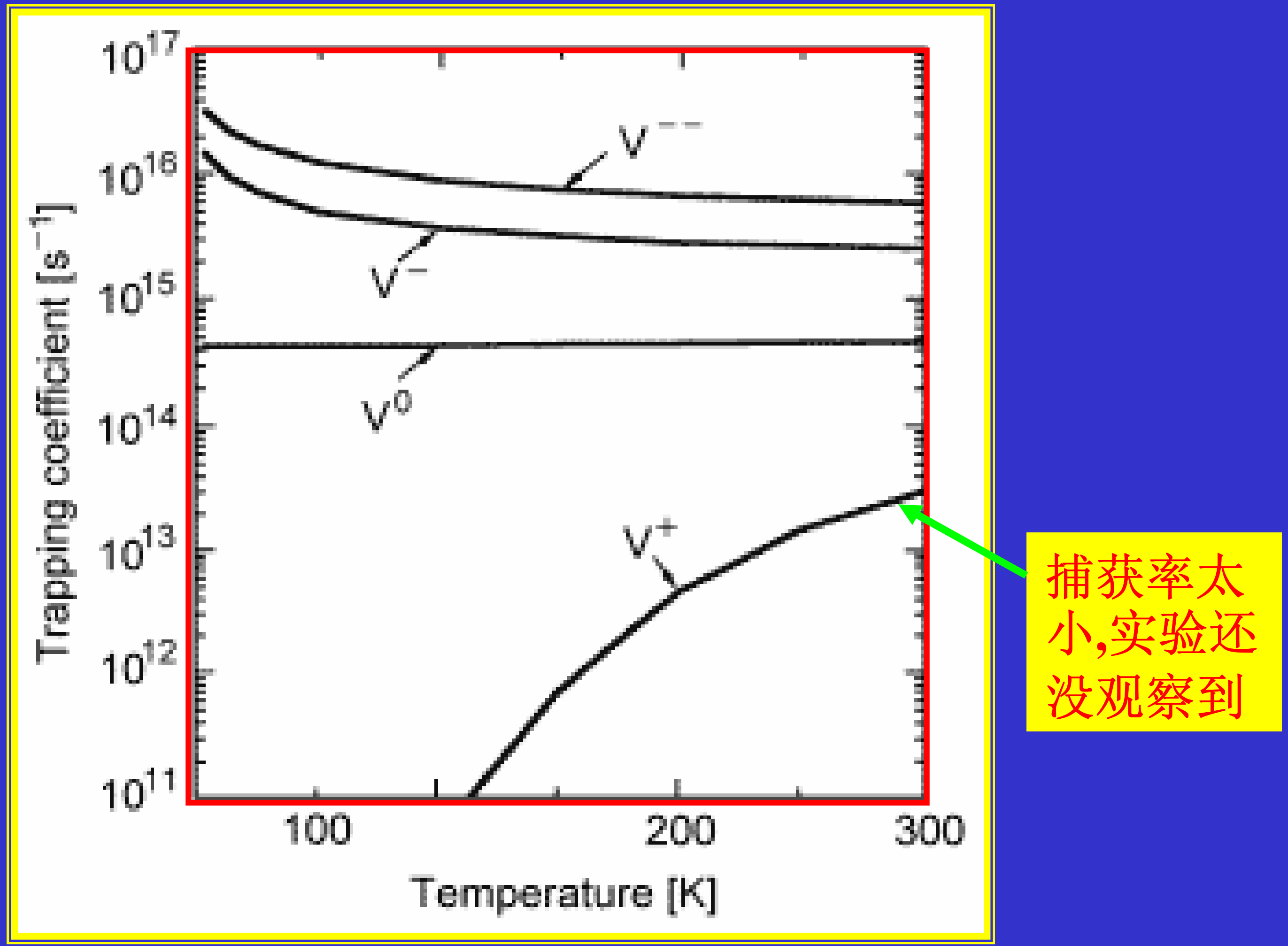
Vacancies may be charged



For a negative vacancy:

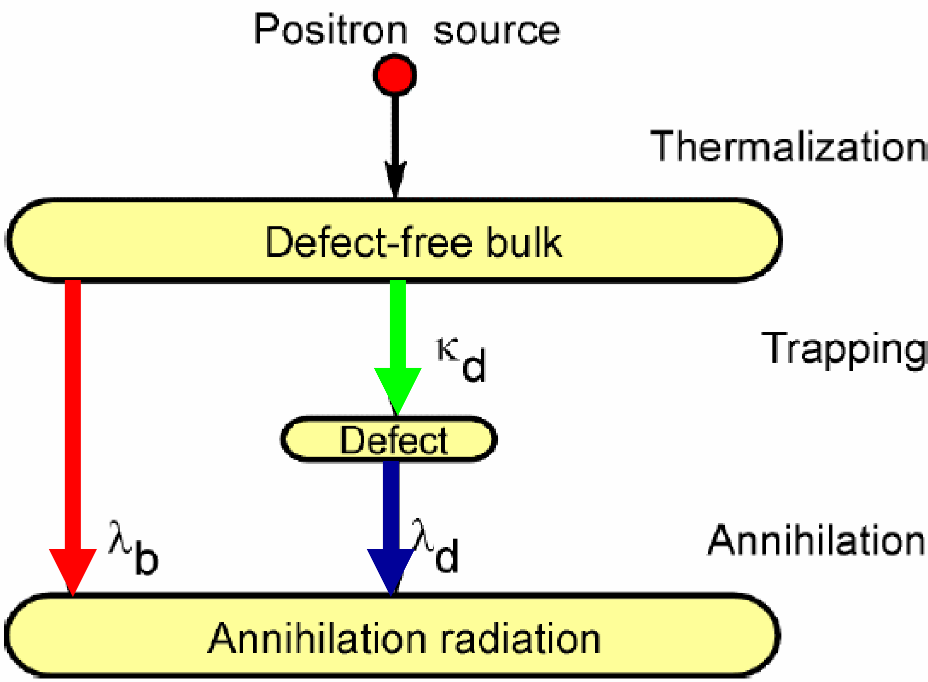
- Coulomb potential is rather extended but weak
- it supports trapping only at low temperatures
- at higher temperatures: detrapping dominates and vacancy behaves like a vacancy in a metal or a neutral vacancy

Positive vacancies repel positrons



Si的三种电荷态空位的捕获系数与温度的关系

Positron Trapping in a Single Defect Type



$$\frac{dn_b(t)}{dt} = -(\lambda_b + \kappa_d)n_b(t)$$

$$\frac{dn_d(t)}{dt} = -\lambda_d n_d(t) + \kappa_d n_b(t)$$

solution: decay spectrum

$$D(t) = I_1 \exp\left(-\frac{t}{\tau_1}\right) + I_2 \exp\left(-\frac{t}{\tau_2}\right)$$

abbreviations:

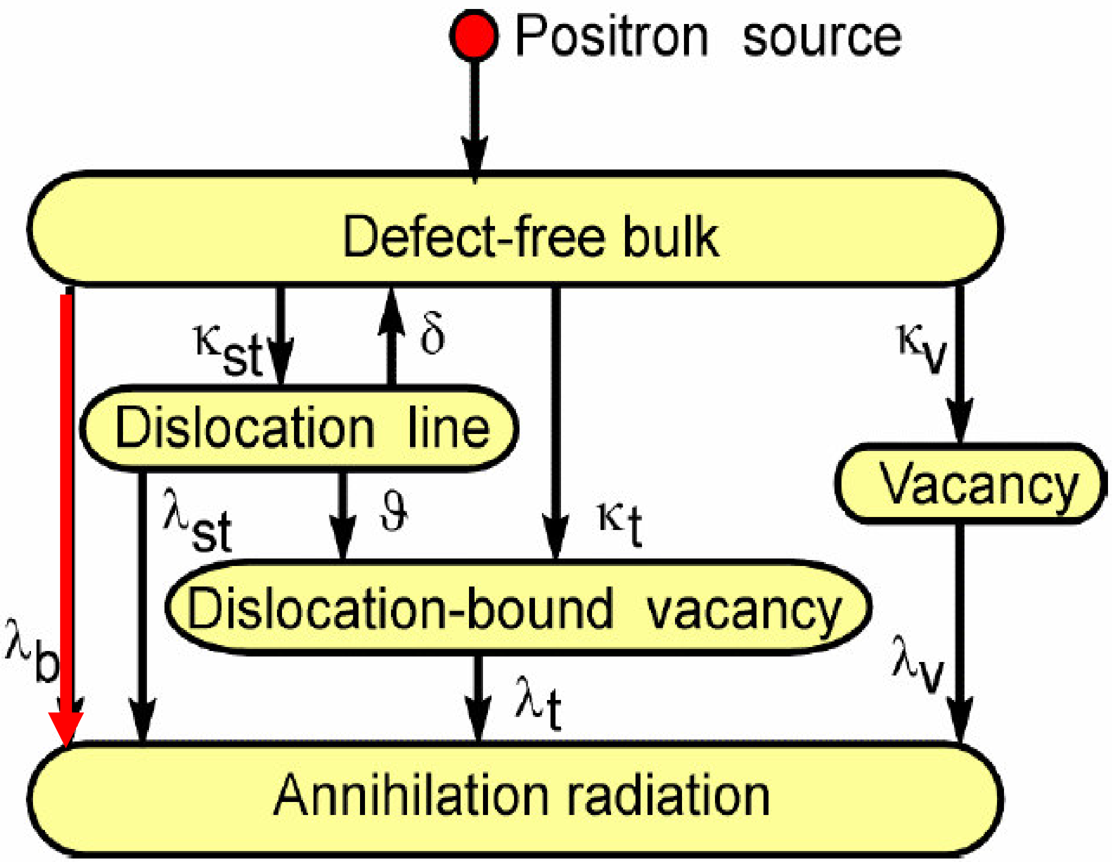
$$\tau_1 = \frac{1}{\lambda_b + \kappa_d}, \quad \tau_2 = \frac{1}{\lambda_d},$$

$$I_1 = 1 - I_2, \quad I_2 = \frac{\kappa_d}{\lambda_b - \lambda_d + \kappa_d}$$

The t_i and I_i are measured ⇒ k is obtained:

$$\boxed{\kappa_d = \mu C_d} = \frac{I_2}{I_1}\left(\frac{1}{\tau_b} - \frac{1}{\tau_d}\right)$$

Positron Trapping in a Dislocation



the dislocation line (shallow trap) acts as a "funnel" for the trapping in deep traps

b ... bulk

v ... vacancy

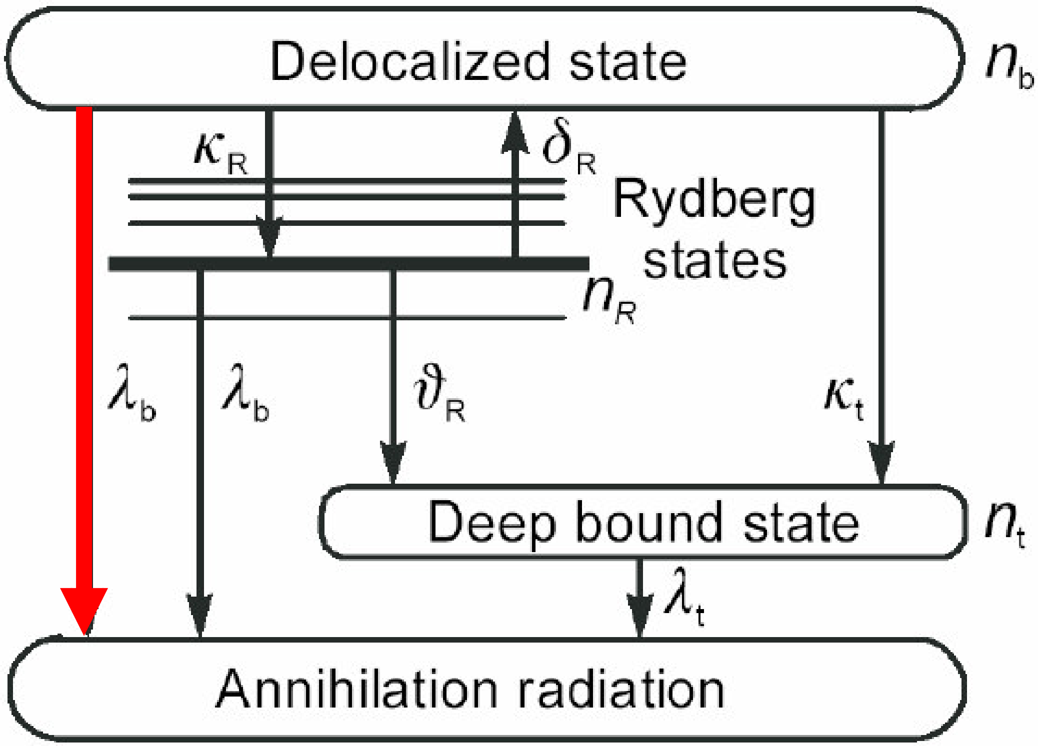
t ... deep trap

st ... shallow trap

λ_i ... annihilation rates κ_i, ϑ ... trapping rates

δ ... detrapping (escape) rate

Positron trapping by negative vacancies



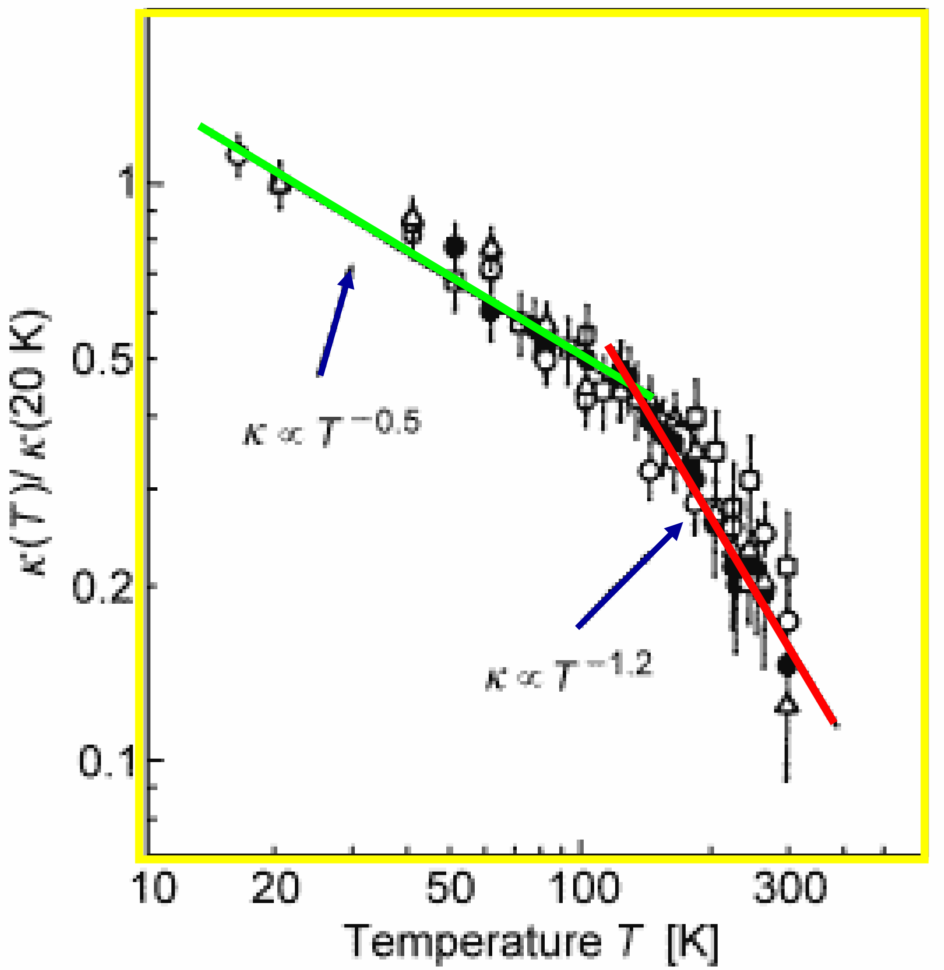
- trapping process can be described quantitatively by trapping model
- Coulomb potential leads to Rydberg states
- from there: positrons may re-escape by thermal stimulation
- once in the deep state: positron is captured until annihilation
- detrapping is strongly temperature dependent

$$\delta_R = \frac{\kappa_R}{\rho_V}\left(\frac{m^* k_B T}{2\pi\hbar^2}\right)^{3/2} \exp\left(-\frac{E_R}{k_B T}\right)$$

E_R binding energy of positron in Rydberg state $E_R \sim 10\text{meV}$

Manninen, Nieminen, 1981

ρ_V vacancy density



- temperature dependence of positron trapping is rather complex

$$\kappa = \frac{\vartheta_R \rho_v \kappa_{R0} T^{-1/2}}{\vartheta_R \rho_v + \kappa_{R0} \left(\frac{m^* k_B}{2\pi \hbar^2}\right)^{3/2} T \exp\left(-\frac{E_R}{k_B T}\right)}$$

- low temperature: ~$T^{-0.5}$ due to diffusion limitation in Rydberg states
- higher T: stronger temperature dependence due to thermal detrapping from Rydberg state

Positron trapping rate *κ* ***in negatively charged gallium vacancies determined in semi-insulating gallium arsenide as a function of temperature T. The trapping rate is normalized to the value measured at 20 °K. Different symbols stand for different samples.***

Table 1. Compilation of positron trapping coefficients of vacancy-type defects experimentally determined in various semiconductors (Krause-Rehberg and Leipner 1997). Only such experiments where the independent reference method was applied to the same samples were taken into account.

Material	Defect	Trapping coefficient $[10^{15}\ s^{-1}]$	$[10^{-8}\ cm^3 s^{-1}]$	T [K]	Reference method	Authors
Si:P	$(VP)^0$	0.68	1.4	300	Hall effect	a
		> 1.3	> 2.6	300	Resistivity	b
Si:P	$(VP)^-$	18	36	300	Hall effect	a
		> 2	> 4	300	Resistivity	b
Si	V_2^0	0.8 ± 0.40	1.5 ± 0.8	300	EPR	c
		0.8	1.6	300	Hall effect	a
Si	V_2^-	2.6 ± 1.3	5.2 ± 2.6	300	EPR	c
		10	20	300	Hall effect	a
Si	V_2^{2-}	5.2 ± 2.7	10.5 ± 5.3	300	EPR	c
		29	58	300	Hall effect	a
Si	V_2^+	< 0.1	< 0.2	300	Hall effect	a
GaP	V_P^0	0.8 ± 0.3	1.5 ± 0.6	473	Hall effect	d
GaP	V_P^-	1.9 ± 0.5	3.8 ± 1.0	473	Hall effect	d
GaP	V_P^+	< 0.1	< 0.2	473	Hall effect	d
GaAs:Te	$(V_{Ga}Te_{As})^-$	1.1 ± 0.2	2.5 ± 0.5	300	Hall effect	e
GaAs:Si	$(V_{Ga}Si_{Ga})^-$	0.7 ± 0.2	1.6 ± 0.5	300	STM	f
GaAs	V_{Ga}^- (EL2*)	> 3	> 7	25	IR absorption	g
		> 30	> 68	20	IR absorption	h
GaAlSb	V_{Ga}^- (DX)	1 ± 0.3	2.9 ± 1	300	DLTS	i
HgCdTe	V_{Hg}^{2-}	2.1 ± 0.3	7 ± 1	300	Hall effect	j
		0.1 ± 0.025	0.3 ± 0.1	800	Hall effect	j
PbSe	V_{Pb}^{2-}	0.1 ± 0.01	0.3 ± 0.03	300	Hall effect	k
CdTe	$V_{Cd}^{2-}Cl_{Te}^+$	1.7 ± 0.4	5.2 ± 1.2	300	PL	l

T temperature of the positron experiment; EPR—electron paramagnetic resonance; STM—scanning tunneling microscopy; IR—infrared; DLTS—deep level transient spectroscopy; PL—photoluminescence.
[a]Kawasuso et al. (1995c), [b]Mäkinen et al. (1992a), [c]Mascher et al. (1989b), [d]Krause-Rehberg et al. (1993c), [e]Krause-Rehberg et al. (1995b), [f]Gebauer et al. (1997c), [g]Krause et al. (1990b), [h]Le Berre et al. (1994), [i]Krause-Rehberg et al. (1993b), [j]Krause-Rehberg et al. (1995a), [k]Polity et al. (1993), [l]Krause-Rehberg et al. (1998).

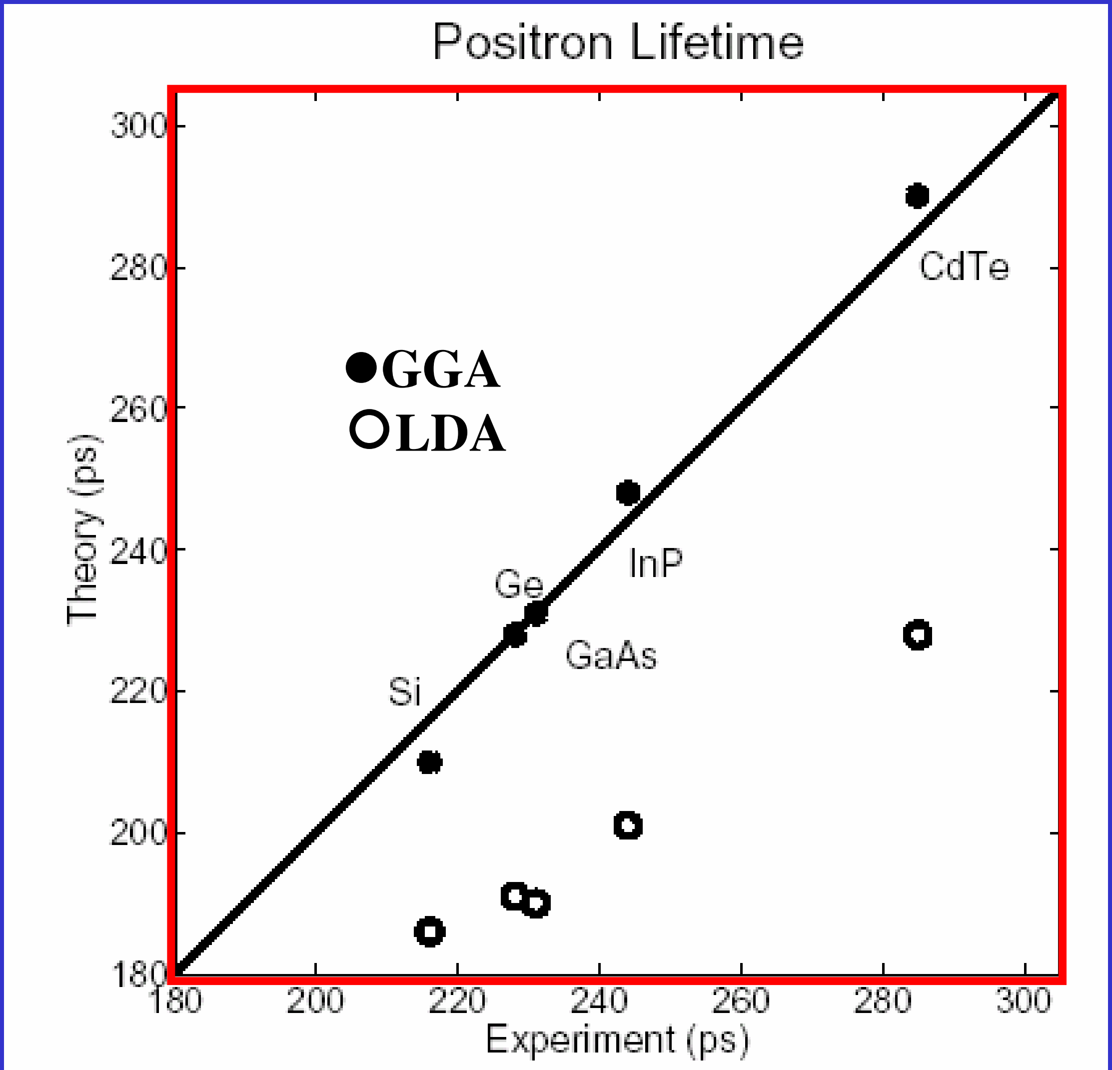
	Defect	τ_d [ps]		Defect	τ_d [ps]		Defect	τ_d [ps
C	V	146	Si	V	256	Ge	V	263
	V_2	206		V_2	309		V_2	316
AlP	V_{Al}	265	GaP	V_{Ga}	264	InP	V_{In}	295
	V_P	261		V_P			V_P	275
	$V_{Al}V_P$	319		$V_{Ga}V_P$	316		$V_{In}V_P$	340
AlAs	V_{Al}	271	GaAs	V_{Ga}	265	InAs	V_{In}	299
	V_{As}	274		V_{As}	268		V_{As}	285
	$V_{Al}V_{As}$	439		$V_{Ga}V_{As}$	321		$V_{In}V_{As}$	347
AlSb	V_{Al}	298	GaSb	V_{Ga}	287	InSb	V_{In}	315
	V_{Sb}	319		V_{Sb}	307		V_{Sb}	322
	$V_{Al}V_{Sb}$	455		$V_{Ga}V_{Sb}$	350		$V_{In}V_{Sb}$	369
CdTe	V_{Cd}	321	HgTe	V_{Hg}	304			
	V_{Te}	339		V_{Te}	315			
	$V_{Cd}V_{Te}$	384		$V_{Hg}V_{Te}$	362			
GaN	V_{Ga}	273						
	V_N	-						
	$V_{Ga}V_N$	348						
SiC	V_{Si}	196						
	V_C	153						
	2V	214						

τ_d is the defect-related lifetime.

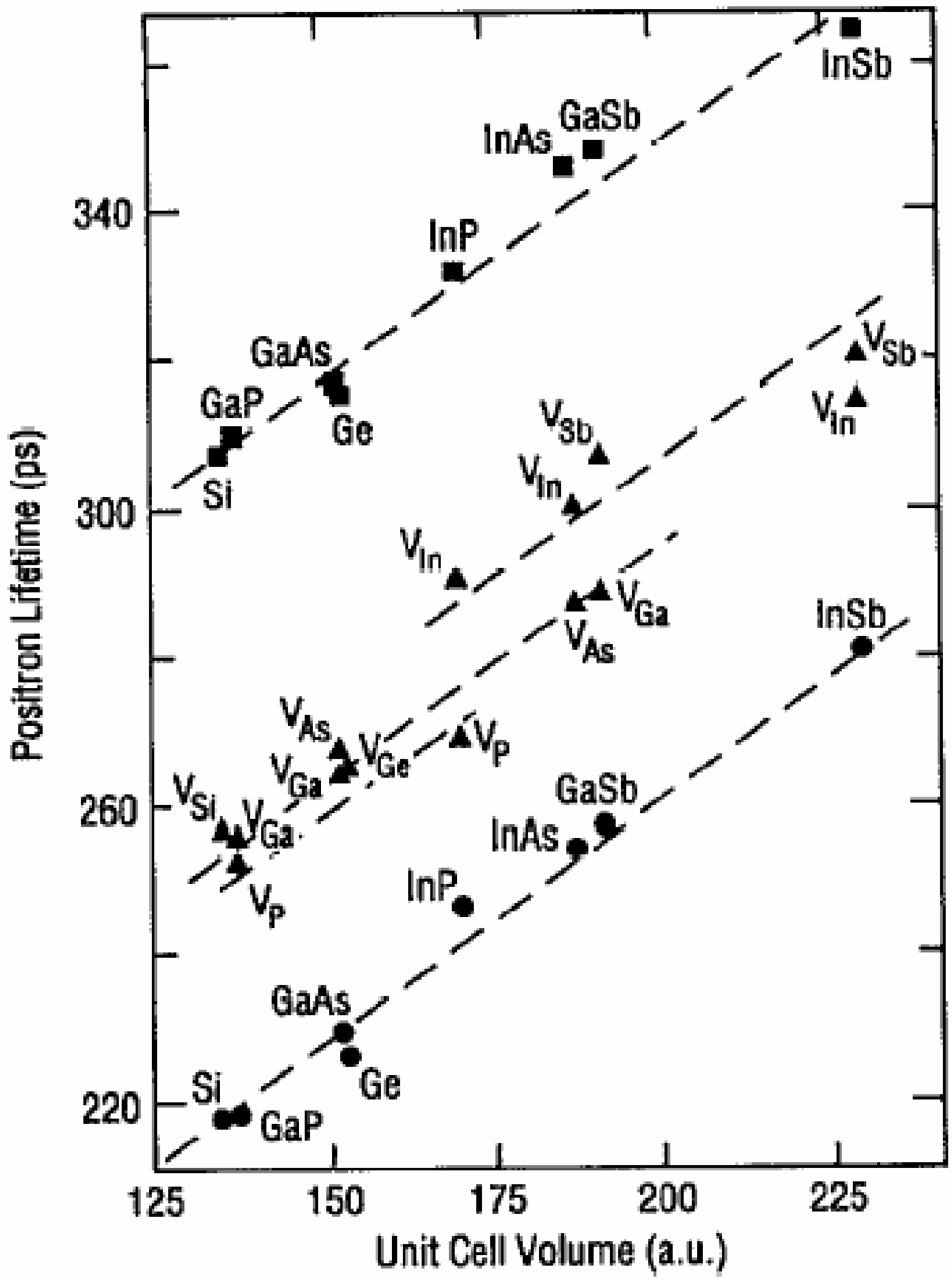
Table 3.8. Positron bulk lifetimes (in ps) calculated according to the generalized gradient approximation (GGA) and compared with results from the local density approximation (LDA). The pseudo-potential calculations were carried out by Panda et al. (1997), and the linear muffin tin orbital in the atomic sphere approximation (LMTO-ASA) and the atomic superposition calculations by Barbiellini et al. (1995, 1996).

	Pseudo-potential		LMTO-ASA		Atomic superposition		
	τ_{th}^{LDA}	τ_{th}^{GGA}	τ_{th}^{LDA}	τ_{th}^{GGA}	τ_{th}^{LDA}	τ_{th}^{GGA}	τ_{b}^{exp}
C	87	100	86	96	—	—	105
Si	190	216	186	210	184	207	218
Ge	198	228	191	228	190	229	228
SiC	130	145	124	139	121	134	142
GaAs	197	232	190	231	190	232	229
InP	213	246	201	248	200	247	241
ZnS	—	—	179	223	179	232	230
CdTe	245	292	228	290	228	310	280
HgTe	—	—	222	285	222	310	274

τ_{th}^{LDA} and τ_{th}^{GGA} are the bulk lifetimes calculated for the local density approximation (LDA) and the generalized gradient approximation (GGA), respectively. τ_{b}^{exp} is the most reliable experimental bulk lifetime.


Positron Lifetime
300
280
260
240
220
200
180
180
200
220
240
260
280
300
Theory (ps)
Experiment (ps)
●GGA
○LDA
CdTe
InP
Ge
GaAs
Si

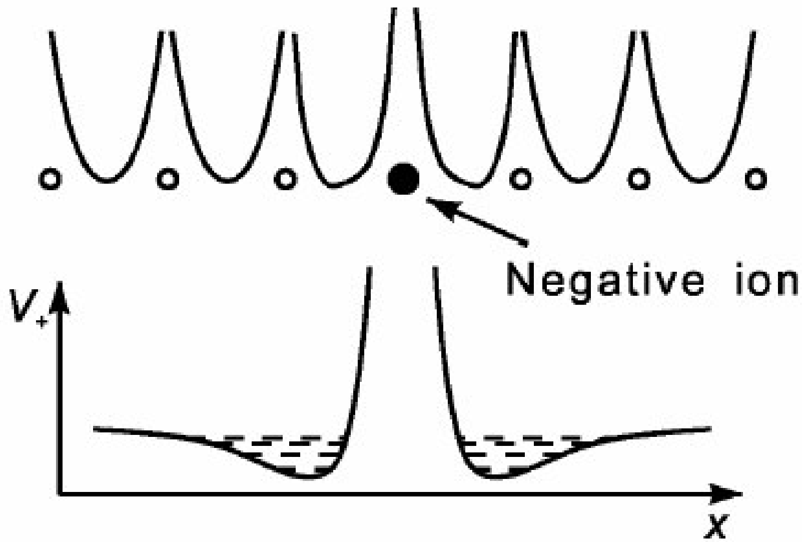
两种计算方法比较



Calculated values of the positron lifetime as a function of unit-cell volume. The symbols denote theoretical lifetime values from

- (O) perfect crystals
- (Δ) monovacancies
- (□) divacancies

Negative ions act as shallow positron traps



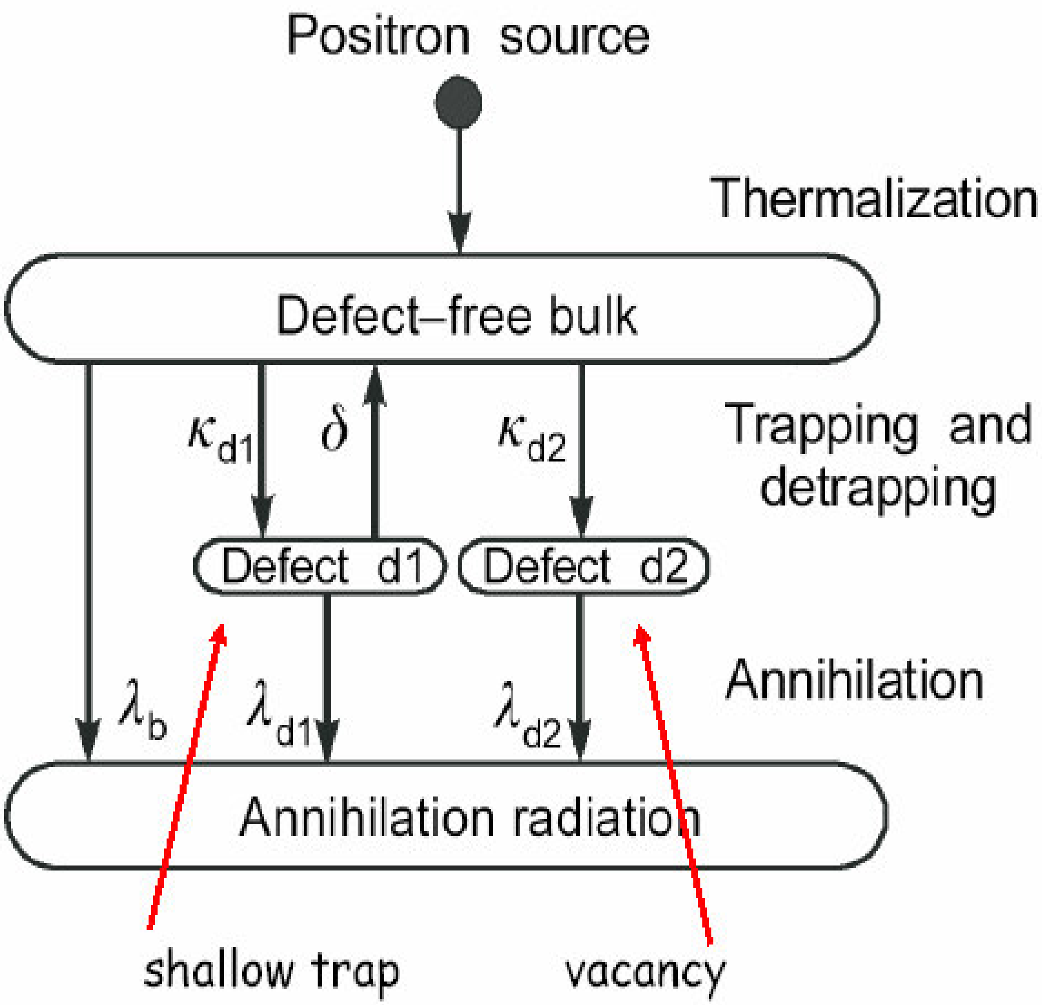
E_{ST}~30-40meV

- at low T: negatively charged defects without open volume may trap positrons
- "shallow" due to small positron binding energy
- annihilation parameters close to bulk parameters
- acceptor-type impurities, dopants, negative antisite defects
- thermally stimulated detrapping can be described by:

$$\delta = \frac{\kappa}{\rho_{st}} \left(\frac{m^* k_B T}{2\pi \hbar^2} \right)^{3/2} \exp\left(-\frac{E_{st}}{k_B T} \right)$$

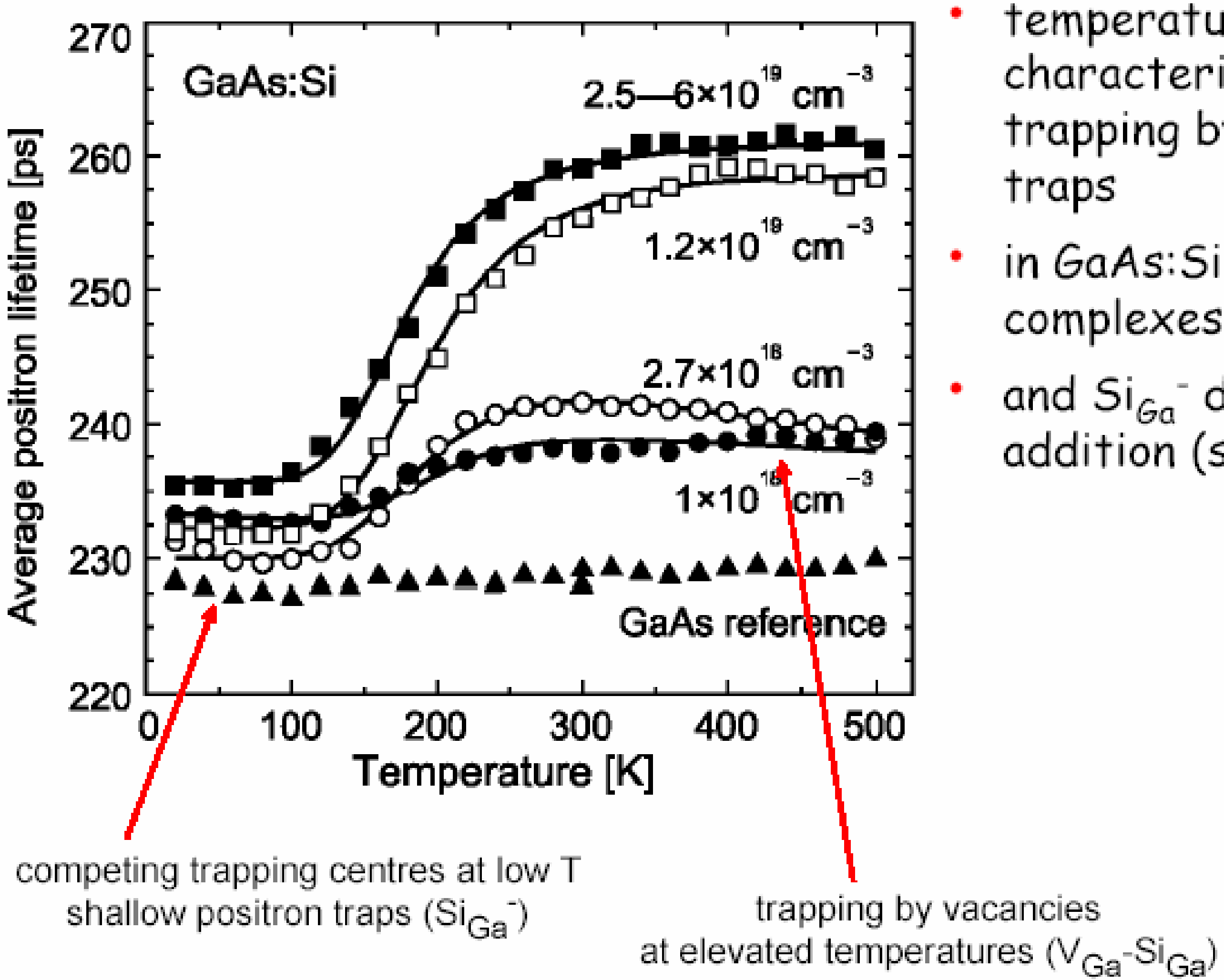
Saarinen et al., 1989

Shallow positron traps



- positron trapping model gets more complex
- however: trapping at shallow traps can be avoided at high temperatures

Effect of shallow positron traps



- temperature dependence is characterized by competing trapping by vacancies and shallow traps
- in GaAs:Si we observe V_{Ga}-Si_{Ga} complexes at high temperatures
- and Si_{Ga}^{-} donors at low T in addition (shallow traps)

The detrapping δ and tripping κ_{st}:

$$\frac{\delta}{\kappa_{st}} = \frac{1}{c_{st}}\left[\frac{m^*}{2\pi\hbar^2}\right]^{3/2}(k_B T)^{3/2}\exp\left[-\frac{E_b}{k_B T}\right]$$

$$\frac{\delta}{\kappa_{st}} = \left[\frac{I_2}{I_1\kappa_v - I_2(\lambda_b-\lambda_2)} - \frac{1}{\kappa_{st}}\right](\lambda_{st}-\lambda_2),$$

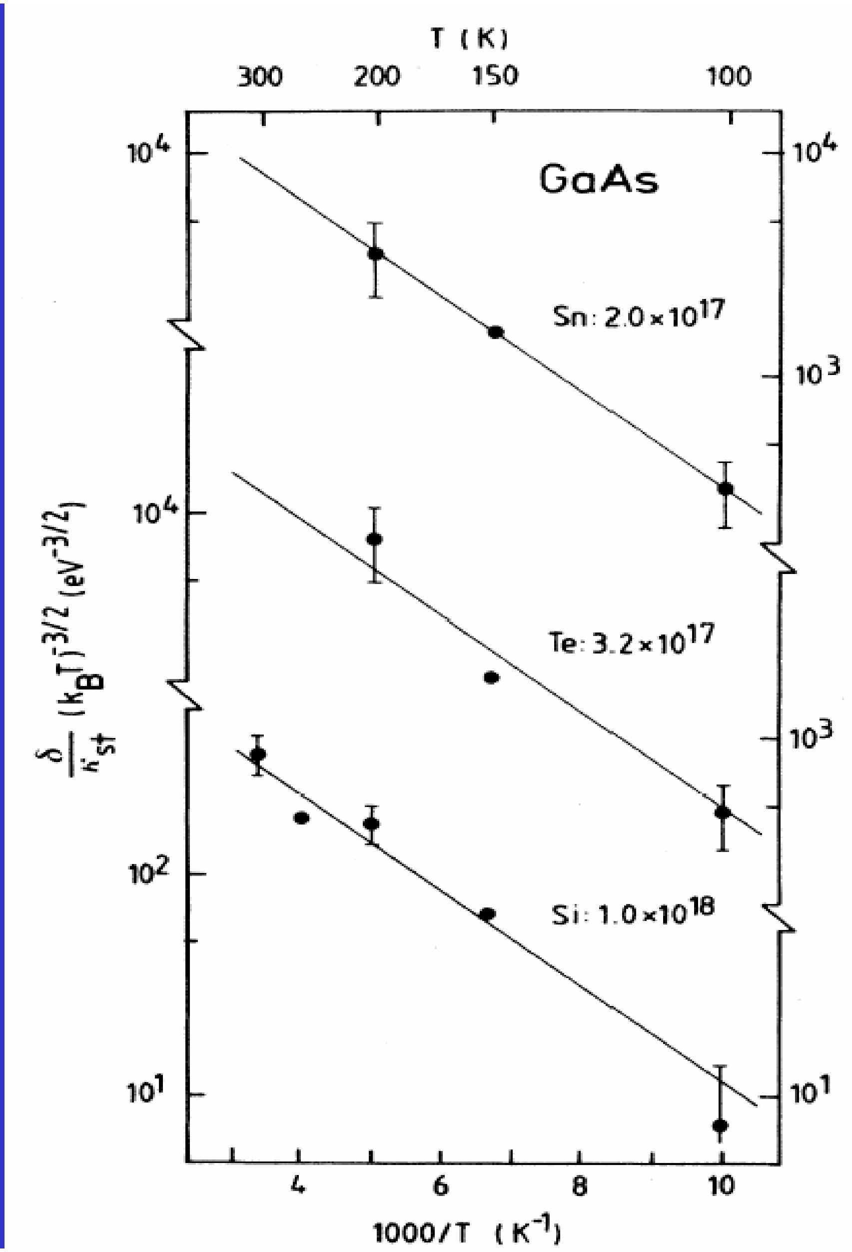
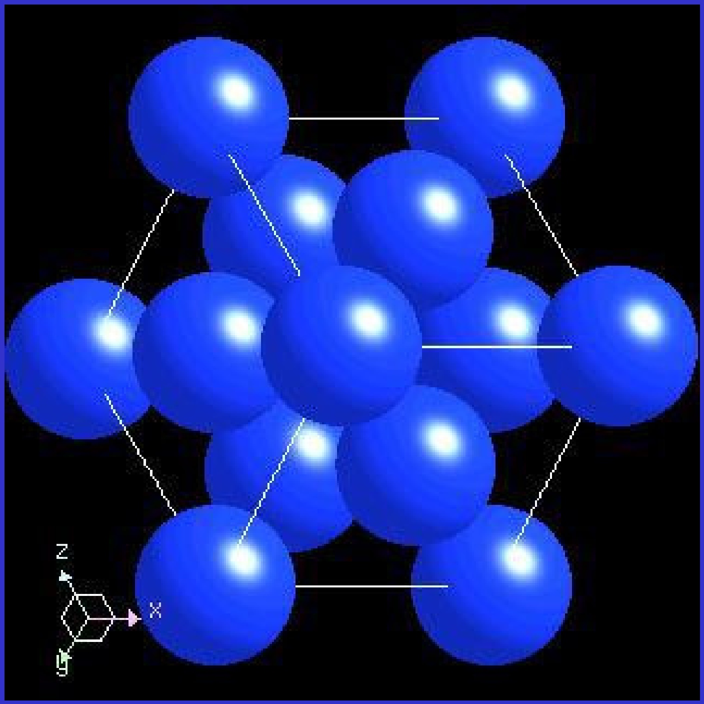


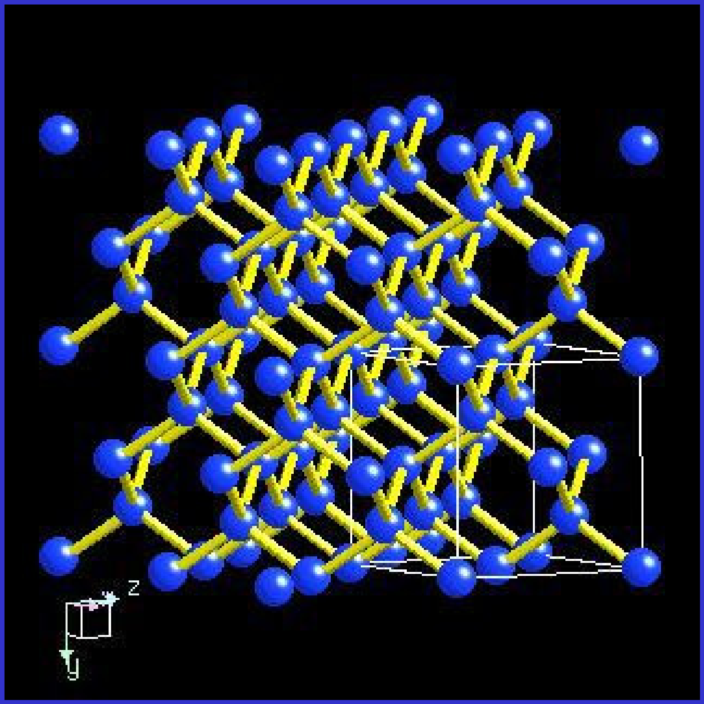
FIG. 6. The ratio of the detrapping and trapping rates in heavily doped *n*-type GaAs calculated from the decompositions of the lifetime spectra using Eq. (20). The solid lines are the fits of Eq. (19) to the experimental data with $E_b = 43$ meV.

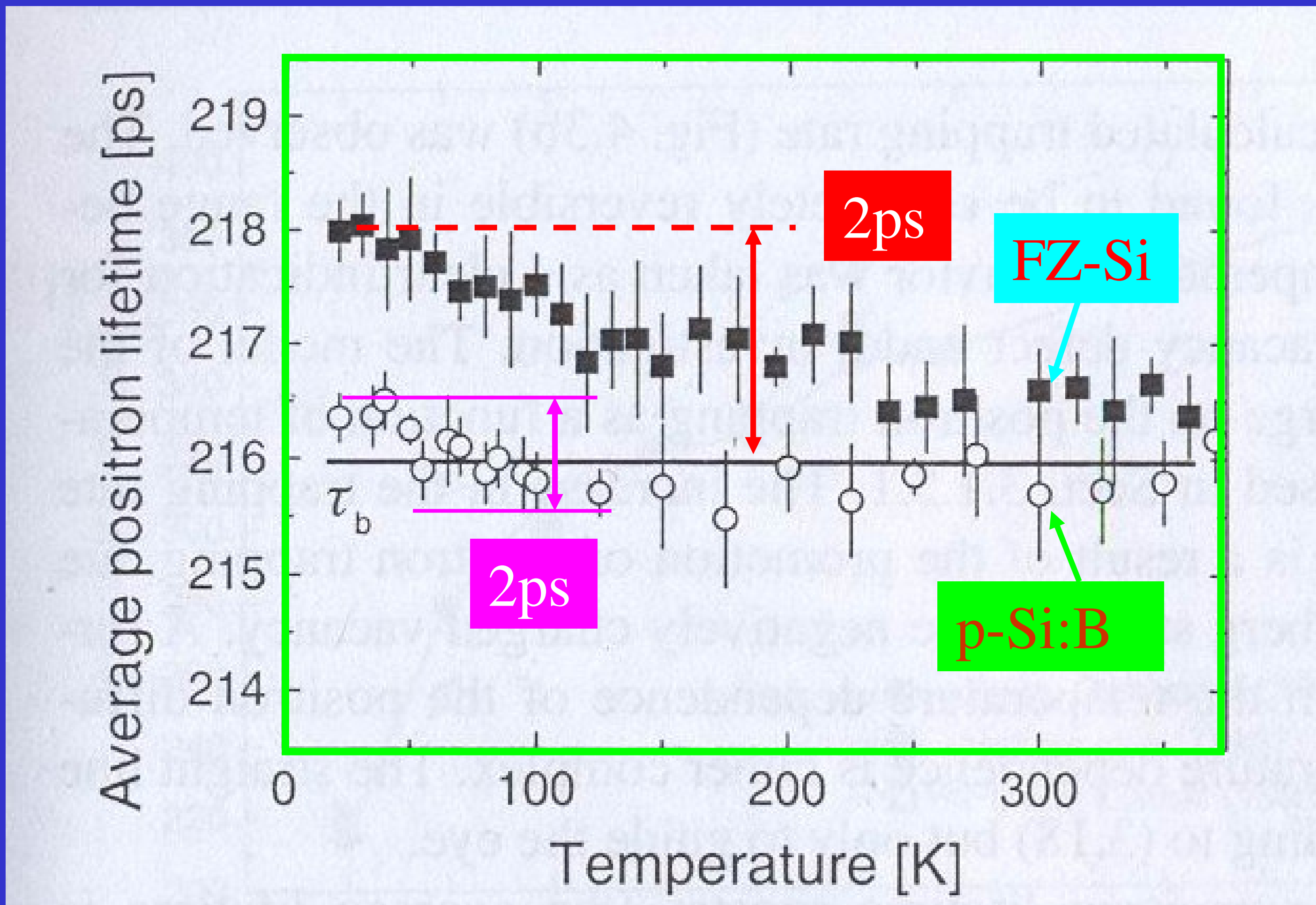
正电子寿命实验值与平均值

Host	τ_{expt} (ps)	τ^*_{expt} (ps)
Si	218,[a] 219,[b] 222[c]	220
Ge	228,[c] 230[d]	229
AlP		
AlAs		
AlSb		
GaP	223,[e] 225[f]	224
GaAs	220,[g] 230,[h] 231,[c] 232,[i] 235[j]	232
GaSb	247,[f] 260,[k] 260[l]	260
InP	235,[f] 242,[c] 244,[m] 247[k]	244
InAs	247,[f] 257[c]	257
InSb	258,[f] 280,[k] 282[n]	280
CdTe	289,[o] 291[f]	
HgTe	274[o]	
BeO		
BP		
C	115[f]	115
GaN	180[k]	180
MgO	166[p]	166
SiC	157[f]	157

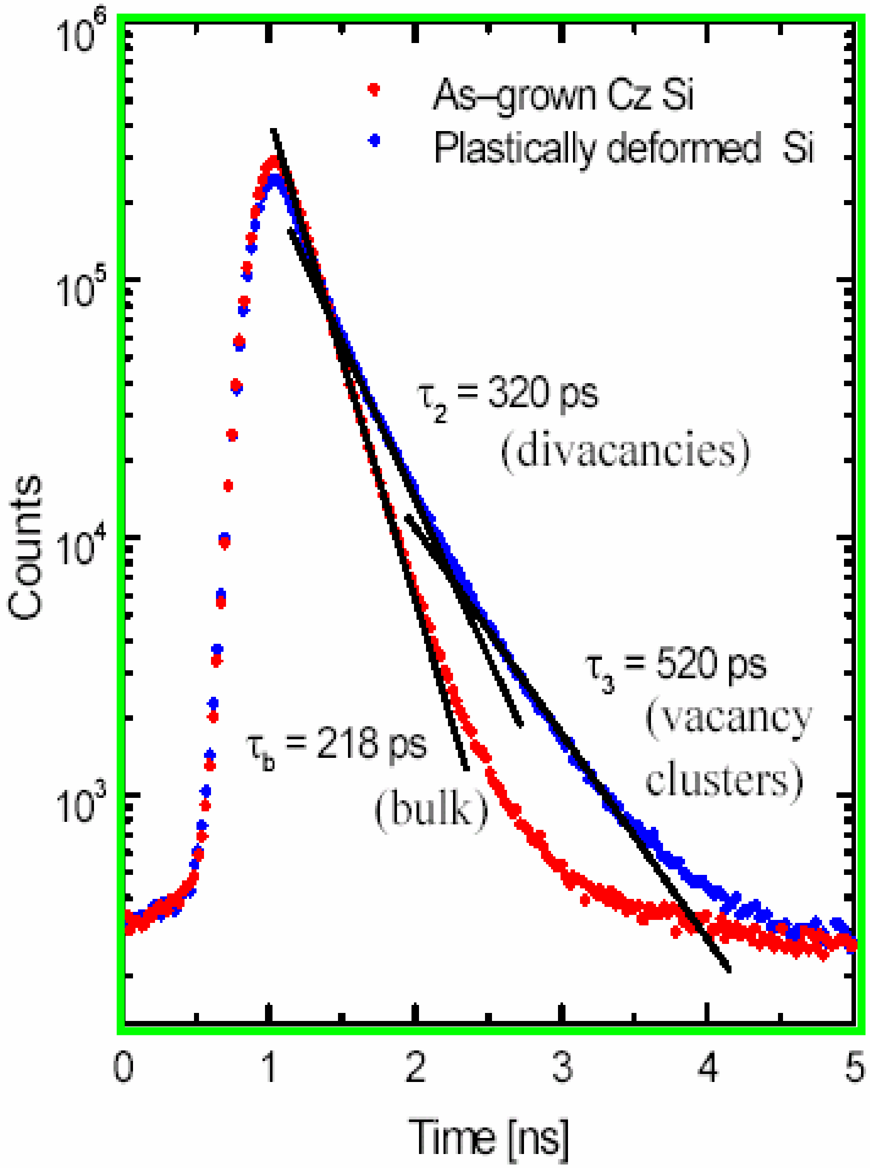
Positron in Si






Average positron lifetime [ps]
219
218
217
216
215
214
0
100
200
300
Temperature [K]
τ_b
2ps
2ps
FZ-Si
p-Si:B

正电子寿命随温度变化



- positron lifetime spectra consist of exponential decay components
- positron trapping in open-volume defects leads to long-lived components
- longer lifetime due to lower electron density
- analysis by non-linear fitting: lifetimes τ_i and intensities I_i

$$N(t) = \sum_{i=1}^{k+1} \frac{I_i}{\tau_i} \exp\left(-\frac{t}{\tau_i}\right)$$

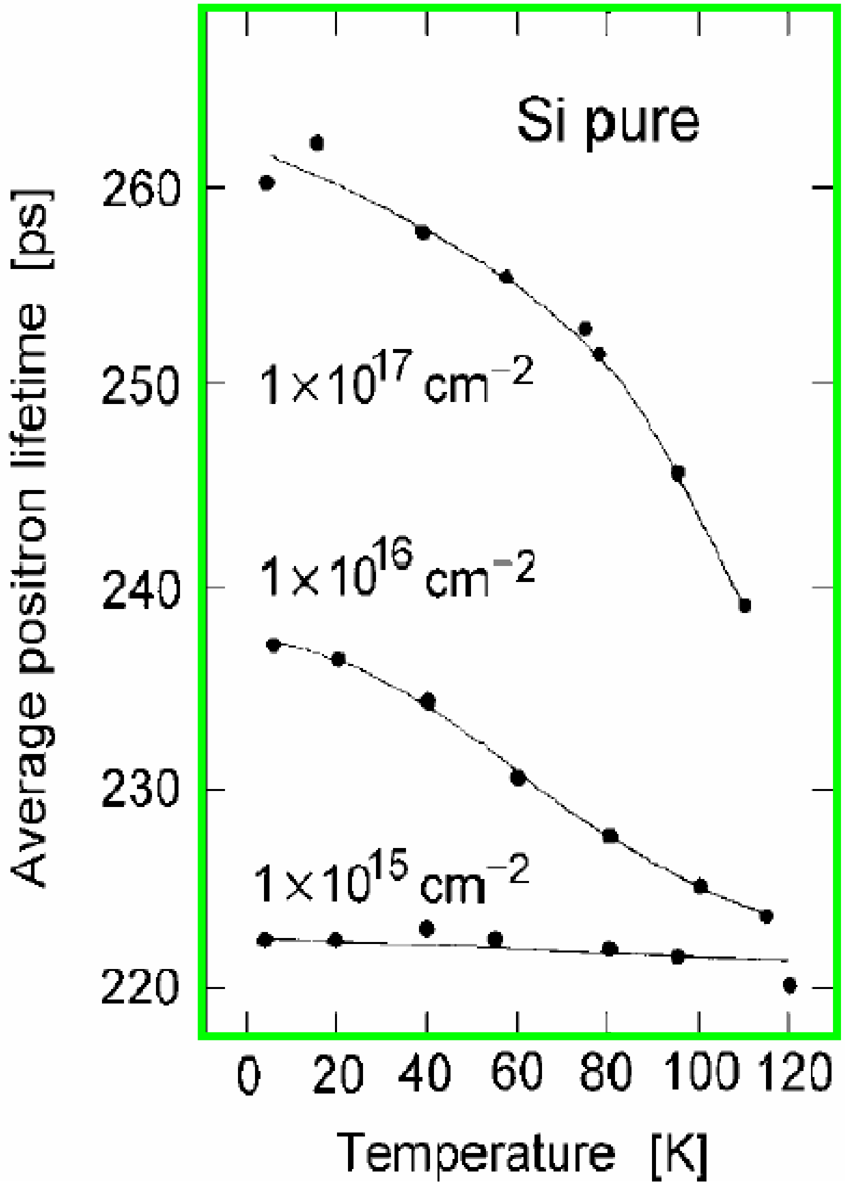
$$\kappa_d = \mu C_d = \frac{I_2}{I_1}\left(\frac{1}{\tau_b} - \frac{1}{\tau_d}\right)$$

trapping coefficient (μ)

trapping rate (κ_d)

defect concentration (C_d)

Temperature-dependent positron trapping

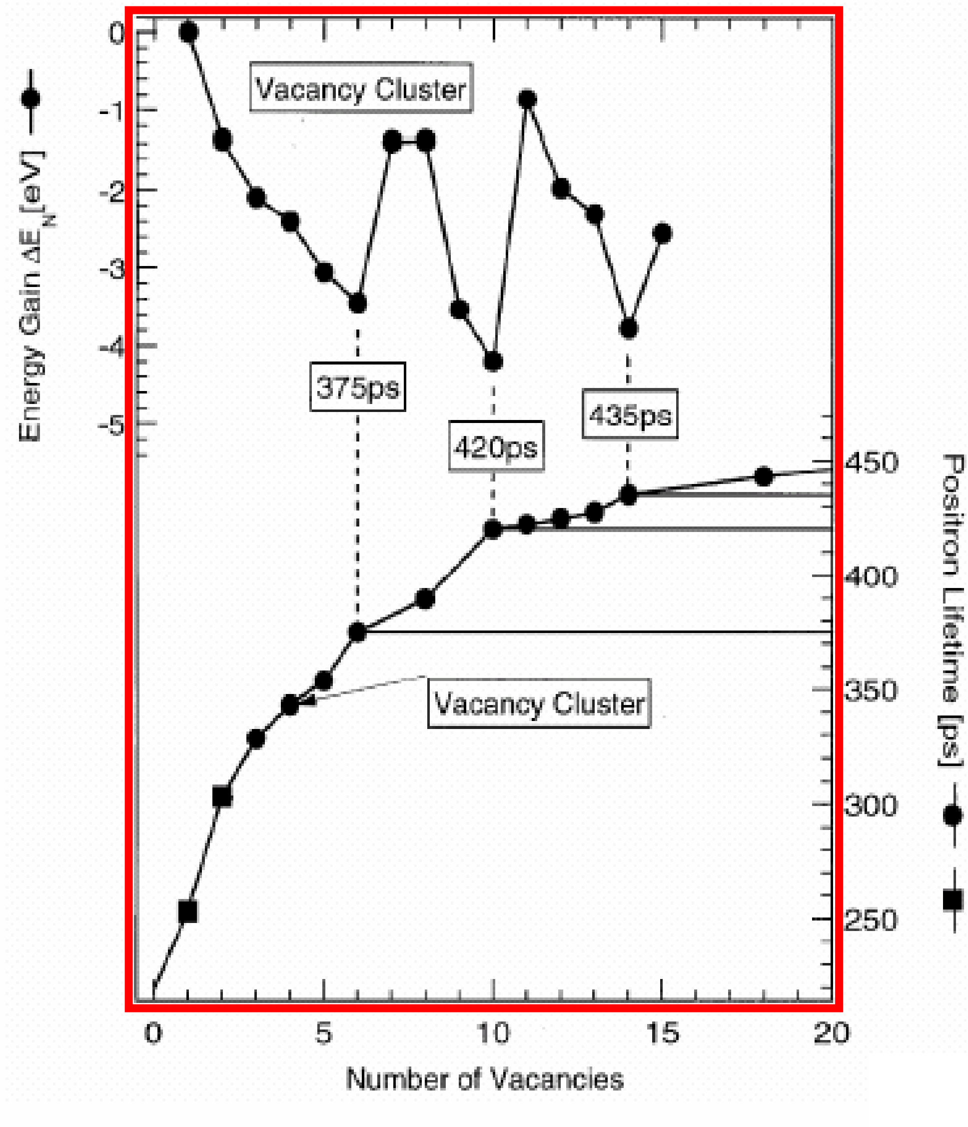


- temperature dependence of positron trapping can be used to determine the charge state of vacancies
- trapping to positive vacancies possible at elevated T
- however: has never been observed
- example: Positron trapping in e-irradiated Si
- trapping by negatively charged divacancies

(Mäkinen et al. 1989)

Electron-irradiation Si

Theoretical calculation of vacancy clusters in Si



- there are cluster configurations with a large energy gain
- „Magic Numbers" with 6, 10 und 14 vacancies
- positron lifetime increases distinctly with cluster size
- for n > 10 saturation effect, i.e. size cannot be determined

N·H
ELSEVIER
Physica B 273–274 (1999) 501–504
PHYSICA B
www.elsevier.com/locate/physb

Magic number vacancy aggregates in Si and GaAs – structure and positron lifetime studies

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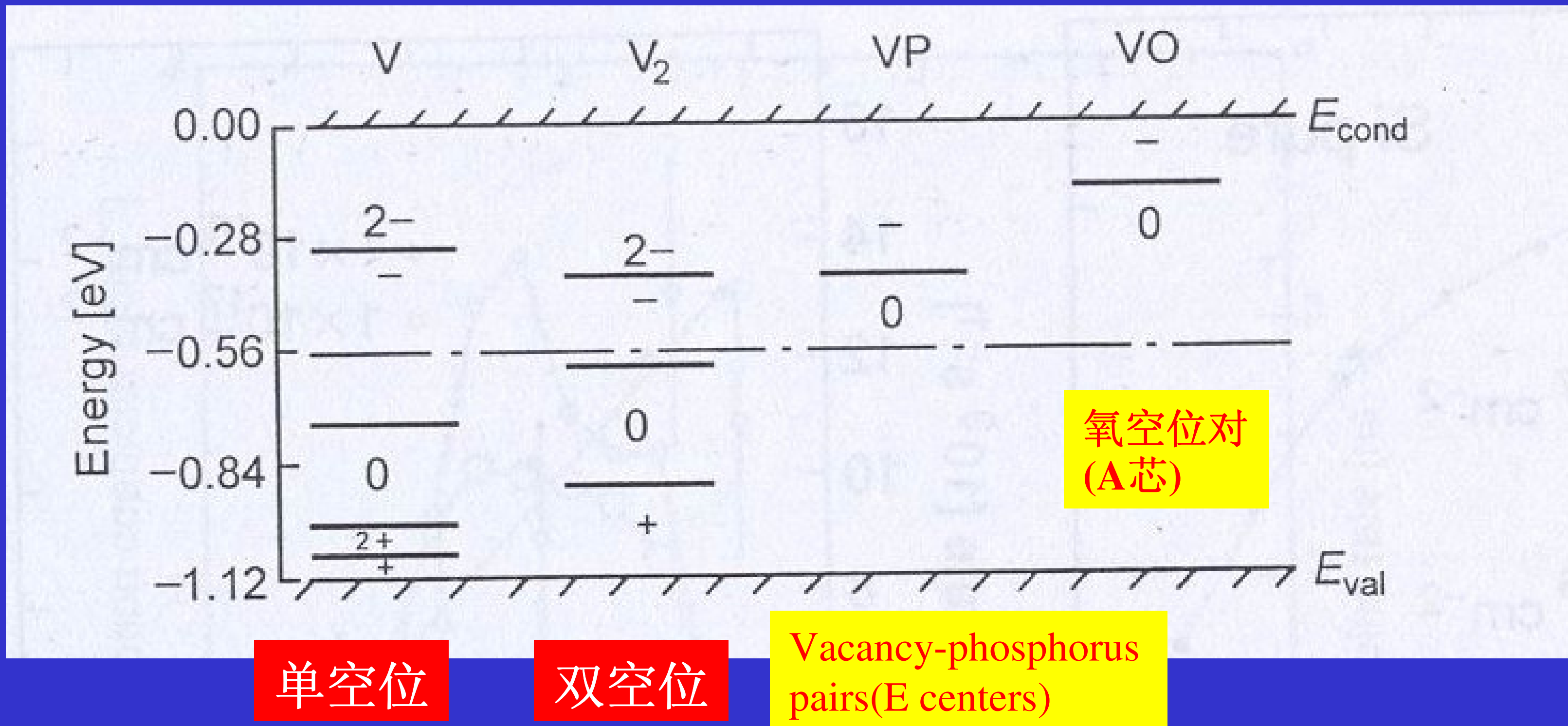
TABLE I. Lifetime results for positrons trapped in defects in Si. The bulk lifetime in Si is ~218 psec at room temperature; it has a weak temperature dependence of 4×10^{-3} psec/°C between 20 and 1200 °C.

Defect type	Lifetime (psec)	Reference
	Vacancies	
monovacancy	266–273	a,b,c,d,e
divacancy	300–325	a,f,g
4-vacancy	435	f
5-vacancy	505	h
6-vacancy (?)	>520	i
	Vacancy-impurity complex	
O-V	270	j
O_2-V	240	j
O-V-B	240	j
$(P\text{-}V)^0$	268,270	k,j
$(P\text{-}V)^-$	248,250	c,k

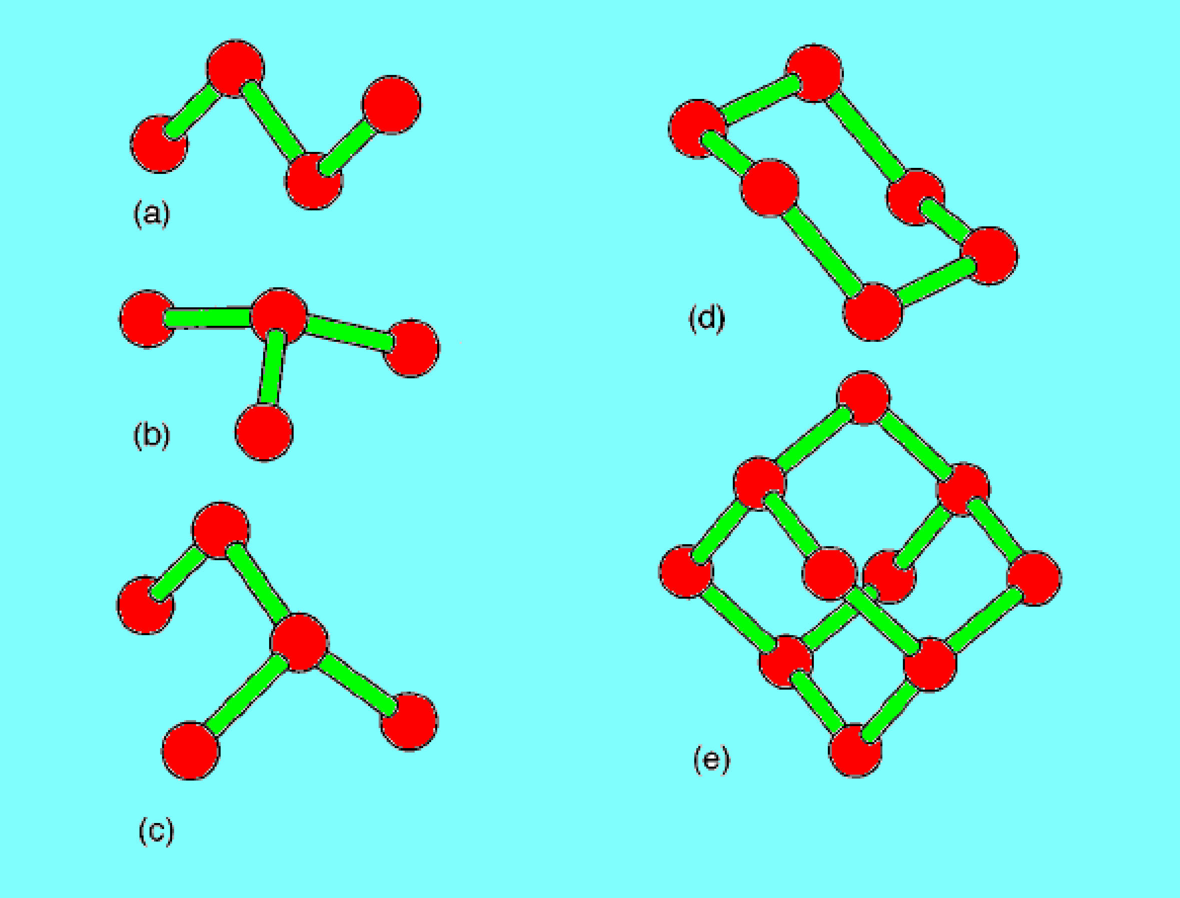
Si中5种电荷态空位

$$\begin{cases} V_{Si}^{2-}:260ps \\ V_{Si}^{1-}:258ps \\ V_{Si}^{0}:255ps \\ V_{Si}^{2+}:\text{不被捕获} \\ V_{Si}^{1+}:\text{不被捕获} \end{cases}$$



各种空位缺陷不同电荷态的能级

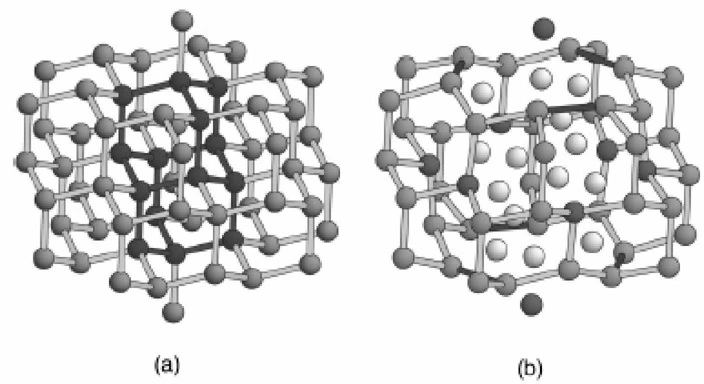
Multivacancies



Configuration of vacant sites in multivacancies: *V*4 with a zigzag chain(a) and a trigonal pyramid (b), *V*5 with a nonplanar shape(c), *V*6 with a closed hexagon (d), and *V*10 with an adamantine cage (e).

Si多空位缺陷的正电子寿命

	Positron lifetime			
	Exp. [a]	No rel. (this work)	Relaxed (this work DFTB)	Full rel. [b]
n	τ(ps)	τ(ps)	τ(ps)	τ(ps)
Bulk	218	218		215
1	282	253	218	279
2	310	303	240	309
3		329	278	320
4		343	291	337
5		353	301	345
6		375	317	348
7		383	330	
8		389	364	
9		398	368	
10		420	385	
11		422	392	
12		425	402	
13		427	406	
14		435	414	



Black atoms and bonds represent the removed atoms forming a cage of *V*14 in the ideal crystal (a).

PHYSICAL REVIEW B VOLUME 53, NUMBER 12

Lifetimes of positrons trapped at Si vacancies

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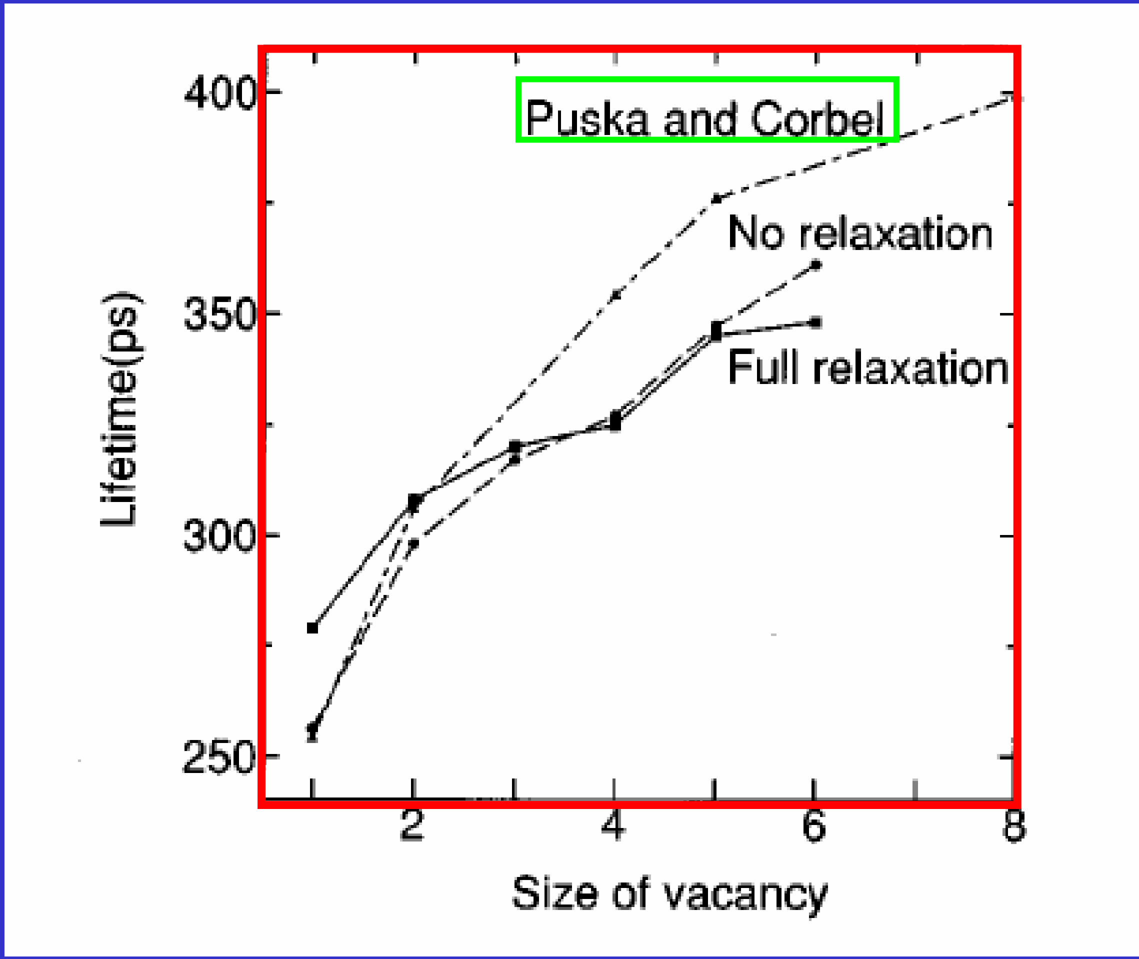
TABLE I. Positron lifetimes in Si. λ_{core} and λ represent annihilation rates for the core and total electron charges, respectively.

	Theory (ps)	$\lambda_{core}/\lambda \times 100$	Expt. (ps)
Bulk	215	2.37	218 (Ref. 5)
V	279	0.67	270 (Ref. 5)
V_2	309	0.50	295–325 (Ref. 8)
V_3	320	0.48	
V_4 (zigzag chain)	325	0.46	
V_4 (trigonal pyramid)	337	0.43	
V_5	345	0.41	
V_6	348	0.45	
V_{10}	386 [a]	0.29	

[a]The present cell size is slightly insufficient to describe V_{10} (see text).



The lifetime vs vacancy of each size. The solid and dashed lines indicate lifetimes for the relaxed and ideal geometries, respectively.

Si多空位缺陷的正电子寿命值和经验公式

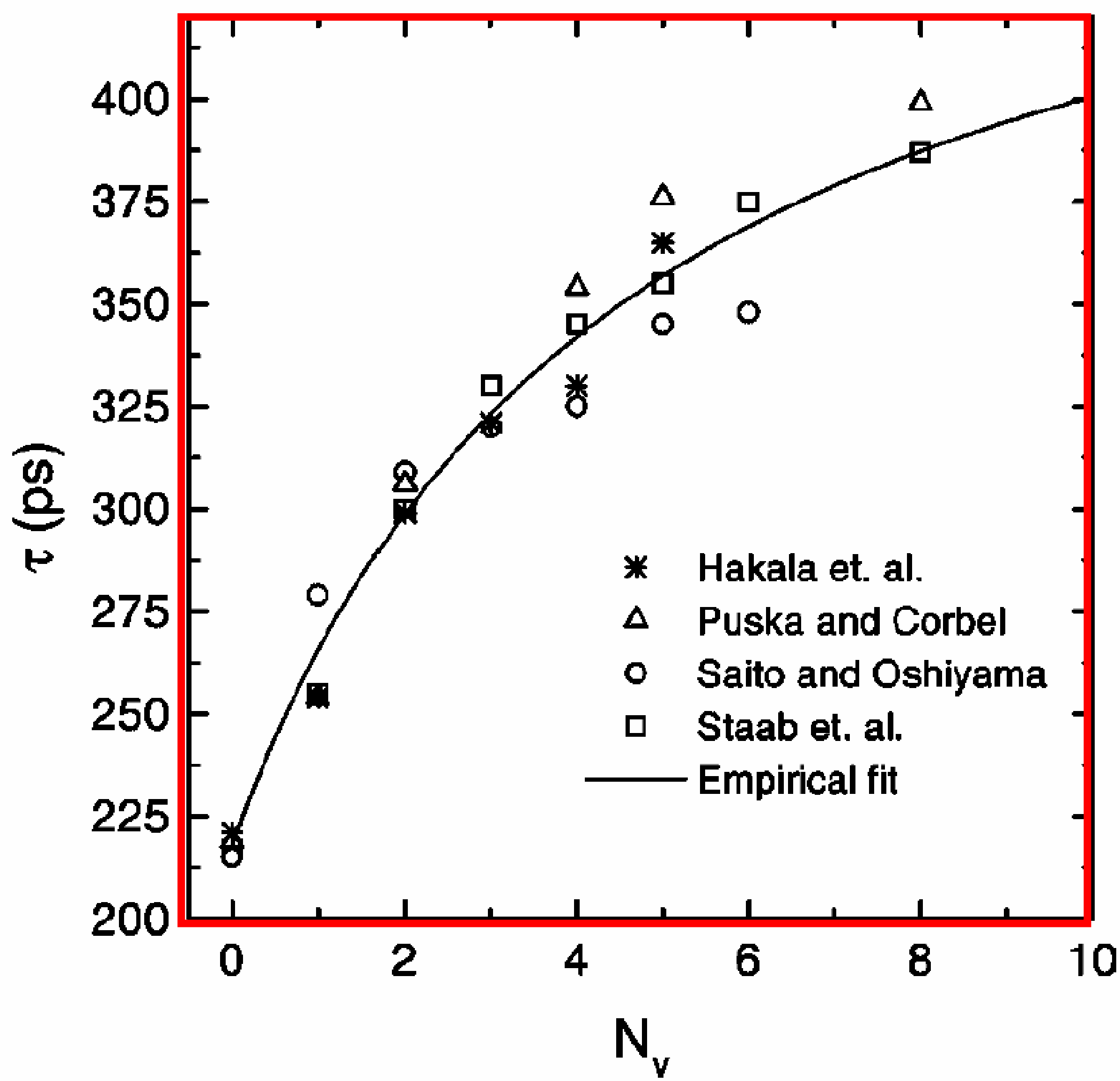
Lifetime (ps)	Bulk	V_1	V_2	V_3	V_4	V_5	V_6	V_7	V_8
Range of lifetime values reported (Refs. 24–27)	215 to 221	254 to 279	299 to 309	320 to 330	325 to 354	345 to 376	348 to 375		387 to 399
Lifetime values from Eq. (1)	218	266	299	323	342	357	369	379	387

$$\tau = \tau_0 + \frac{AN_v}{(B + N_v)}$$

A=266.57ps

B=4.60

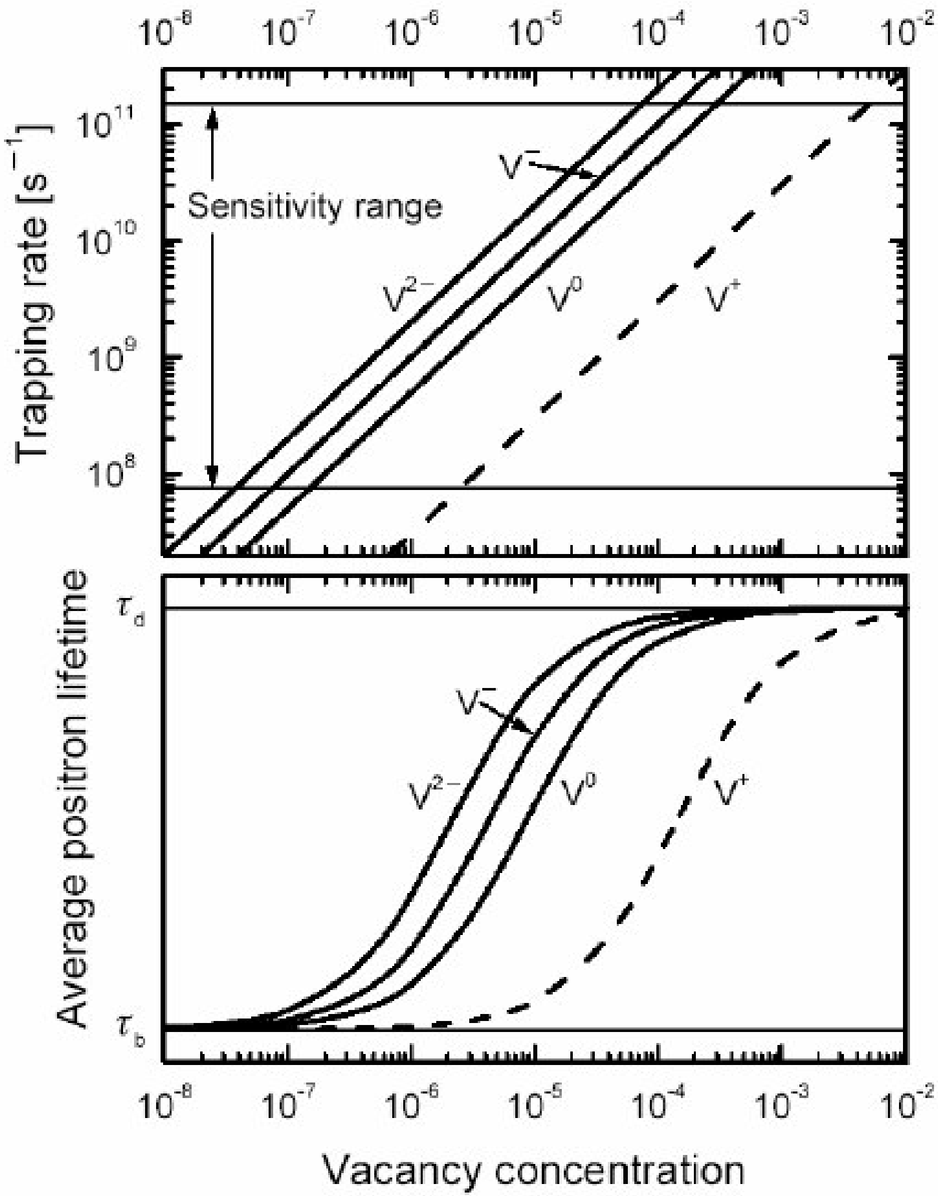
τ_0=218ps



Defect lifetime vs vacancy clusters in Si

TABLE III. Characteristic S and W parameters calculated for the perfect bulk lattice and for the ideal vacancy clusters in Si. The momentum component p_z is along the [111] direction. Before calculating the S and W parameters the theoretical Doppler spectra have been convoluted with a Gaussian with FWHM of $4.7 \times 10^{-3} m_0 c$. S_{val} and $S_{B,\mathrm{val}}$ have been calculated using the valence electron momentum distributions instead of the total distribution.

System	S/S_B	$S_{\mathrm{val}}/S_{B,\mathrm{val}}$	W/W_B
Bulk	$S_B = 0.5344$	$S_B = 0.5410$	$W_B = 0.01701$
V	1.018	1.014	0.86
V_2	1.045	1.038	0.72
V_3	1.053	1.045	0.68
V_4	1.067	1.058	0.64
V_5	1.081	1.072	0.59



Sensitivity limits of PAS for vacancy detection

- **lower sensitivity limit** e.g. for negatively charged divacancies in Si starts at about 10^{15} cm^{-3}
- **upper limit**: saturated positron trapping
- defect identification still possible
- only lower limit for defect density can be given

离子注入

- **H**
- **He**
- **Kr**
- **Ar**
- **O**
- **F**

- **N**
- **As**
- **Ge**
- **B**
- 多种离子混合注入

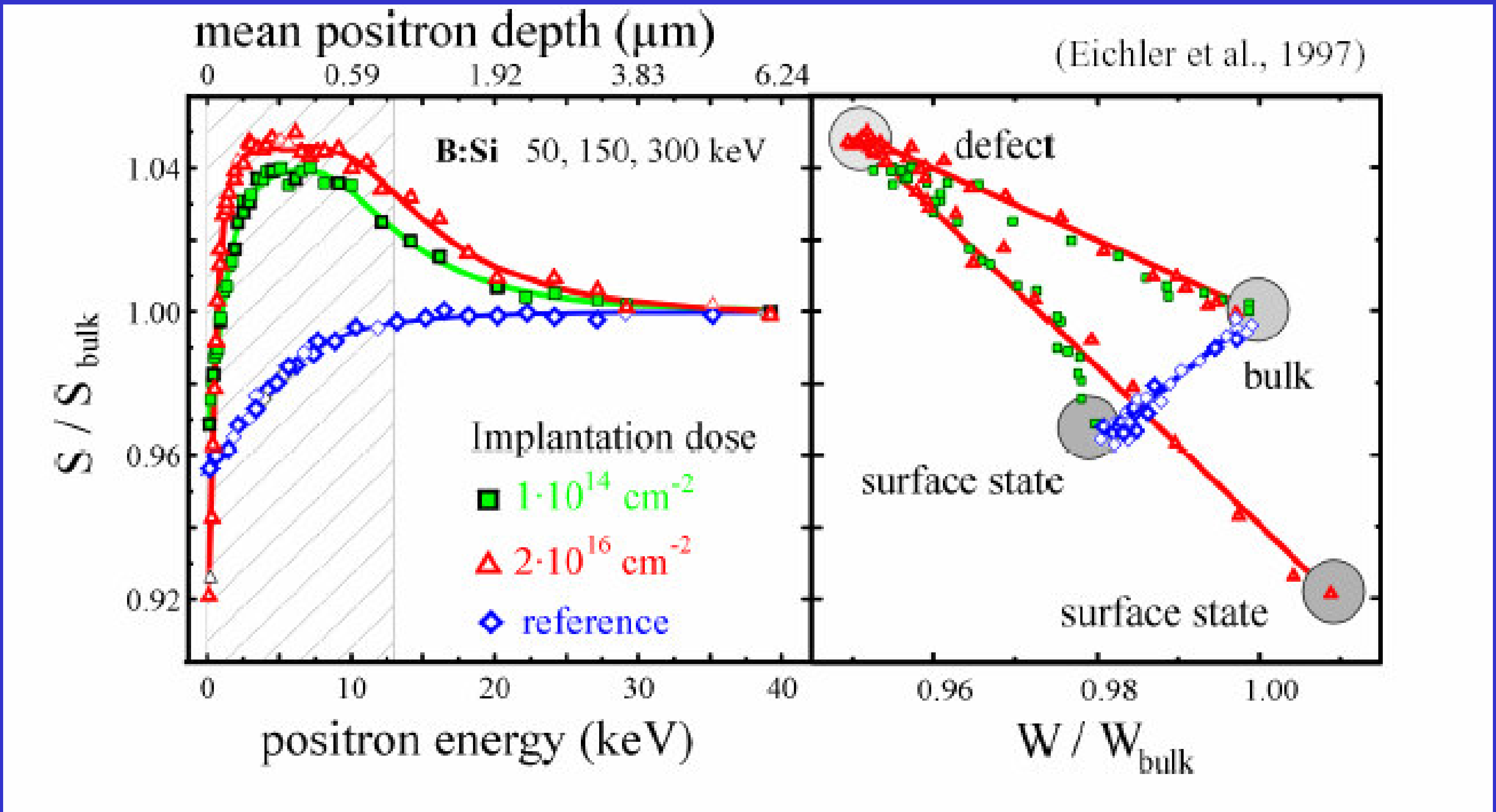
Defects in ion-implanted Si

$$S(E)=F_{\mathrm{surf}}(E)S_{\mathrm{surf}}+F_{\mathrm{vac}}(E)S_{\mathrm{vac}}+F_{\mathrm{bulk}}(E)S_{\mathrm{bulk}},$$

- **S_{suf}, S_{vas}和S_b 表示表面,空位和晶体体S参数**
- **F 为各部分的比例.**

Defects in Si induced by Ion Implantation

B注入Si



B注入Si

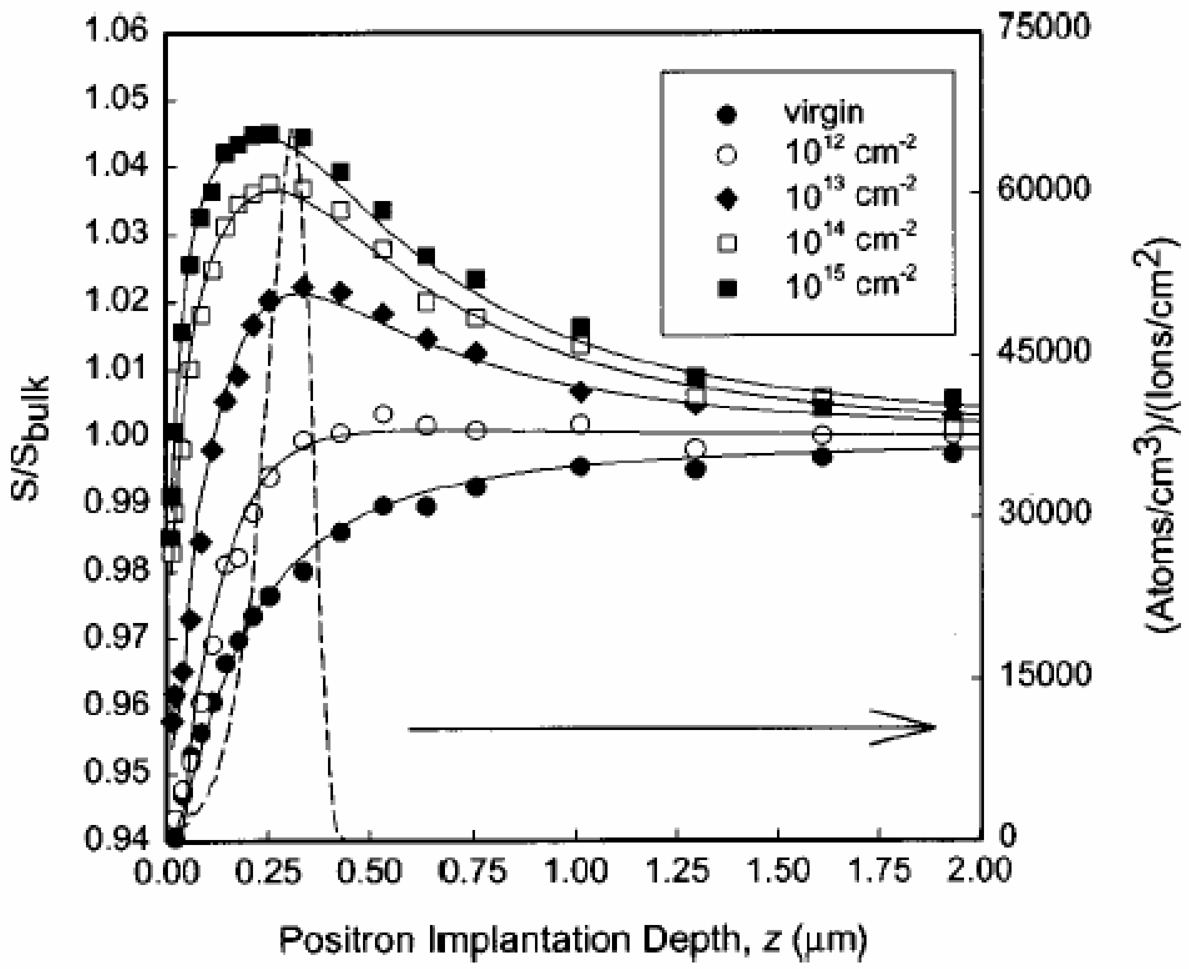


FIG. 2. $S-z$ curves obtained from 80 keV boron-implanted Si. Solid lines represent best fits with POSTRAP5. The dotted line shows the depth distribution of implanted boron, calculated using TRIM code.

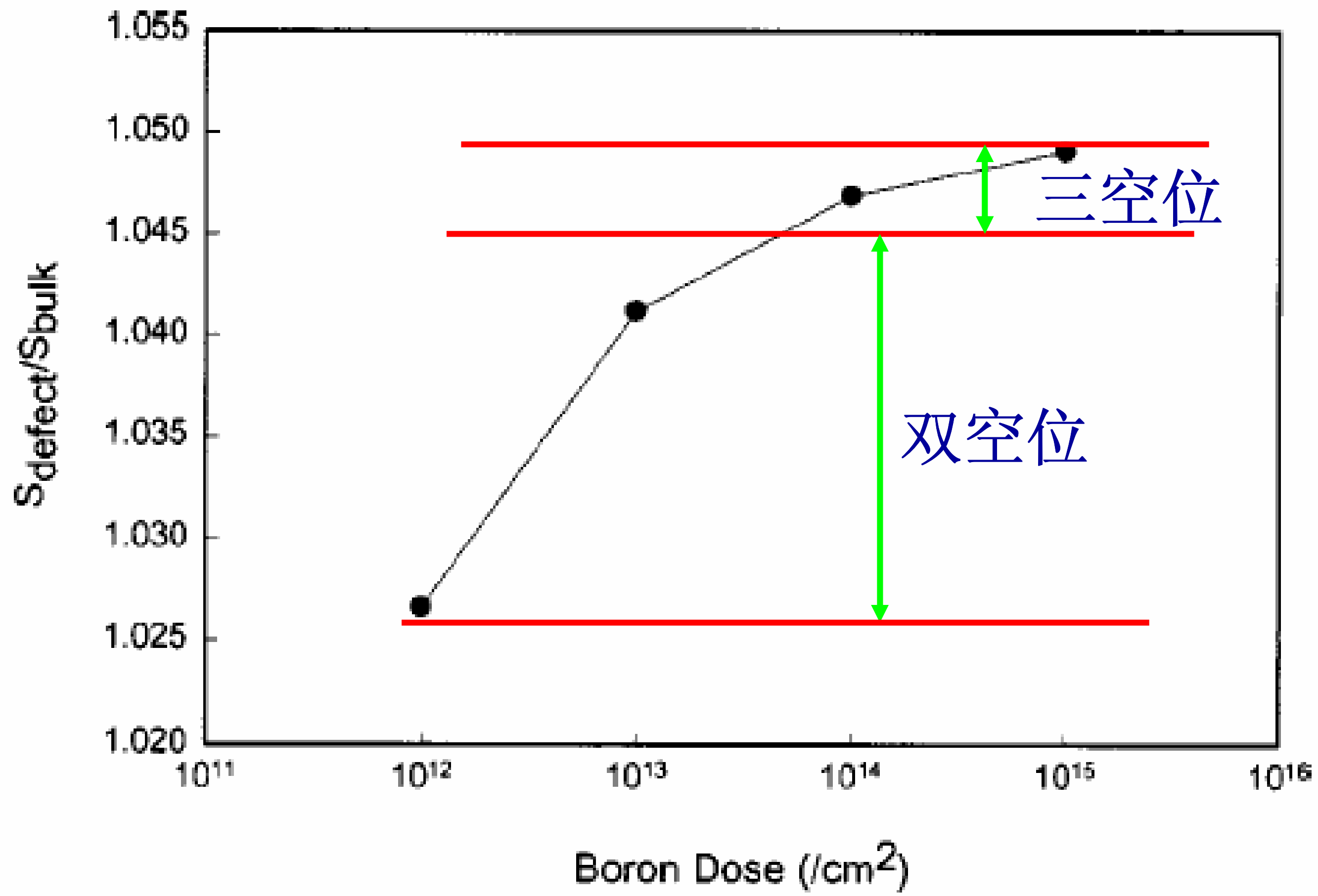
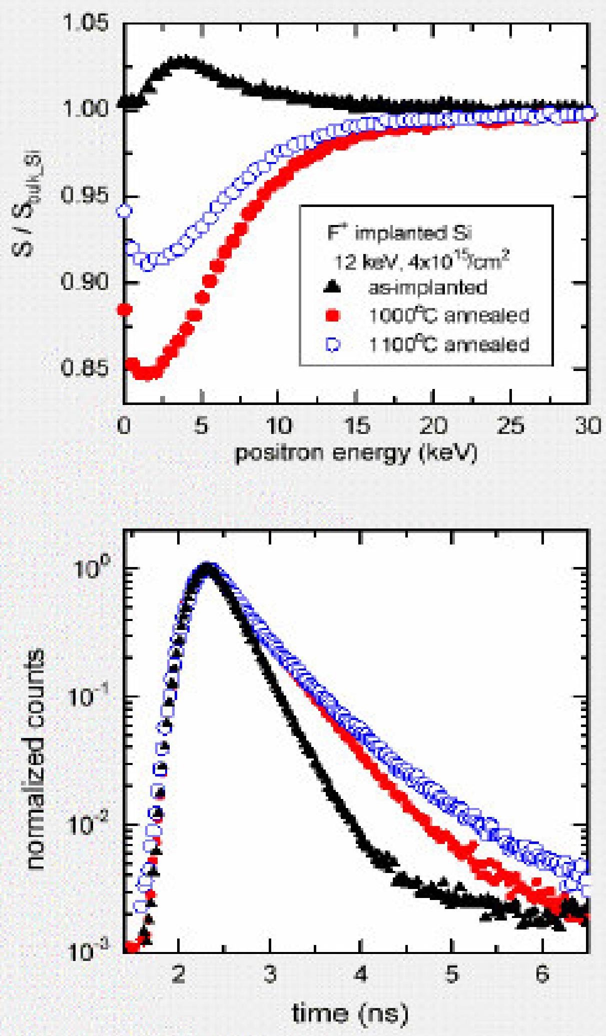
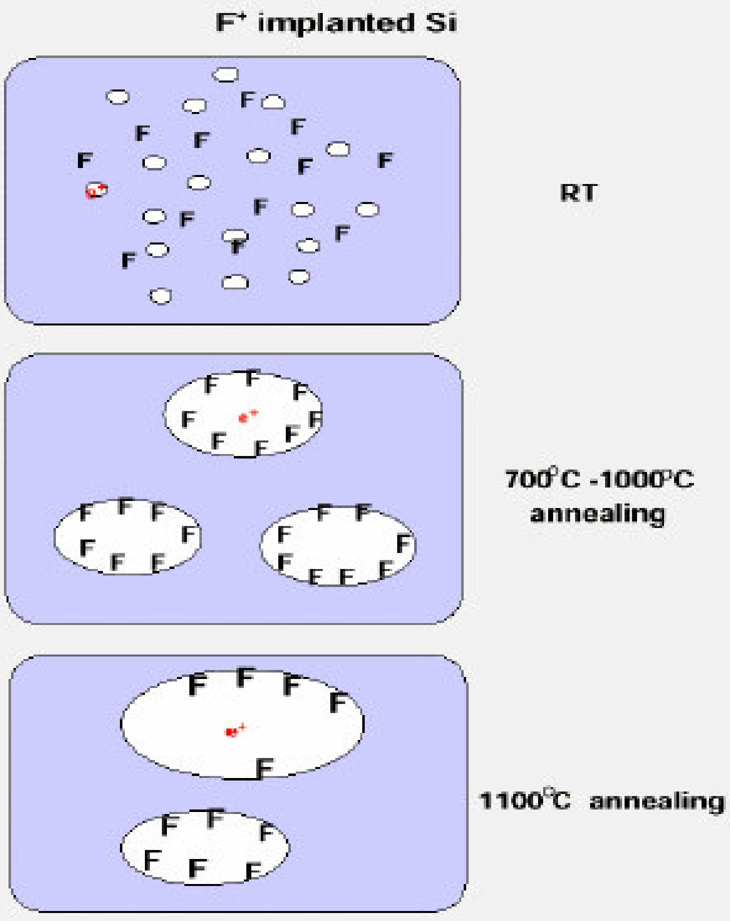


FIG. 3. Normalized S_{defect} values as a function of implanted boron fluences. The S_{defect} value is extracted from the fitting procedure.

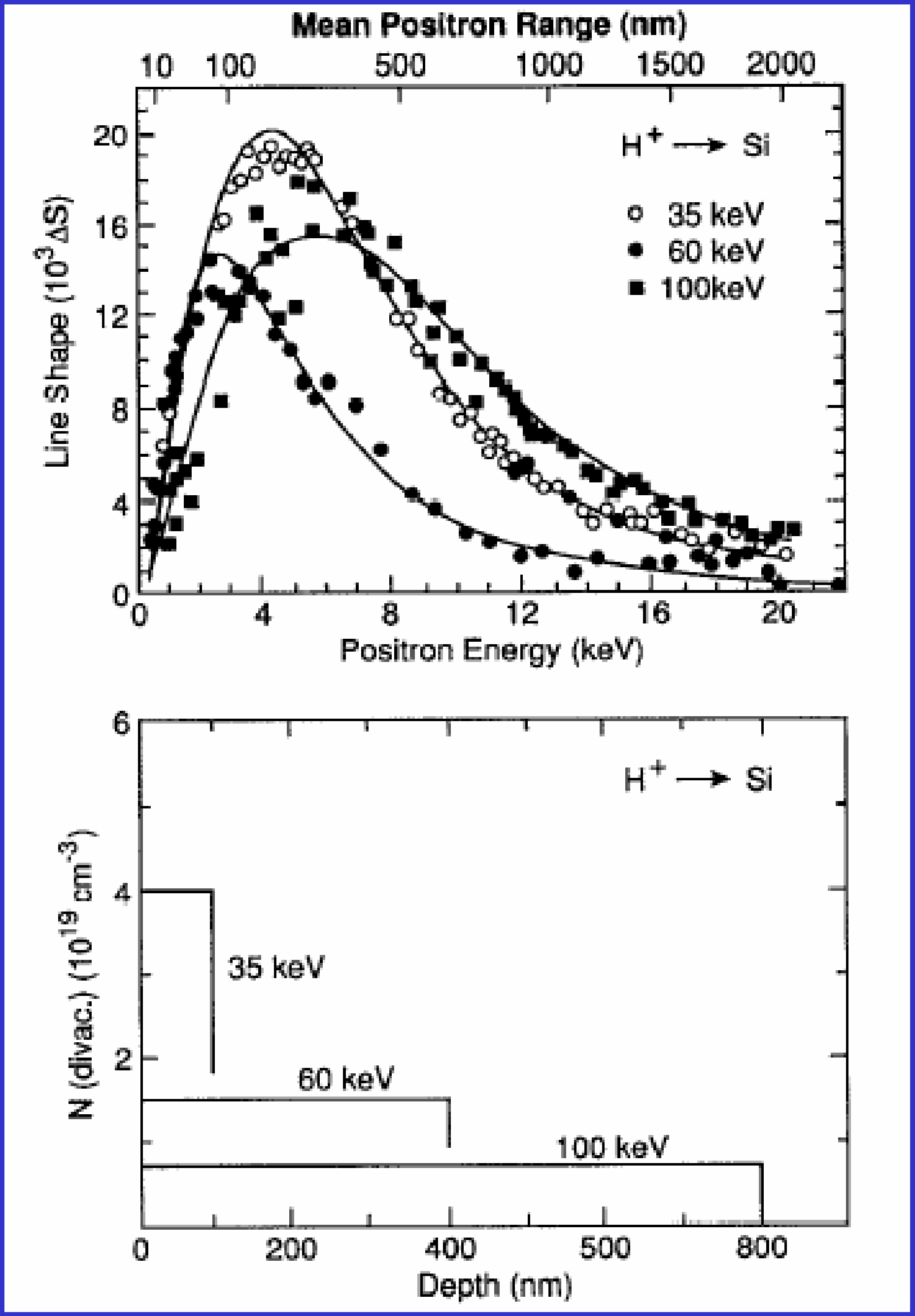
F^+ implanted Si

Shallow Doping



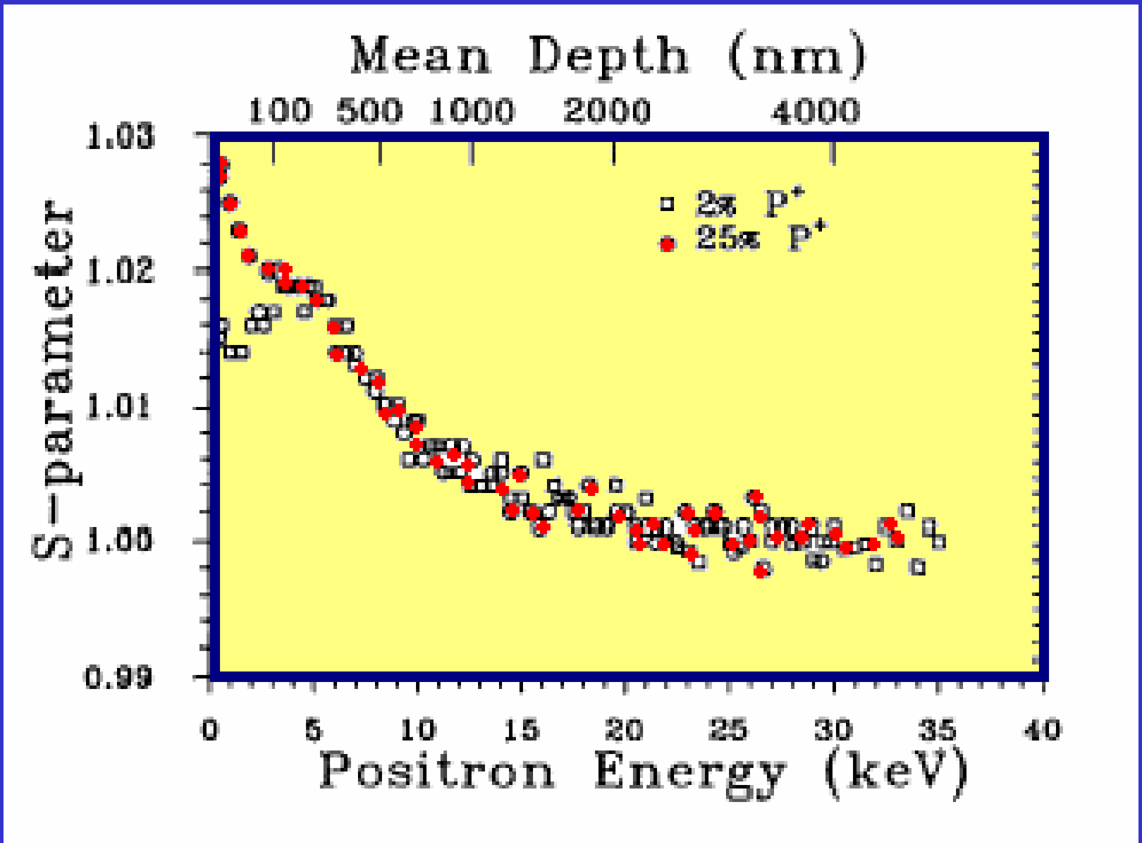


H注入



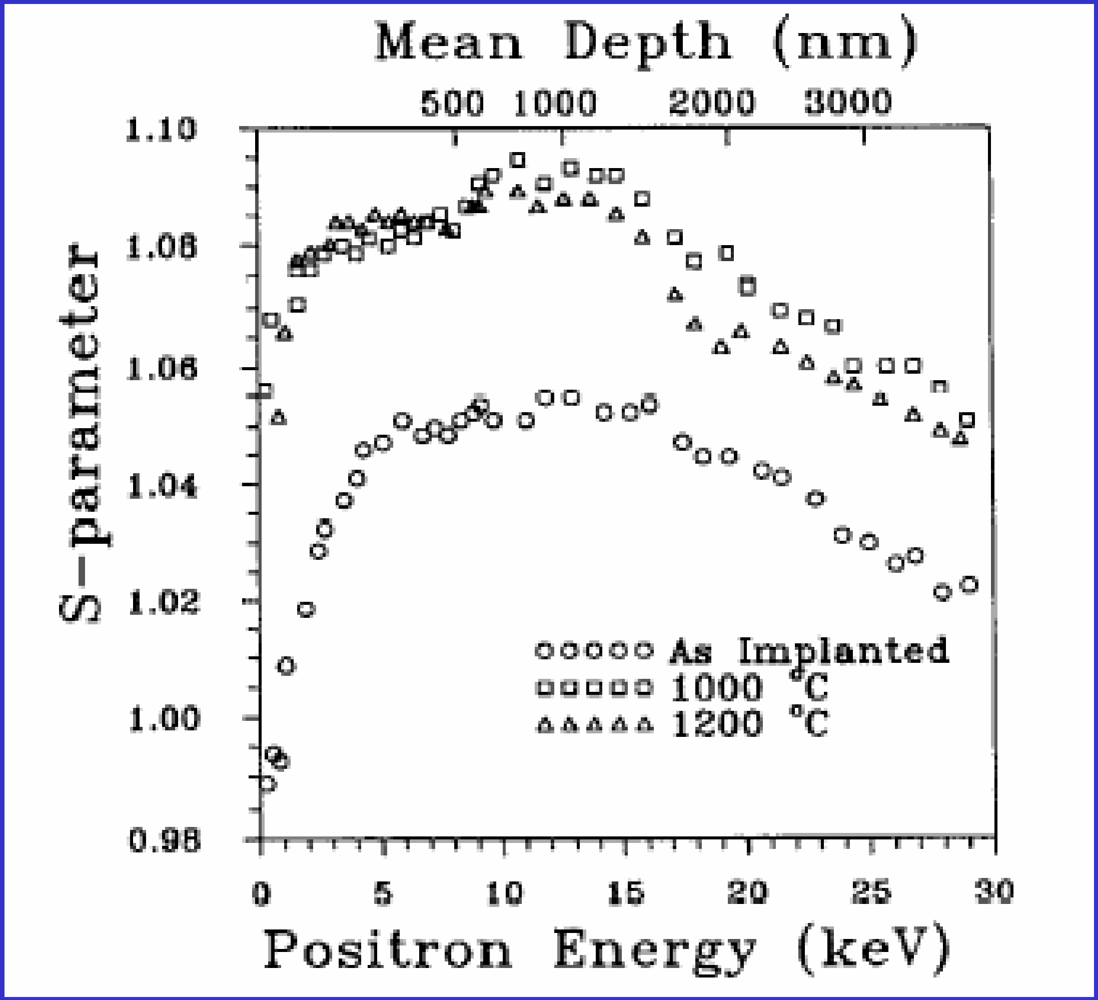
Kwinonen等用能量为**35, 60,** 和 **100 keV,** 剂量为**1** ×**10^6 H+**的**H+**注入到**Si**中, 研究空位的形成. 图为ΔS (=$S_{irradiated}$-$S_{unirradiated}$) 随正电子能量的变化, 缺陷见下图. 这些双空位缺陷在**470-570K**之间可以退火掉.

P注入

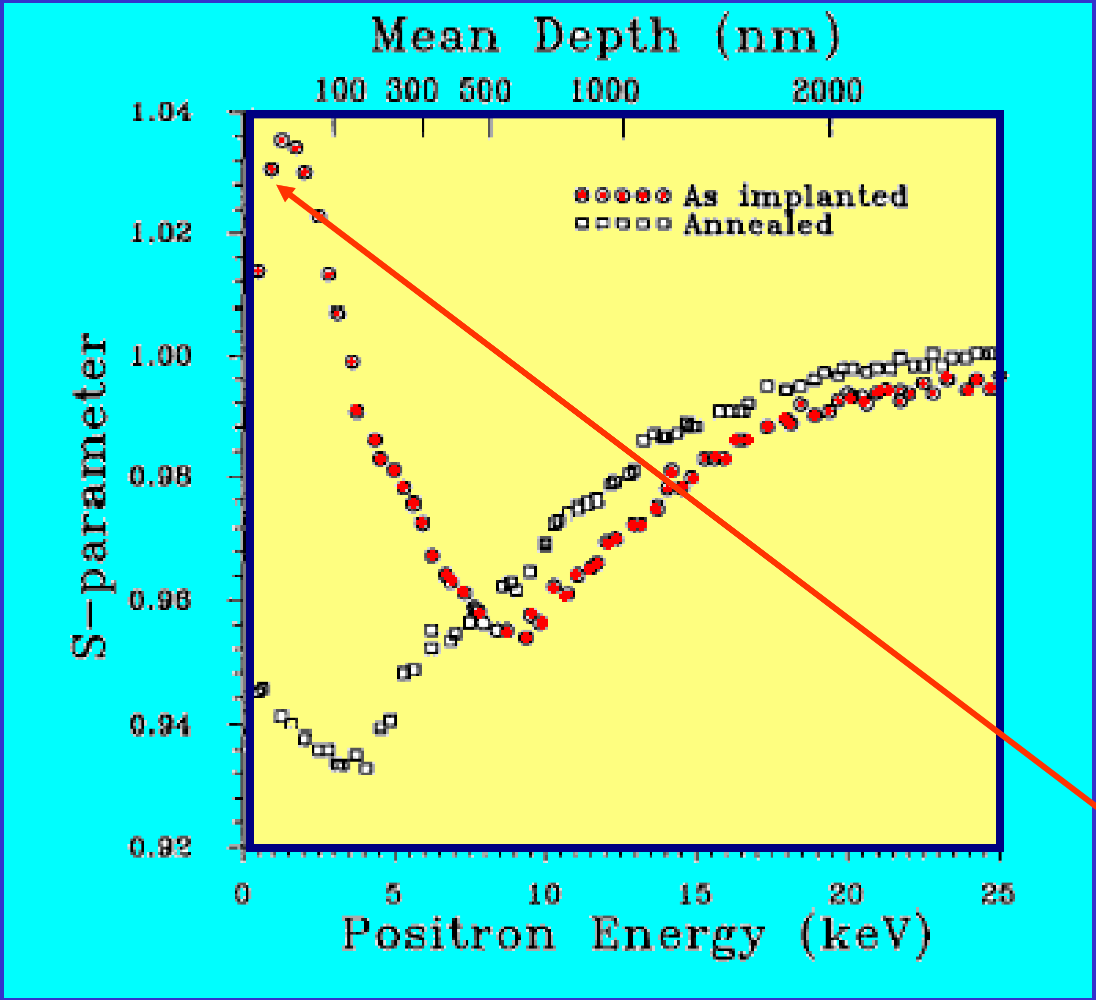


- 260KeV的P+辐照Si

图表明在600C退火后20C测量的S-E曲线,对应于100KeV-P+在2%和25%污染,离表面100nm内两组结果差别很大,100nm是100keV-P+的射程, 高污染注入在表面缺陷较多.



- The effect of isochronal anneal on the S-E data for P^+ implanted Si



O注入

S值高于Sb区(<2keV)

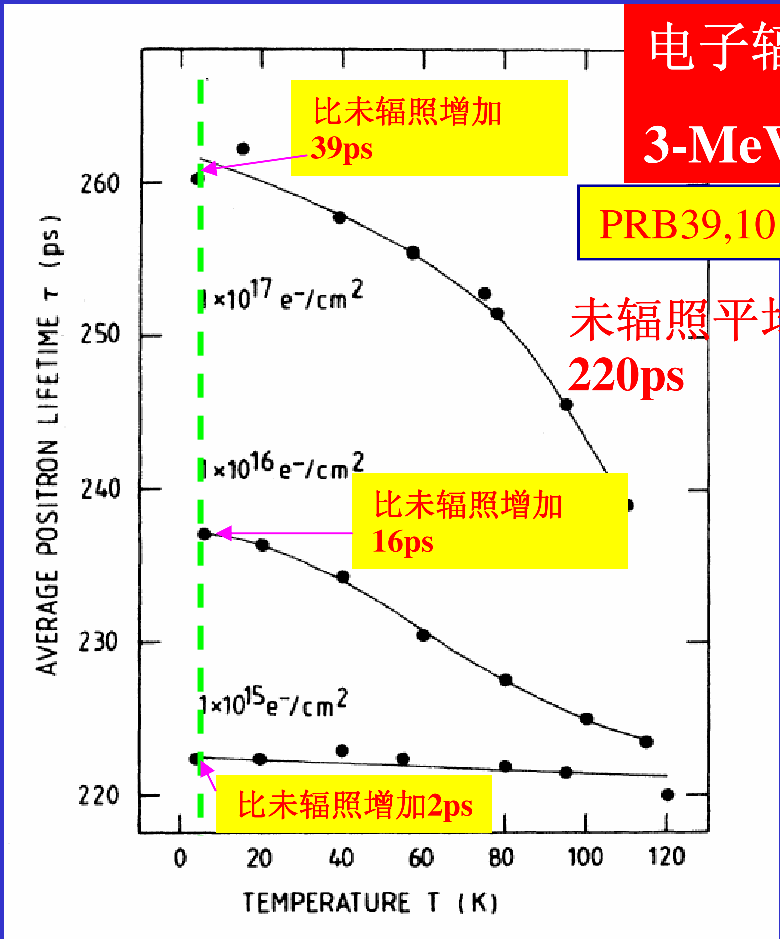
S值小于Sb区(<9keV)

S=Sb, >20keV

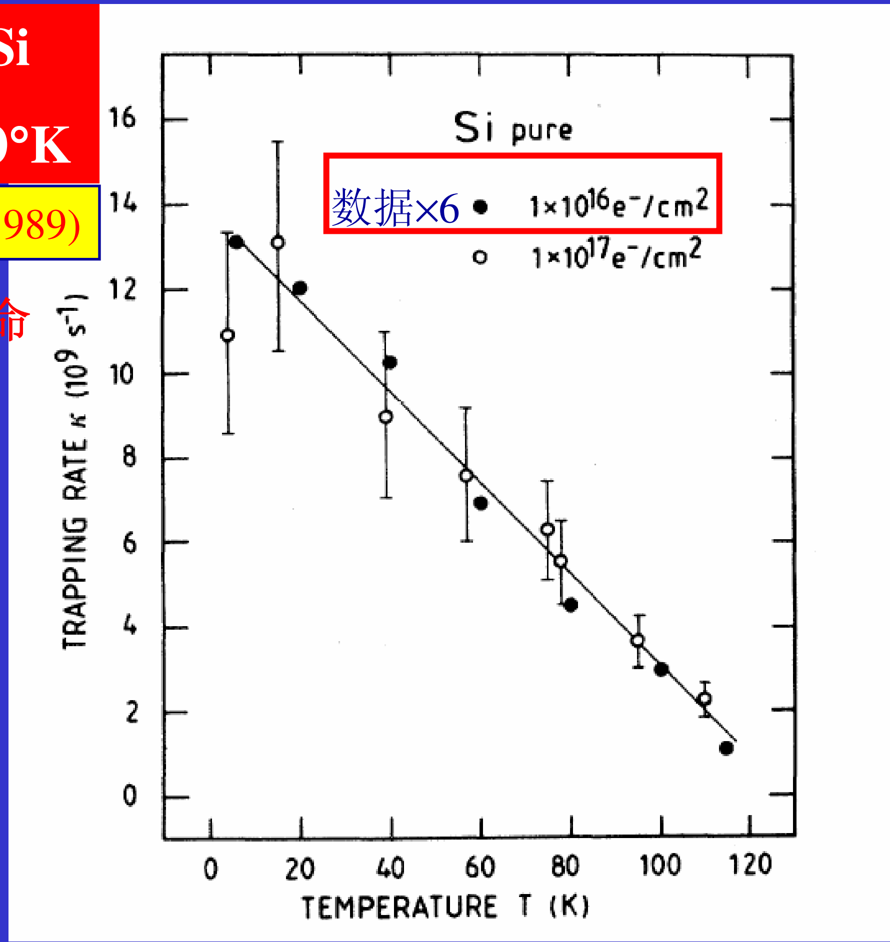
表层有大的S值表明有大的空位团形成，因为辐照在600C完成的，单和双空位能移动.

- (O)600 ºC 时200 keV氧离子注入到Si(100) 中, 剂量为 1.7×10^{17} ions/cm^2.
- (□) 1300 ºC 退火后的数据.

Irradiation induced defects



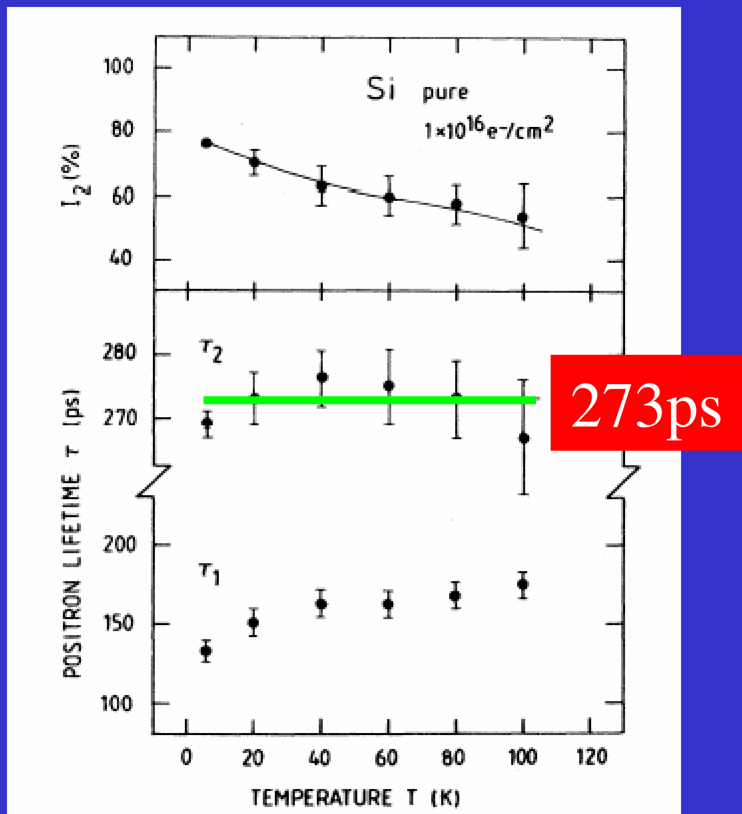
不同辐照剂量下正电子寿命随温度变化

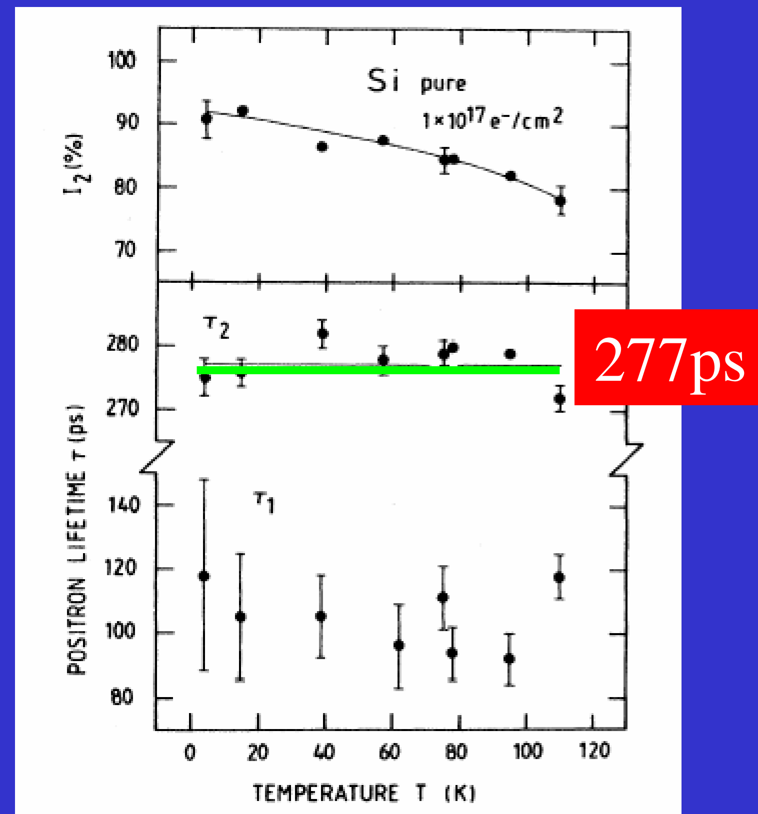


正电子捕获率随温度变化

- 线性减少
- 随温度增加减少10倍
- 辐照剂量大，捕获率大

辐照条件,测量条件同上



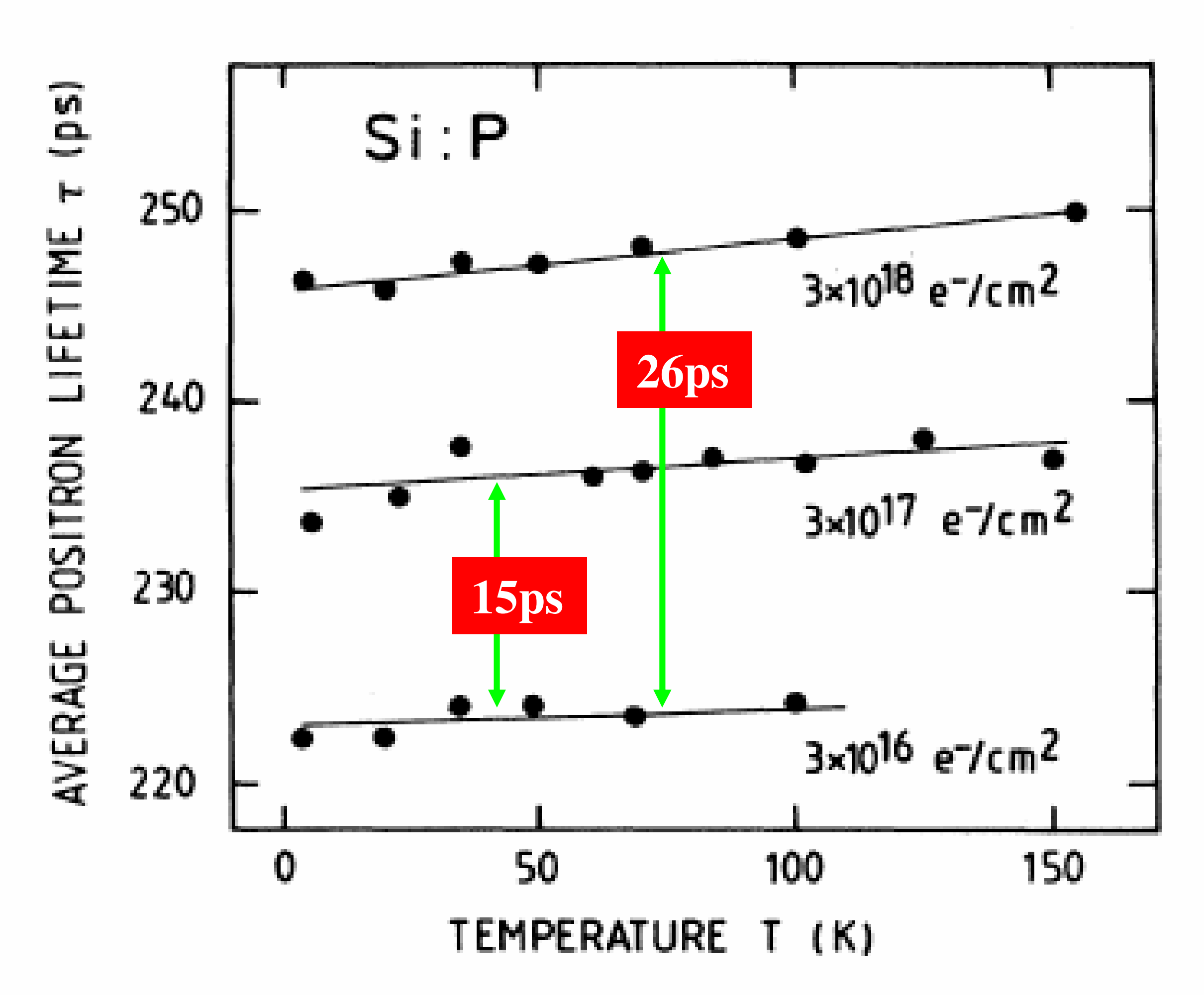


τ_2寿命不随温度变化
只是强度随温度减少

电子辐照Si:P

1.5-MeV, 20°K

不管何种辐照剂量, 平均寿命随温度基本不变.

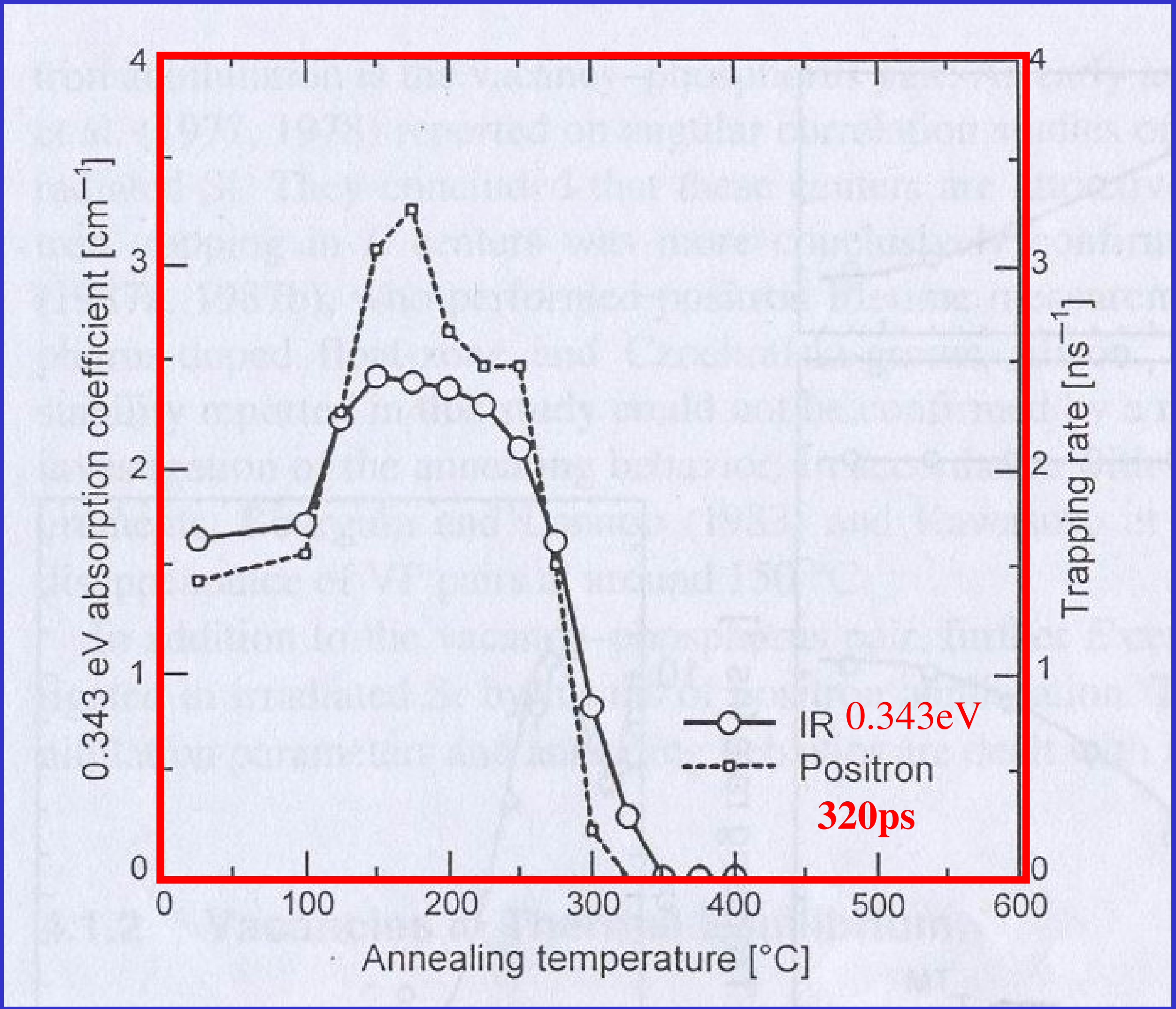


正电子平均寿命随温度变化

Mater.Sci.Forum
175-177, 423(1995)

Si 双空位缺陷寿命
(ps)

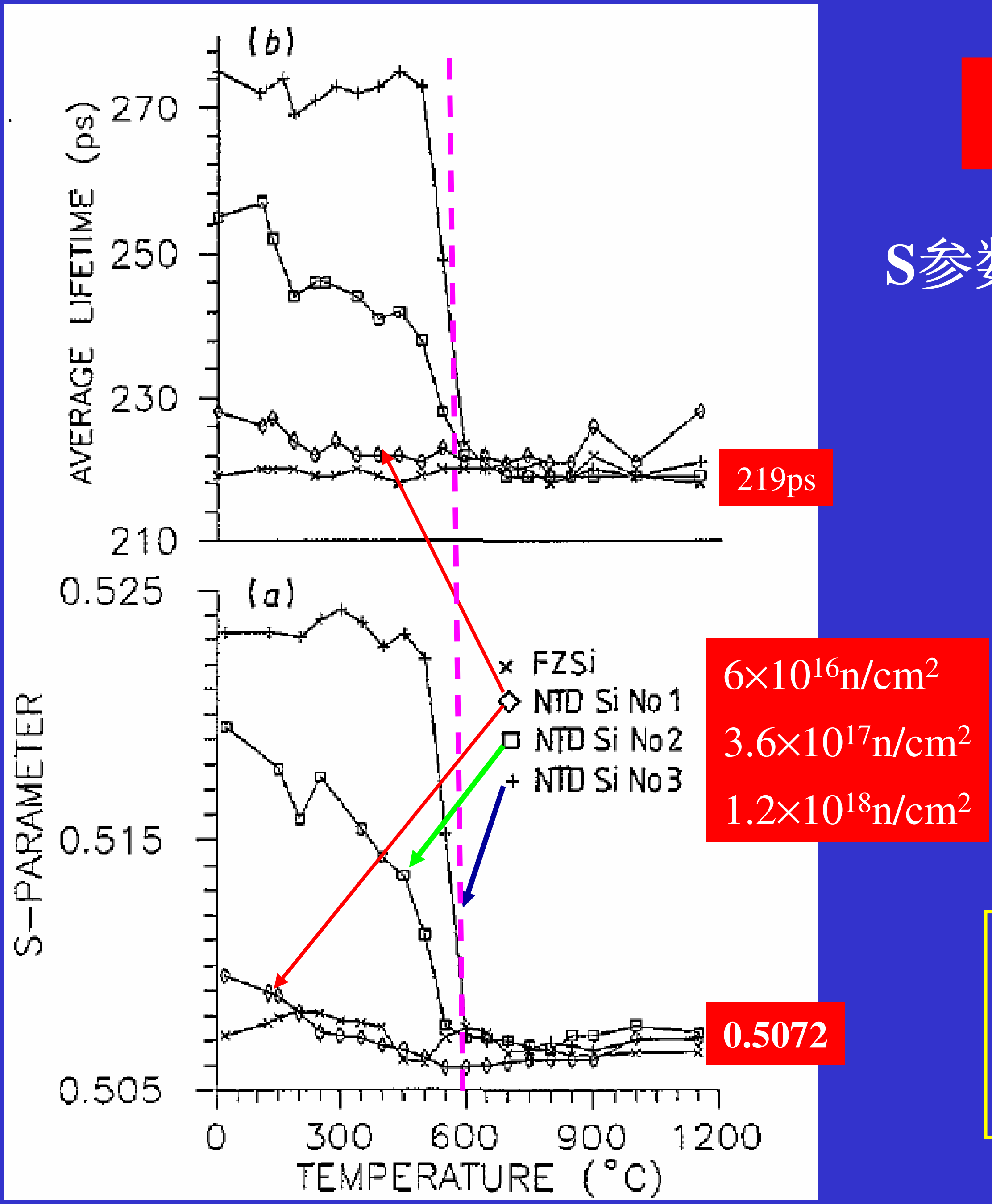
缺陷	10K	320K
V^{2-}_2	260	320
V^{-}_2	278	320
V^{0}_2	290	295



比较红外吸收系数和正电子捕获率

中子辐照FZ Si

S参数和平均寿命随温度变化



Meng and Puff
J.Phys.: Condens.matter
6(1994)4971

PHYSICAL REVIEW B VOLUME 58, NUMBER 16 15 OCTOBER 1998-II

Defects in electron-irradiated Si studied by positron-lifetime spectroscopy

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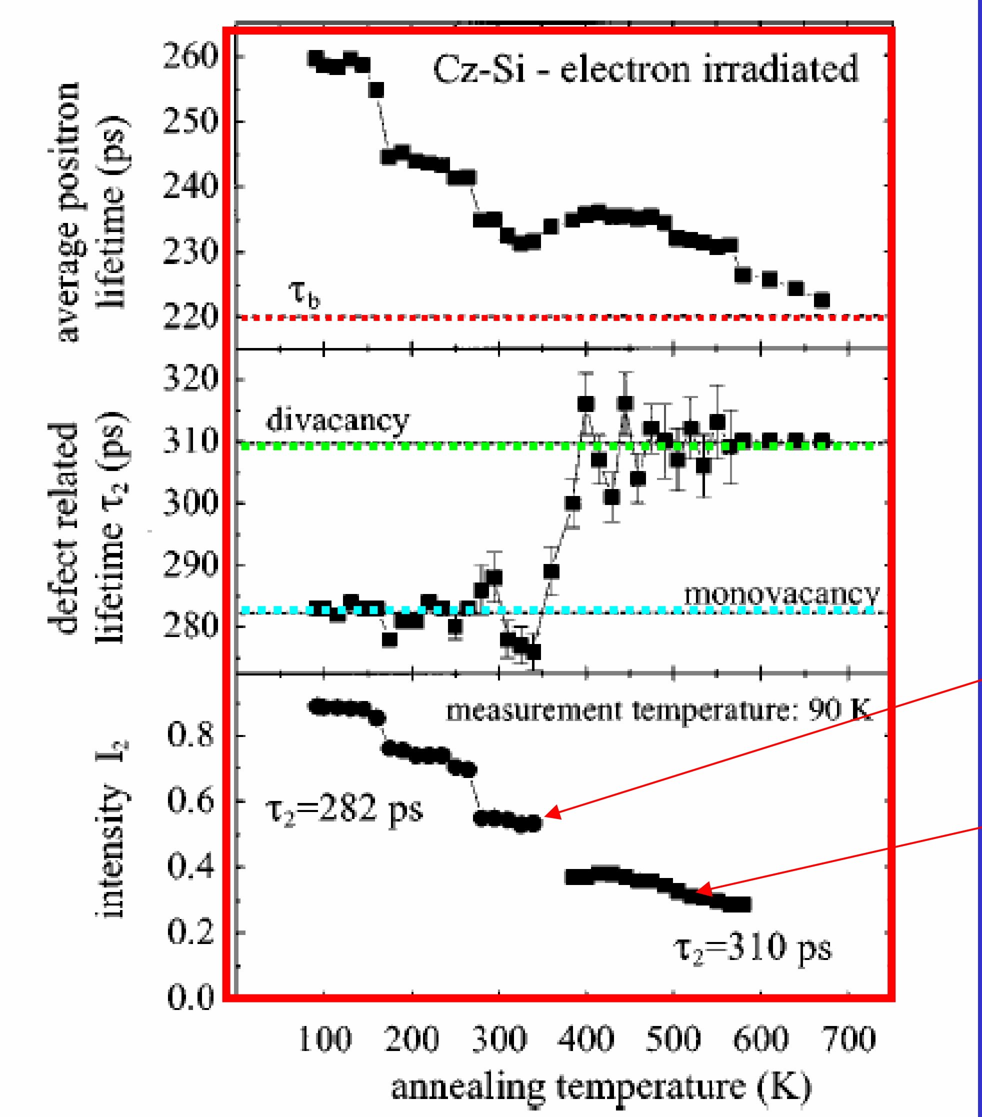
(Received 20 April 1998; revised manuscript received 13 July 1998)

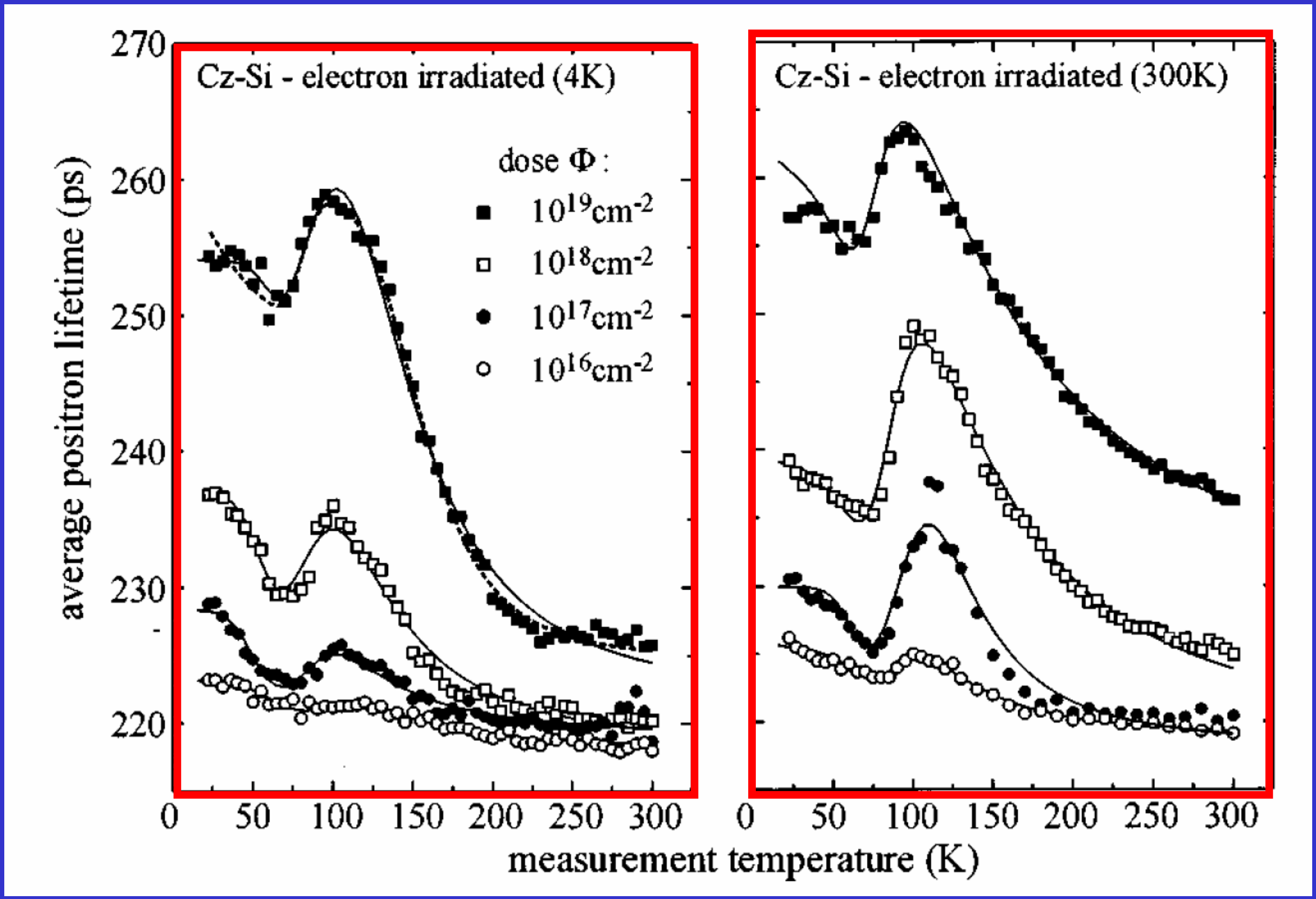


电子辐照条件:
~2 MeV, 4 K, 10^{18} cm^{-2})

正电子寿命随退火温度的变化．测量条件 90° K.

monovacancy

divacancy



4 °K 和室温下300°K不同电子辐照剂量(2 MeV)下正电子寿命随温度的变化.

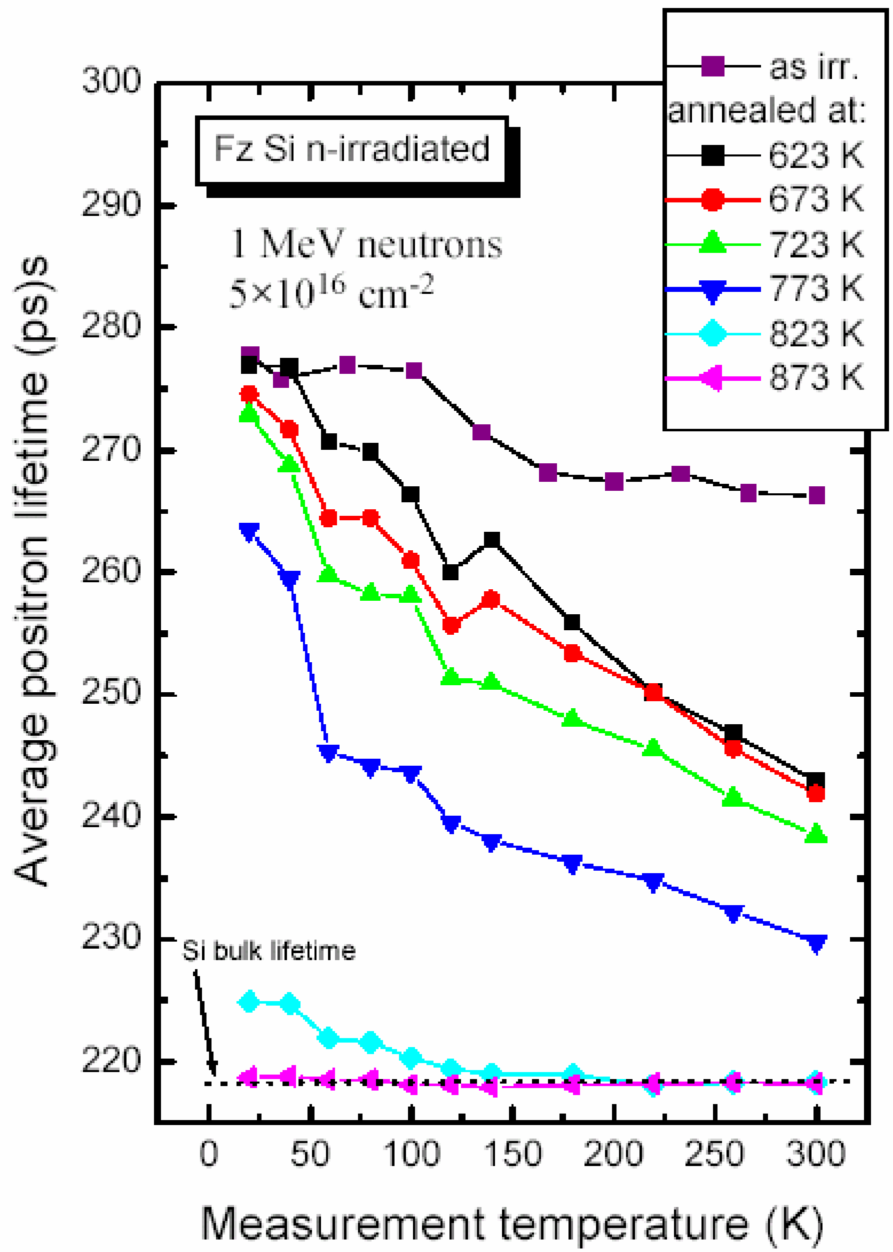
The solid lines correspond to the trapping model taking into account a negatively charged vacancy defect and a negative ion as shallow positron trap.

n-irradiated Si

- radiation defects limit lifetime of detectors in high-luminosity collider experiments (ATLAS, TESLA)
- neutron irradiation generates vacancy-type defects
- in as-irradiated state at RT:

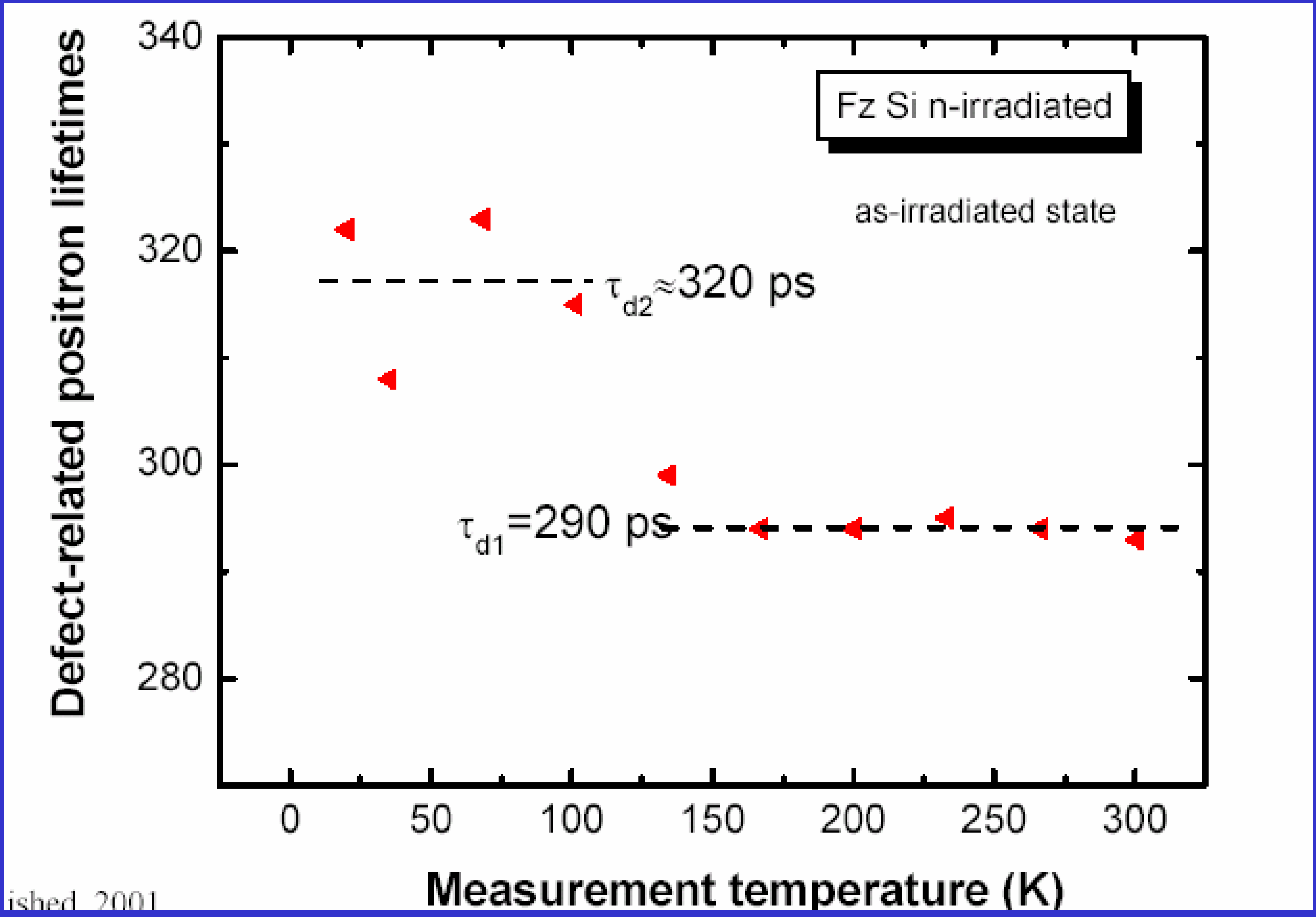
  positron trapping rate: $\kappa = 9.7\times10^{9}\ s^{-1}$
  defect concentration: $C_{def} = 2.5\times10^{17}\ cm^{-3}$
- therefore: $C_{def} \gg [O]$
- probably isolated divacancies and larger vacancy clusters

  (monovacancies anneal at about 170 K; divacancies stable up to 450...500 K)



n-irradiated Si

- two different vacancy-type defects are detected: divacancies and V_3



n-irradiated Si

- after annealing of divacancies (673 K annealing step)

  positron trapping rate:

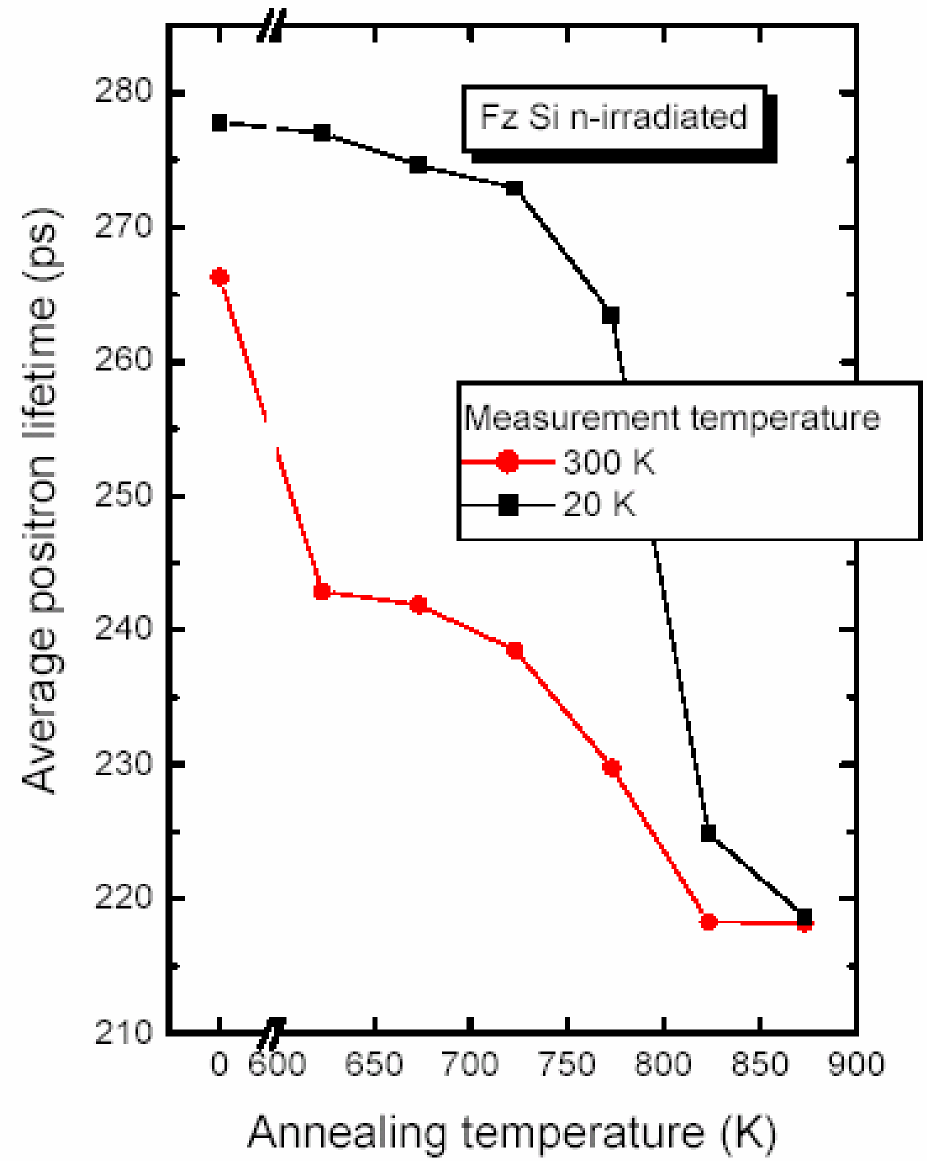
  $\kappa = 2\times10^{9}\ s^{-1}$

  assuming V_3 $\Rightarrow$

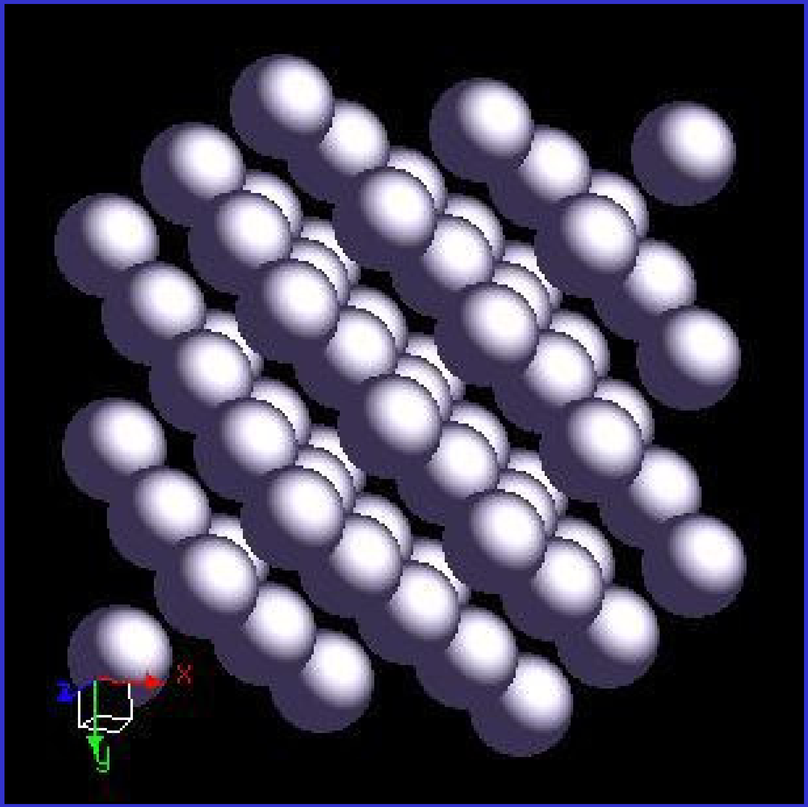
  defect concentration:

  $C_{V3} \approx 3\times10^{16}\ cm^{-3}$

- annealing stages at 300…600K and at 800 K



Positron in Germanium



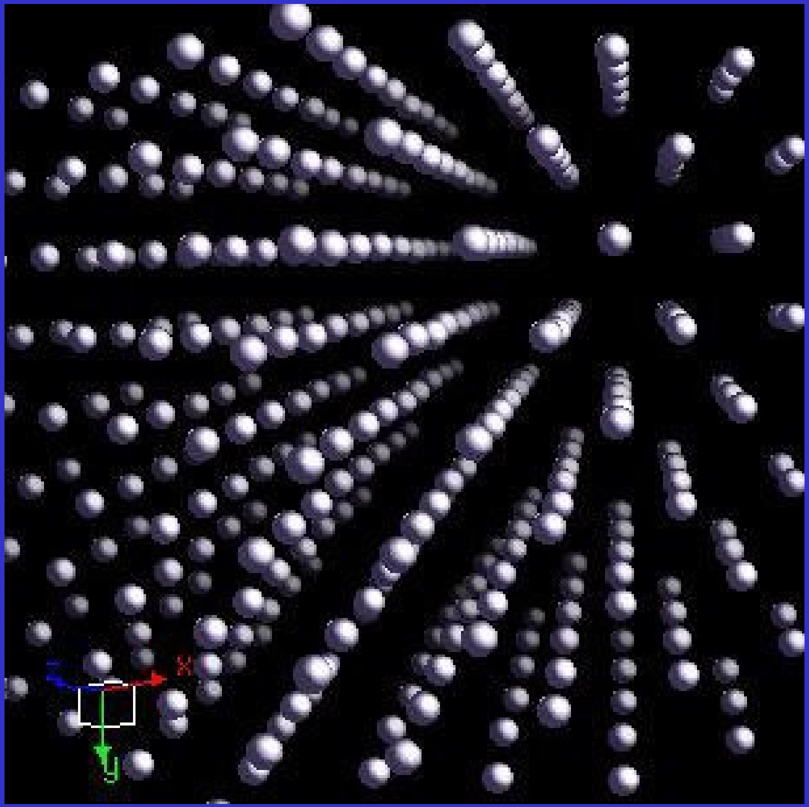
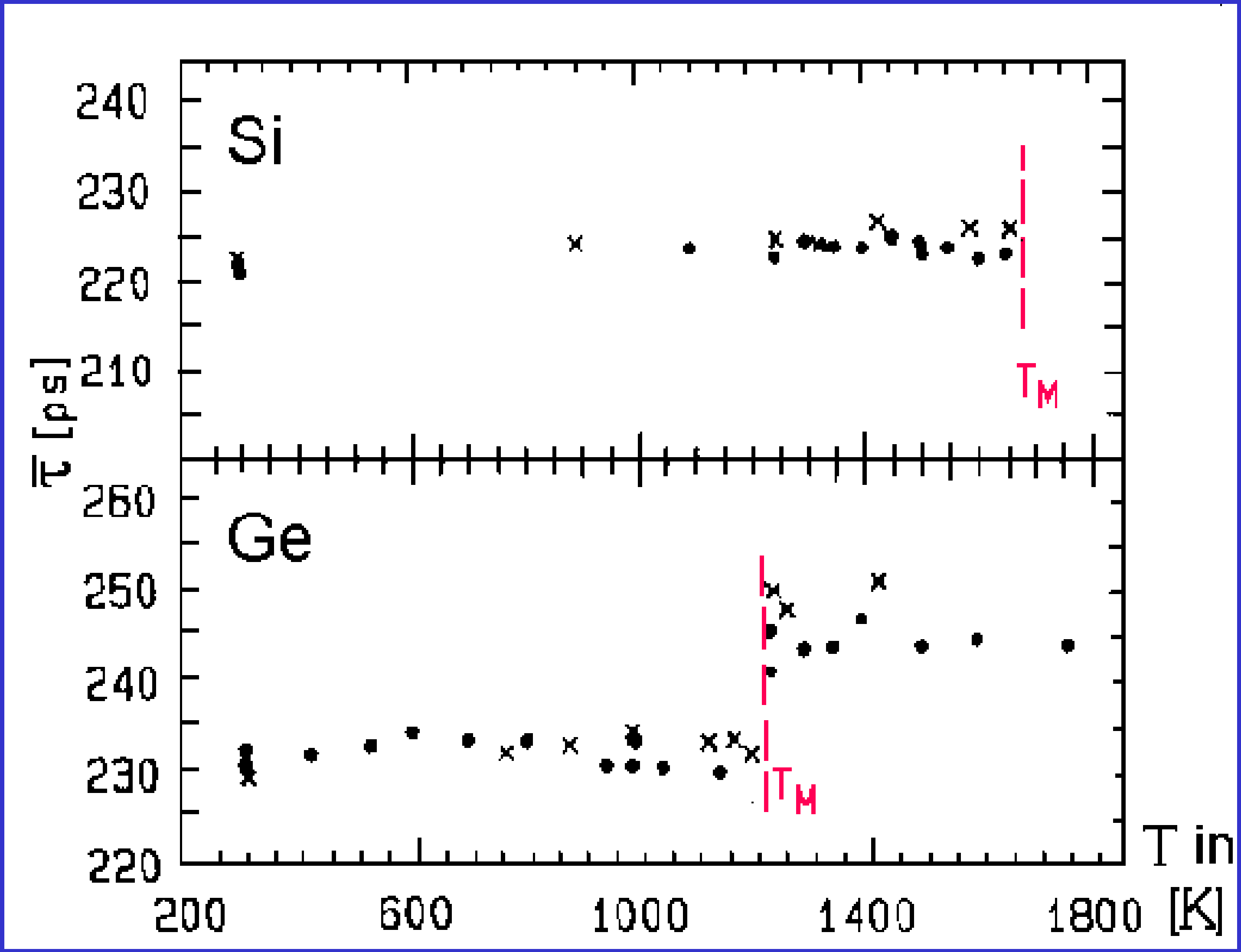


Table 4.3. Positron-lifetime data of germanium.

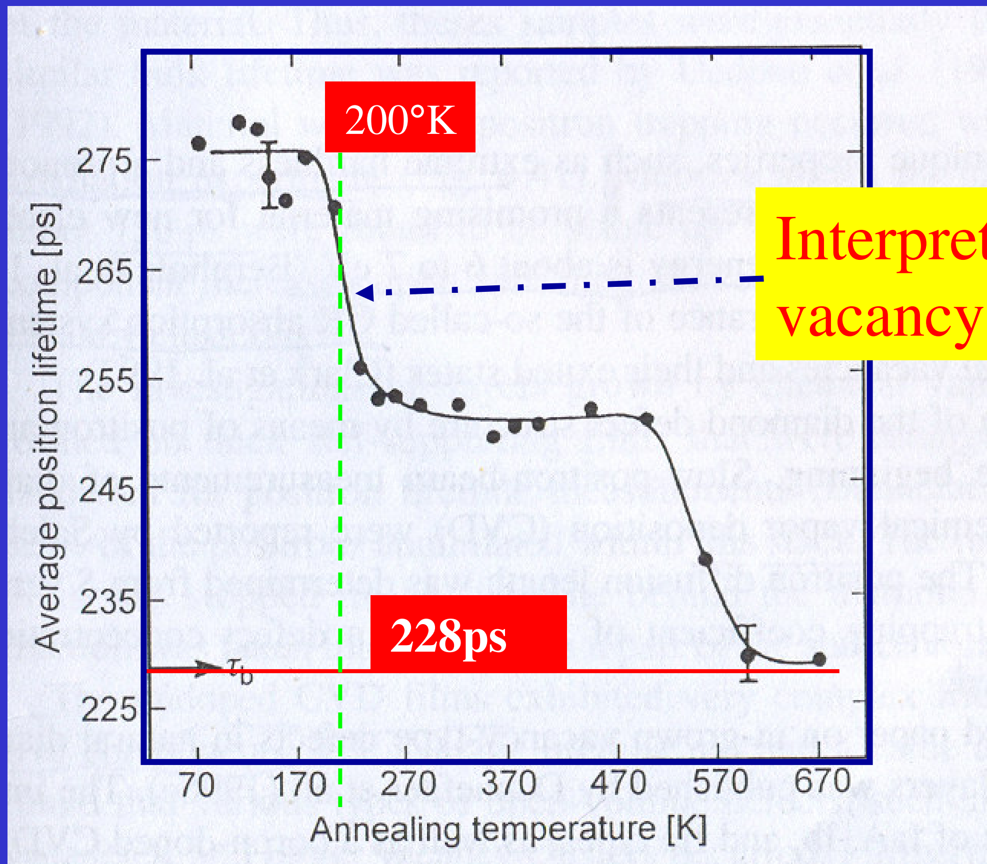
	Positron annihilation characteristics		Dissolution
	Lifetime [ps]	τ_d/τ_b	temperature [K]
Bulk lifetime	228[a,b]	—	—
Monovacancies	278[c], 290[a], 292[d]	1.22, 1.27, 1.28	200[a,c]
Voids	520[c]	2.28	870[c]
Dislocation-related defects	325[e]	1.43	

τ_d is the defect-related positron lifetime, τ_b the positron lifetime in the defect-free bulk.
[a]Corbel et al. (1985), [b]Würschum et al. (1989b), [c]Polity and Rudolf (1999), [d]Moser et al. (1985), [e]Krause-Rehberg et al. (1993a).



Positron life time spectroscopy in **Si** and **Ge** ,

T_M denotes the melting point.



200K处的退火台阶

Interpreted of monovacancies to vacancy-dopant complexes

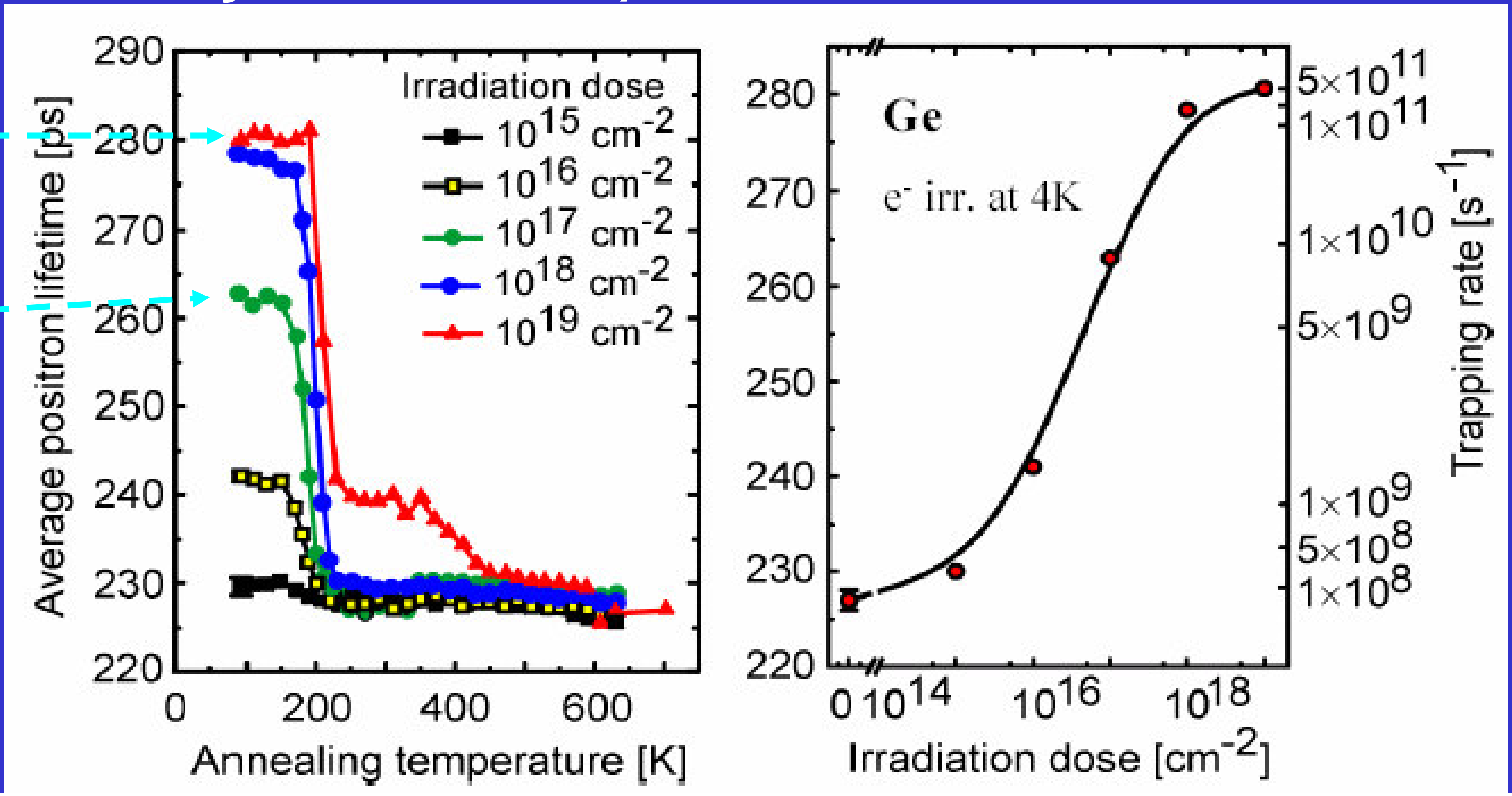
p-Ge在20°K温度下在电子辐照后的寿命随等时退火温度的变化.

Defects in electron -irradiated Ge

- Electron irradiation (2 MeV) induces Frenkel pairs (vacancy - interstitial pairs)
- steep annealing stage at 200 K
- at high irradiation dose: divacancies are formed (thermally more stable)

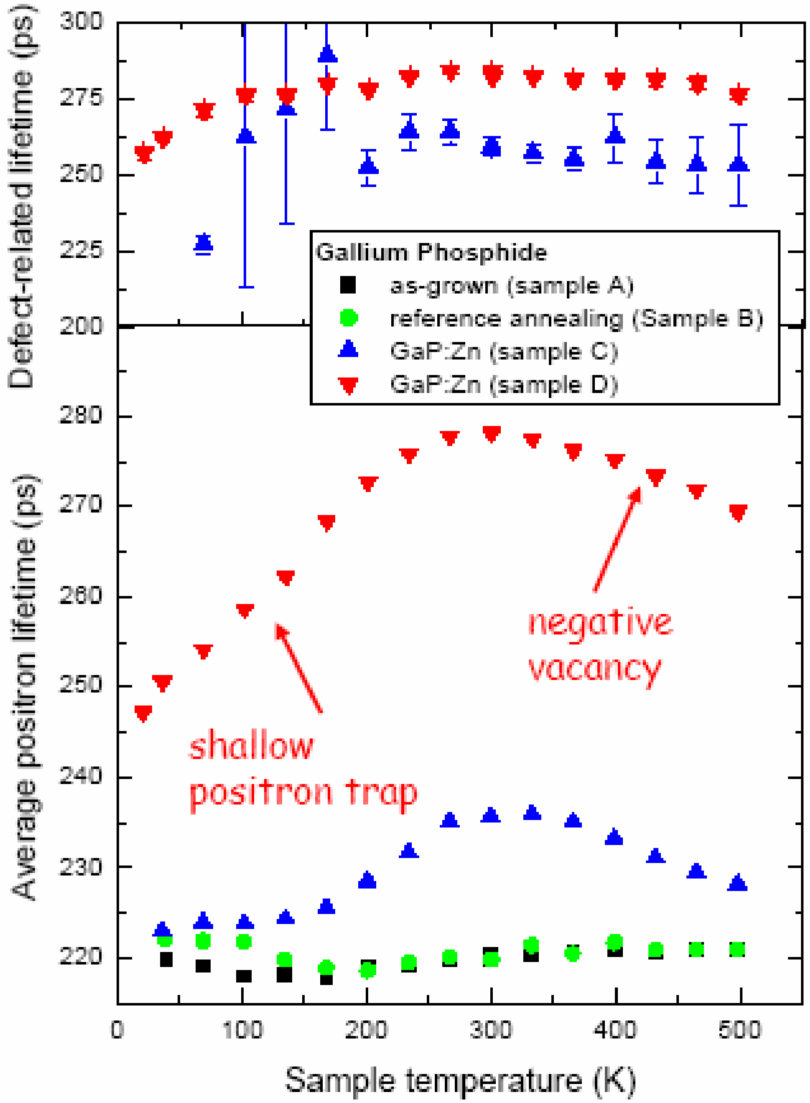
孤立的单空位或双空位
285ps

单空位
263ps



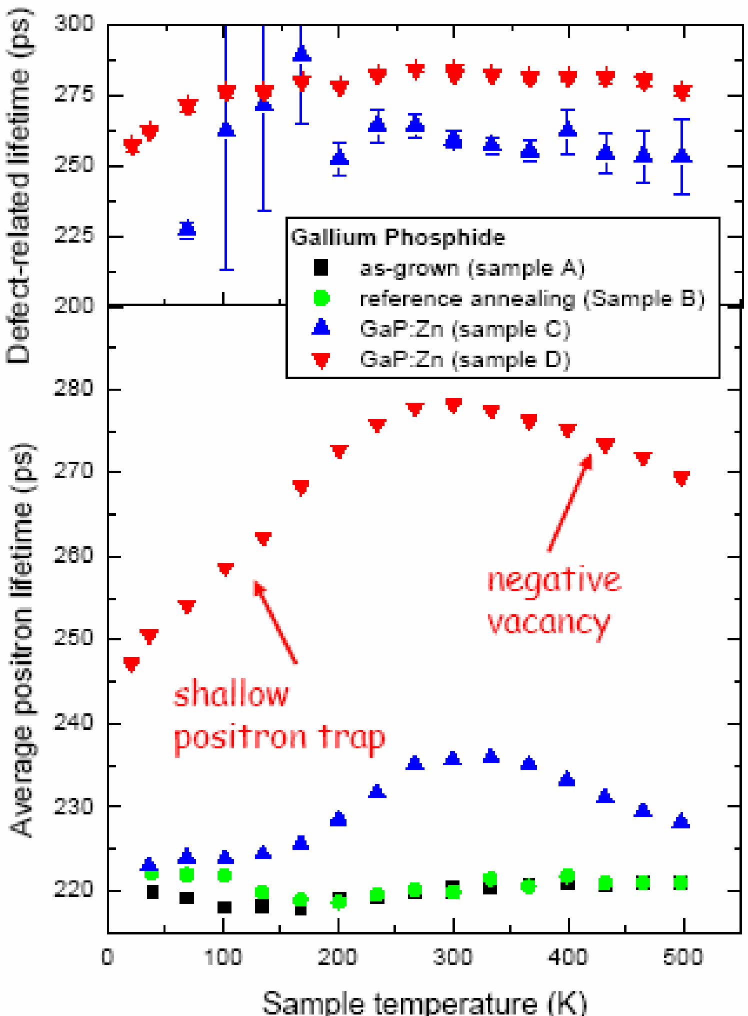
Positron in GaP

Positron lifetime results



- both reference samples: no trapping
- distinct vacancy signal only after Zn in-diffusion
- sample D: almost complete positron trapping at RT
- defect-related lifetime: τ_v = 282 ps
- outward relaxation is expected for both vacancies:
- V_{Ga} -> 3.8% and V_P -> 6.1%
  (G. Schwarz et al., Phys. Rev. 1998)
- lifetimes were theoretically calculated taking into account the relaxation

Positron lifetime results



- defect-related lifetime: τ_v = 282 ps

Defect	e^+ lifetime in ps	remarks
GaP bulk	220	
V_{Ga}	258	unrelaxed
	270	3.8% outward relaxation
V_P	244	unrelaxed
	271	6.1% outward relaxation
V_P-Zn_{Ga}	274	6.1% outward relaxation
V_P-V_{Ga}	307	unrelaxed

- from lifetime: no decision between V_{Ga} and V_P

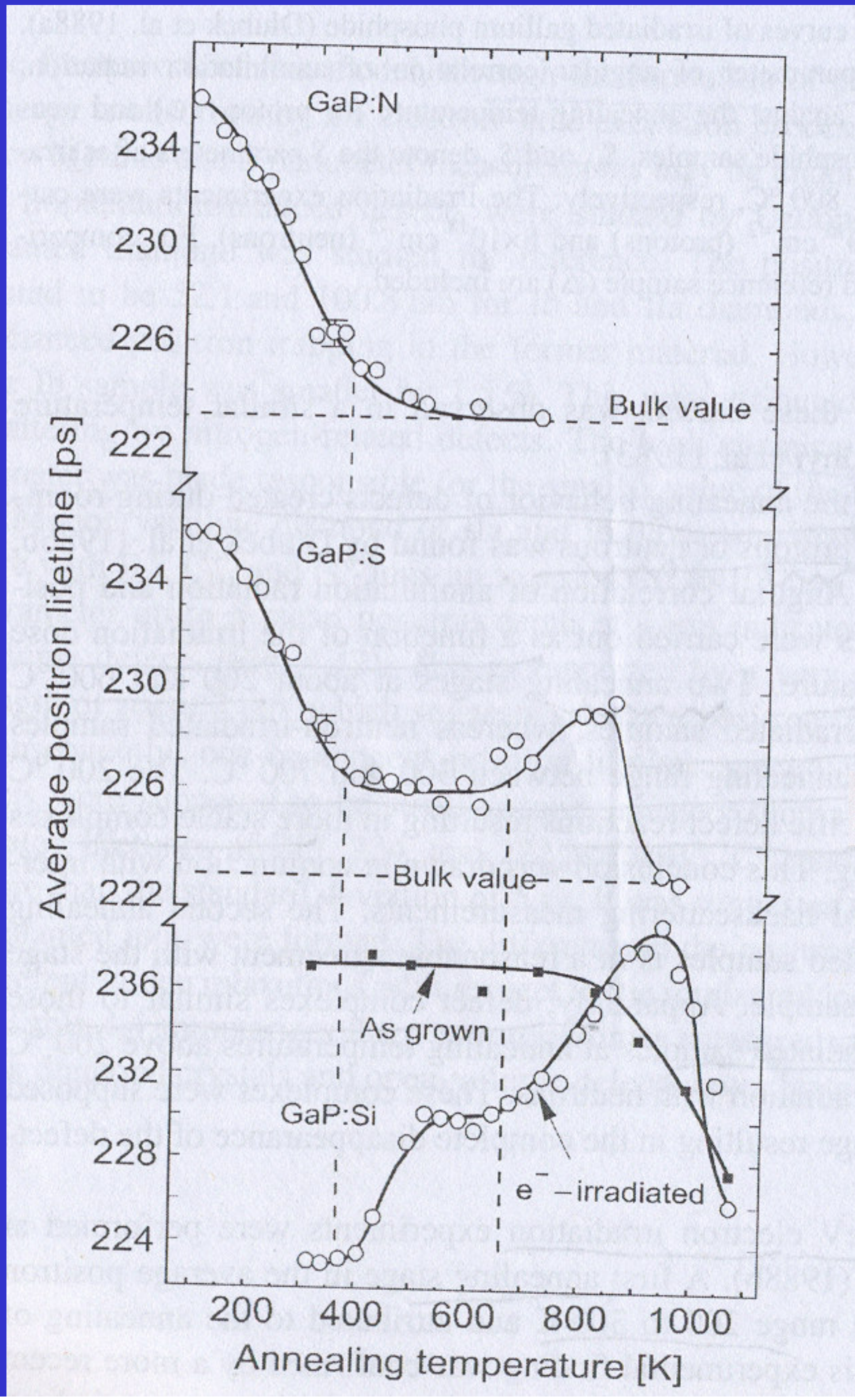
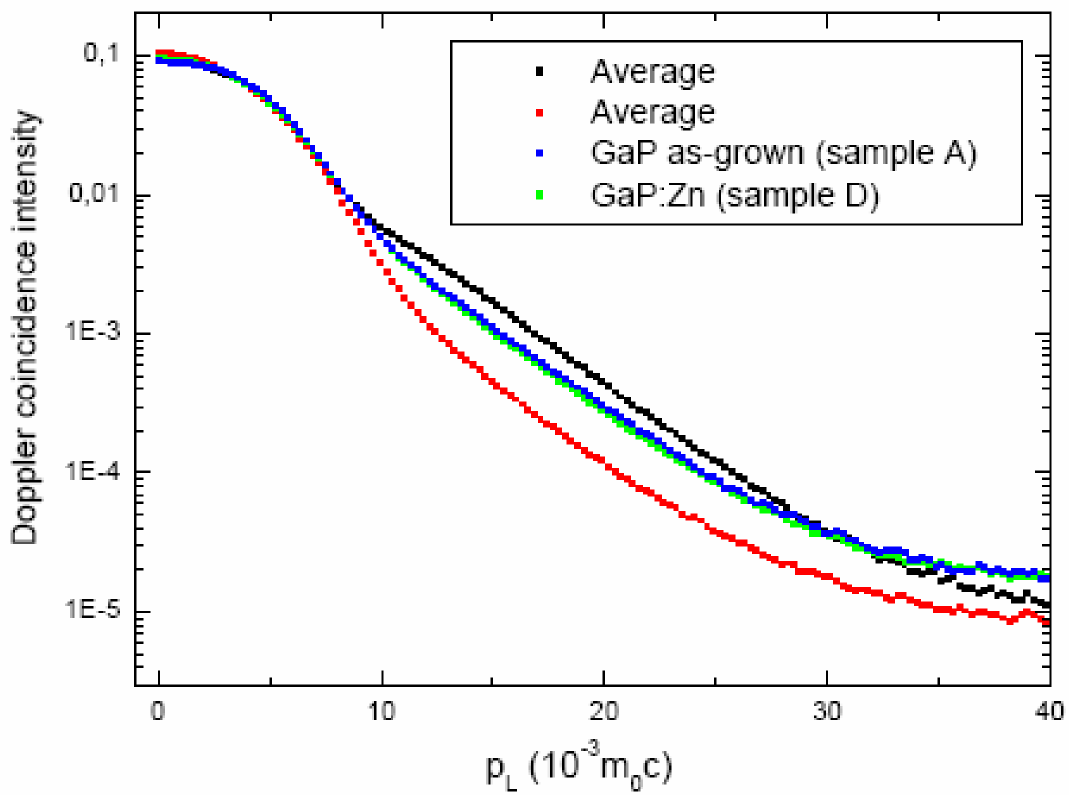


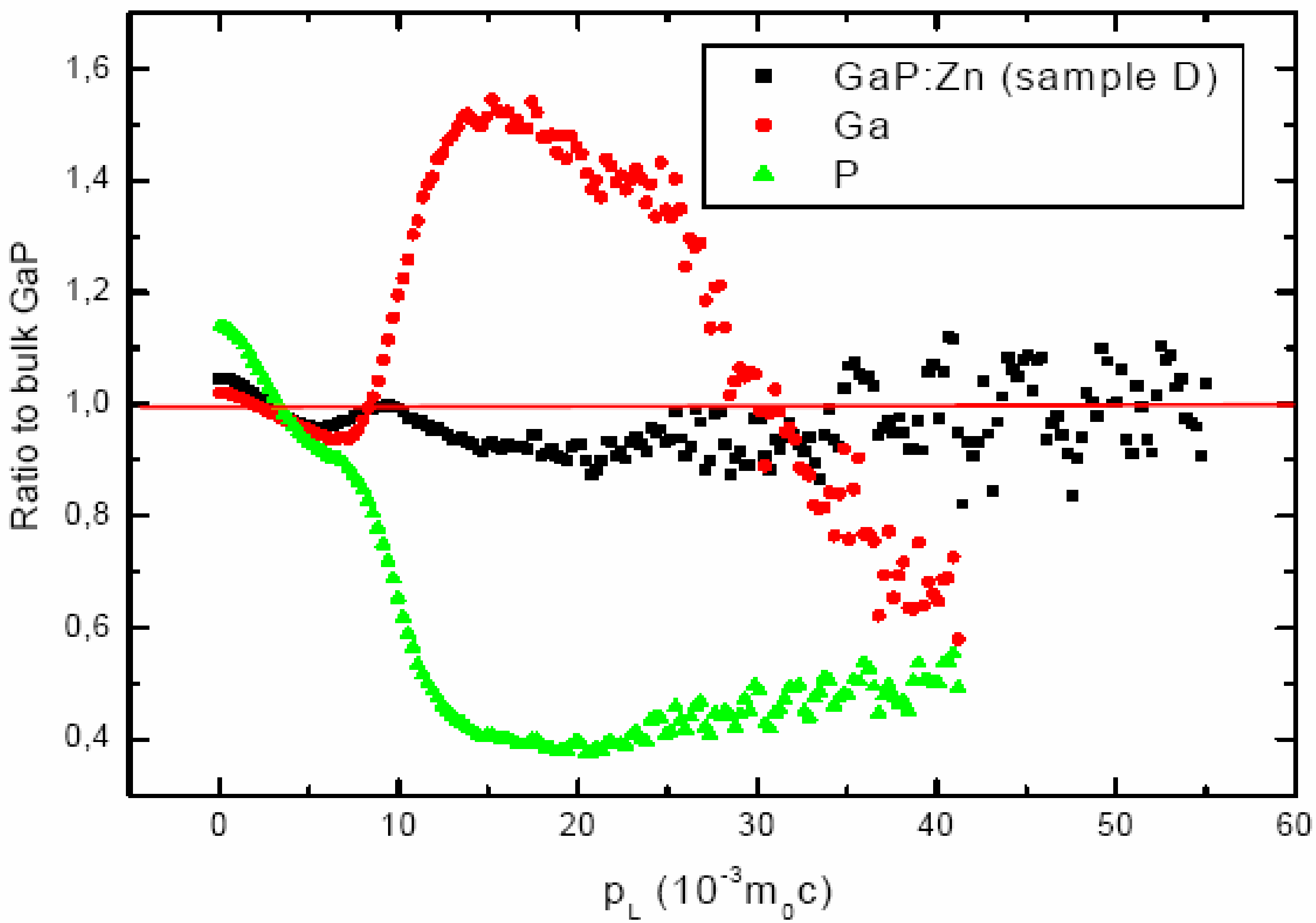
Fig. 5.3. Average positron lifetime as a function of the annealing temperature in nitrogen-, sulfur-, and silicon-doped electron-irradiated gallium phosphide (Polity et al. 1995a).

Doppler Coincidence Experiments

- DBCS was used to study the chemical environment of the detected mono-vacancy
- surprise: although complete trapping -> high-momentum Doppler spectrum close to reference sample
- comparison with theoretically calculated spectra required

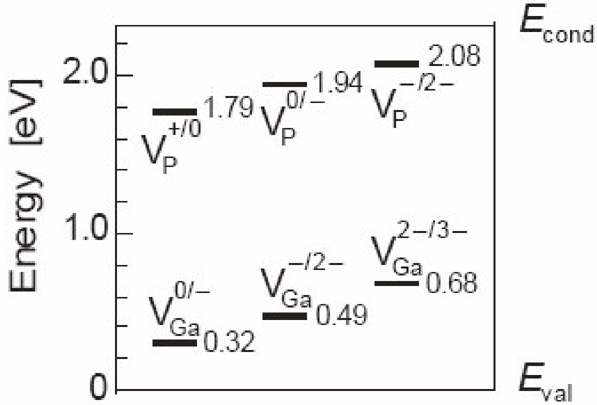


Doppler Coincidence Experiments



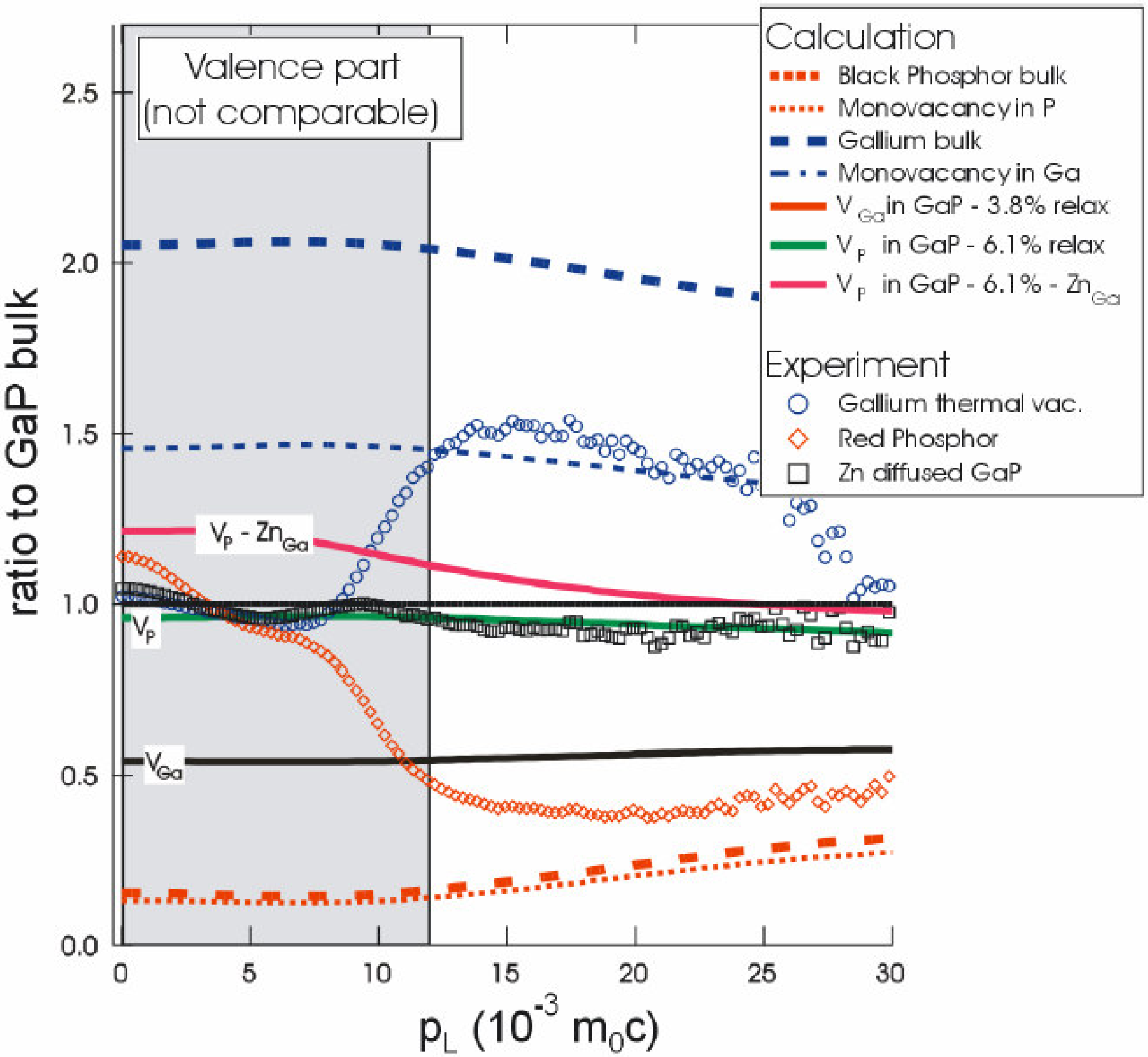
Doppler Coincidence Experiments

- calculations agree well for Ga and P
- V_{Ga} is close to P data, while V_P is very close to the bulk behavior
- conclusion: we detected V_P



(M. Puska, J. Phys. Cond. Mat. 1989)

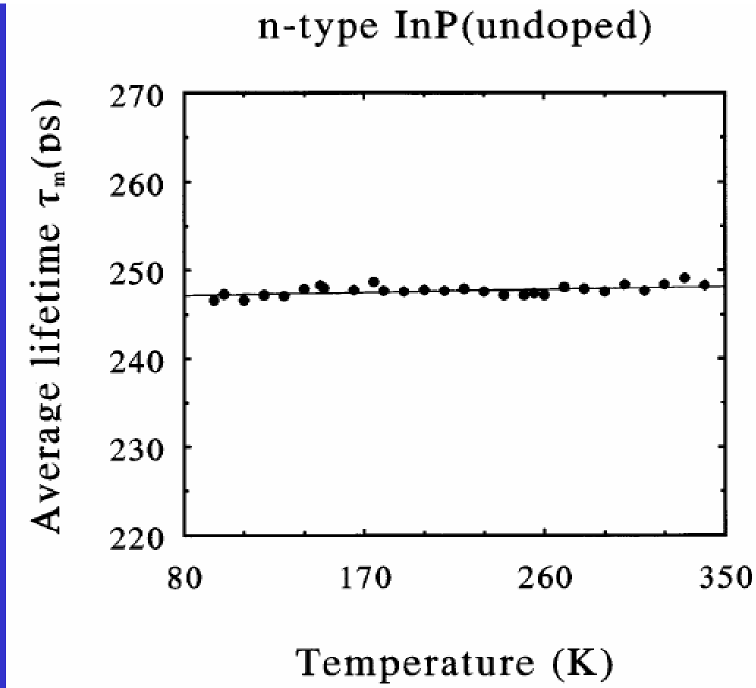
- however: V_P should be positive in p-type GaP
- probably we detect V_P-Zn_{Ga}

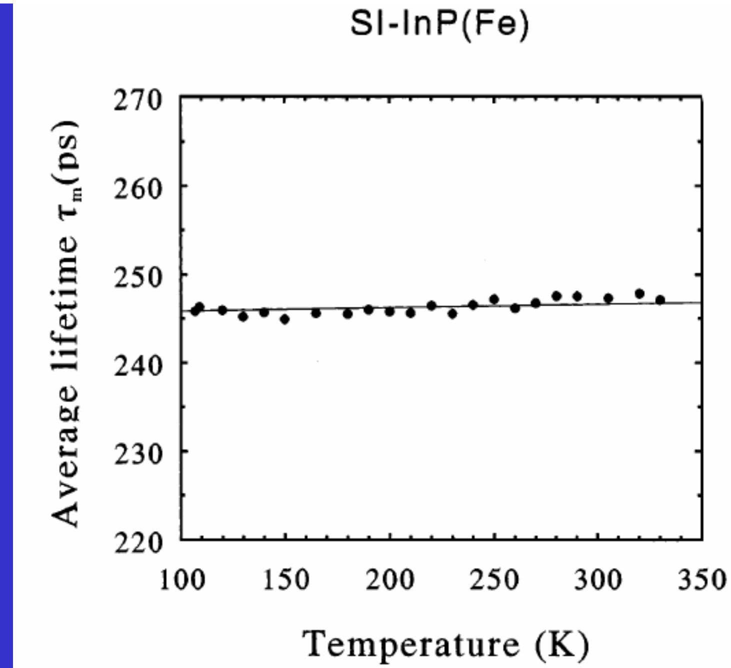


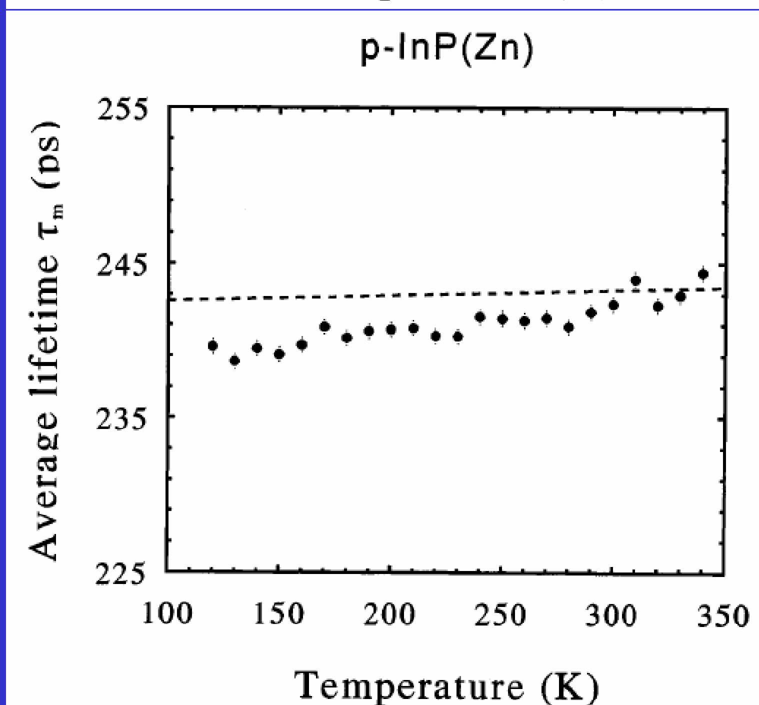
Conclusion

- During Zn in-diffusion: vacancies are formed
- concentration is much higher than thermal vacancies
- Vacancy is located in P sublattice
- V_p should be positive -> thus a defect complex is most probably observed
- best candidate: V_P-Zn_{Ga}

Positron in InP

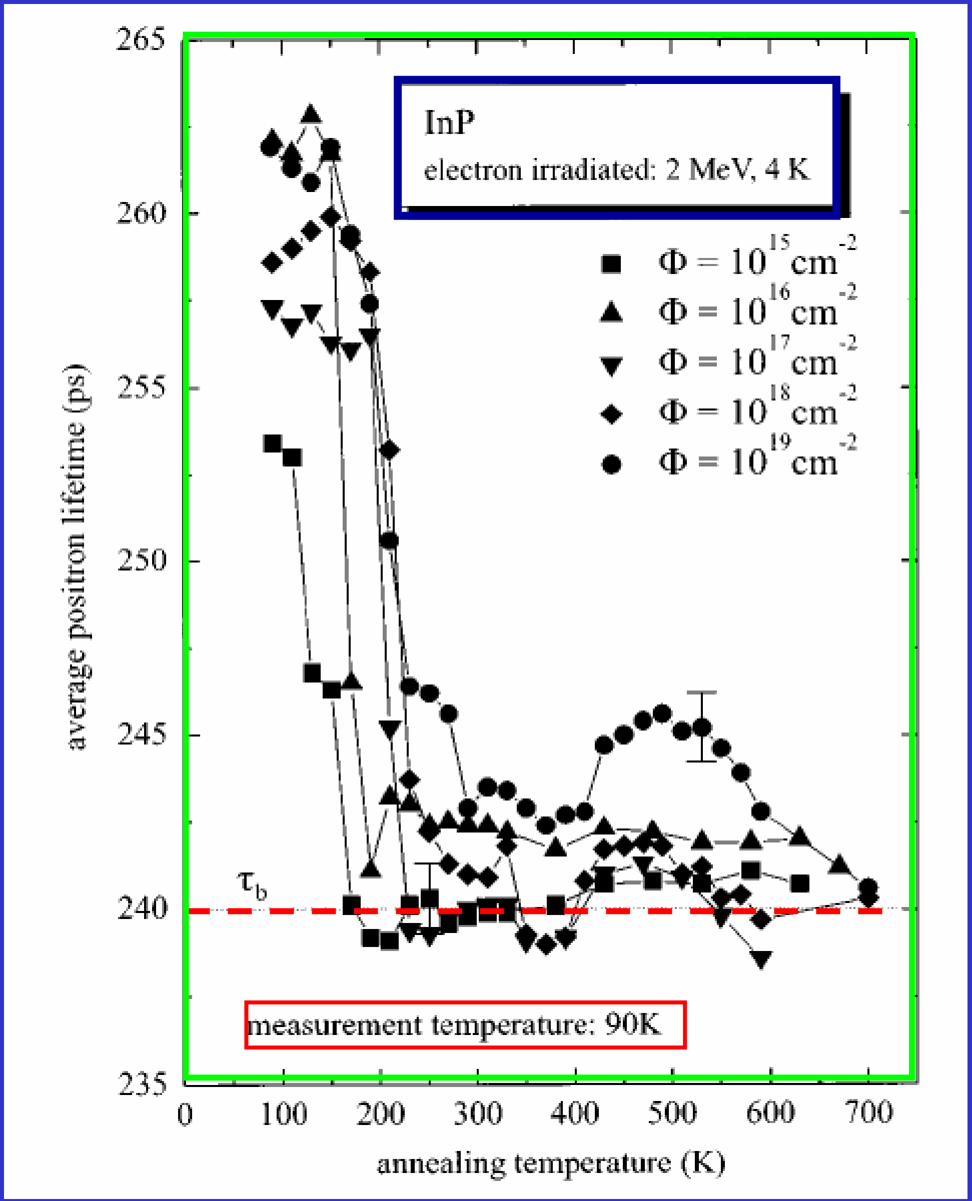






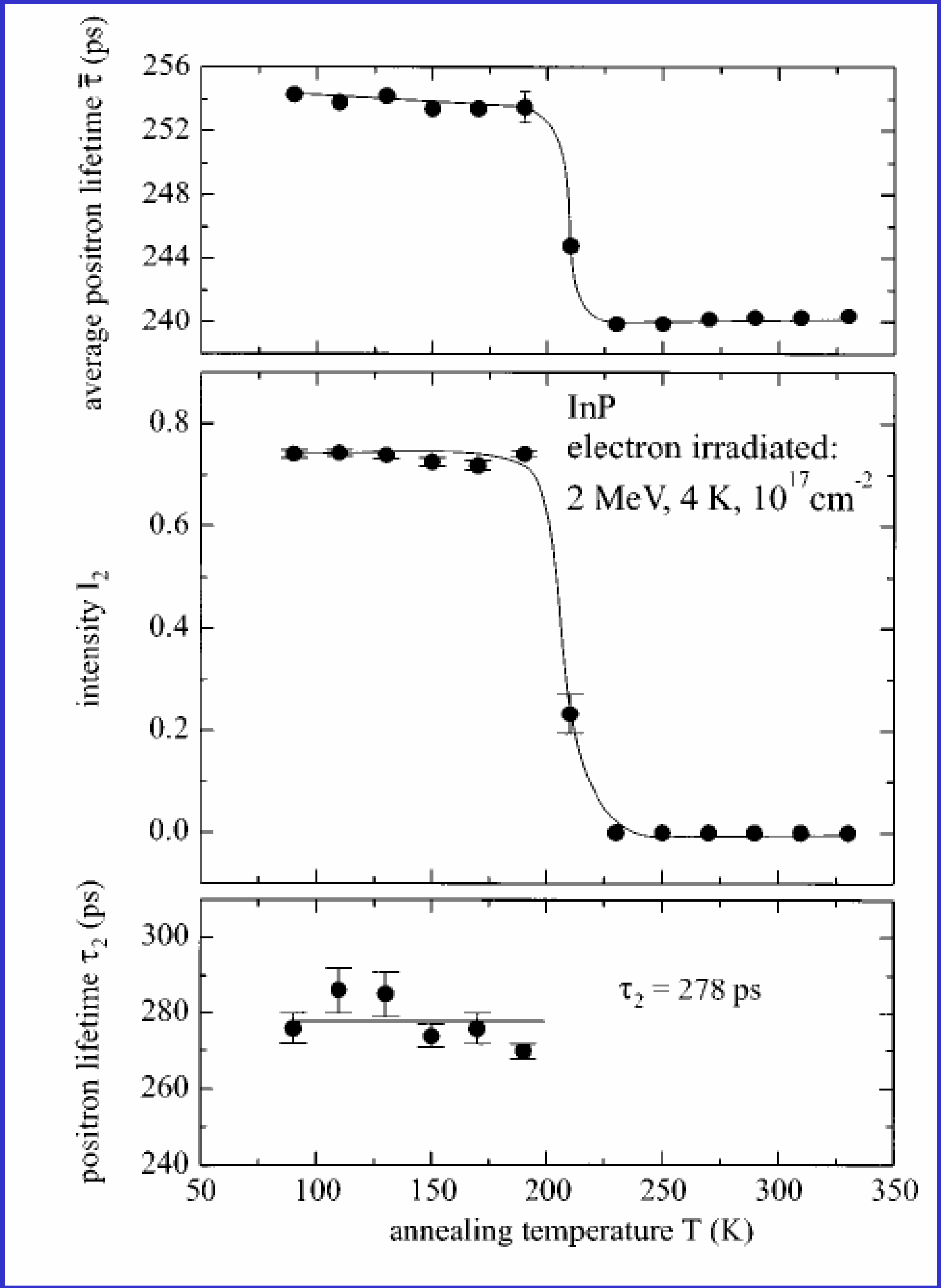
对**n-InP**, 正电子寿命随温度稍微增加, 这完全是热膨胀效应带来.

$$\tau(T)^{1/3} = \tau(T_0)^{1/3}\,[1+\alpha(T-T_0)],$$



n-InP电子辐照后平均正电子寿命随退火温度的变化.

- 在100-270K存在退火台阶;
- 台阶温度在~200K, 台阶温度随辐照剂量增加而增加;
- 退火后都到达体寿命.



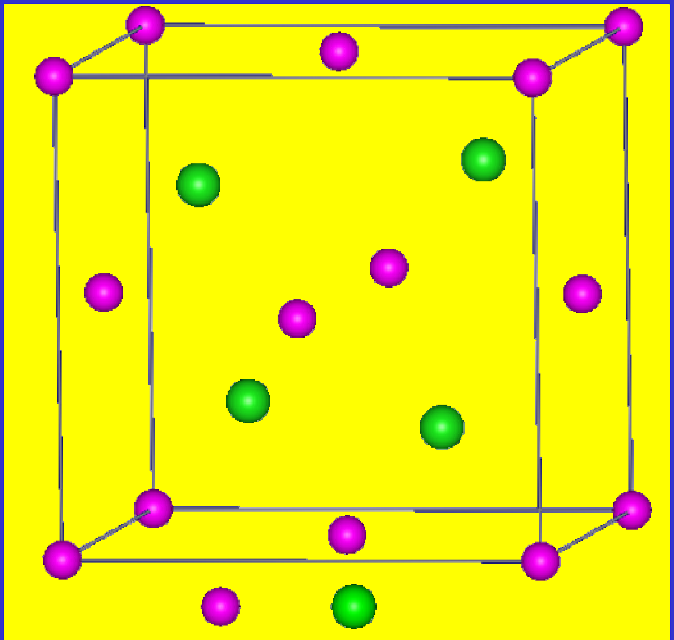
电子辐照*n*-InP的平均寿命，第二寿命和强度随退火温度的变化.

Positron lifetime of bulk and vacancy in InP

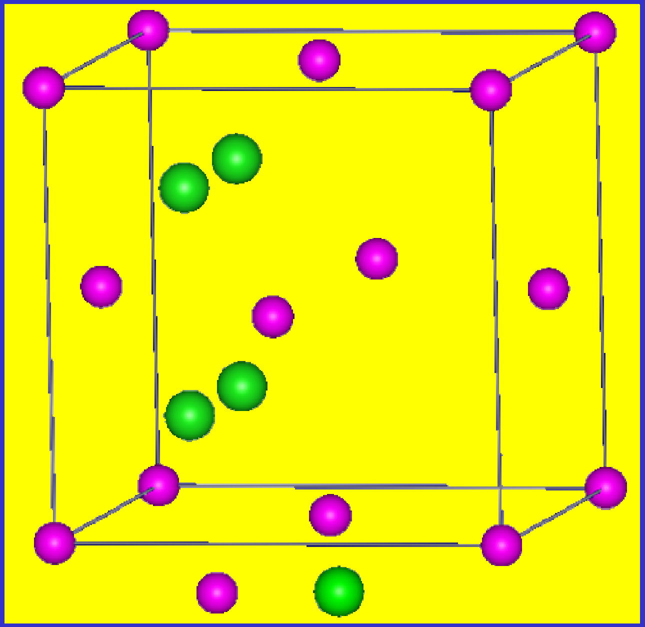
	Positron annihilation characteristics		Dissolution temperature [K]
	Positron lifetime [ps]	τ_d/τ_b	
Bulk lifetime	242[a, b]	—	—
	241[c]		
	243[d, e]		
	244[f]		
In monovacancies	312[g]	1.2[h]	< 250[c, d, e]
	265[i]	1.12[j]	
	297[d]	1.22	
	283[e, f]	1.16	
P monovacancies	263[d,e,f]	1.08	< 250[c]
V_P-zinc complexes	325[a, f]	1.34	680 to 750[a]
Divacancies	323[i]	1.37[j]	473[k]
Voids	420[l]	1.61[m]	873[l]
	486 to 527[b]	2.00 to 2.18	

τ_d is the defect-related positron lifetime, τ_b the positron lifetime in the defect-free bulk.

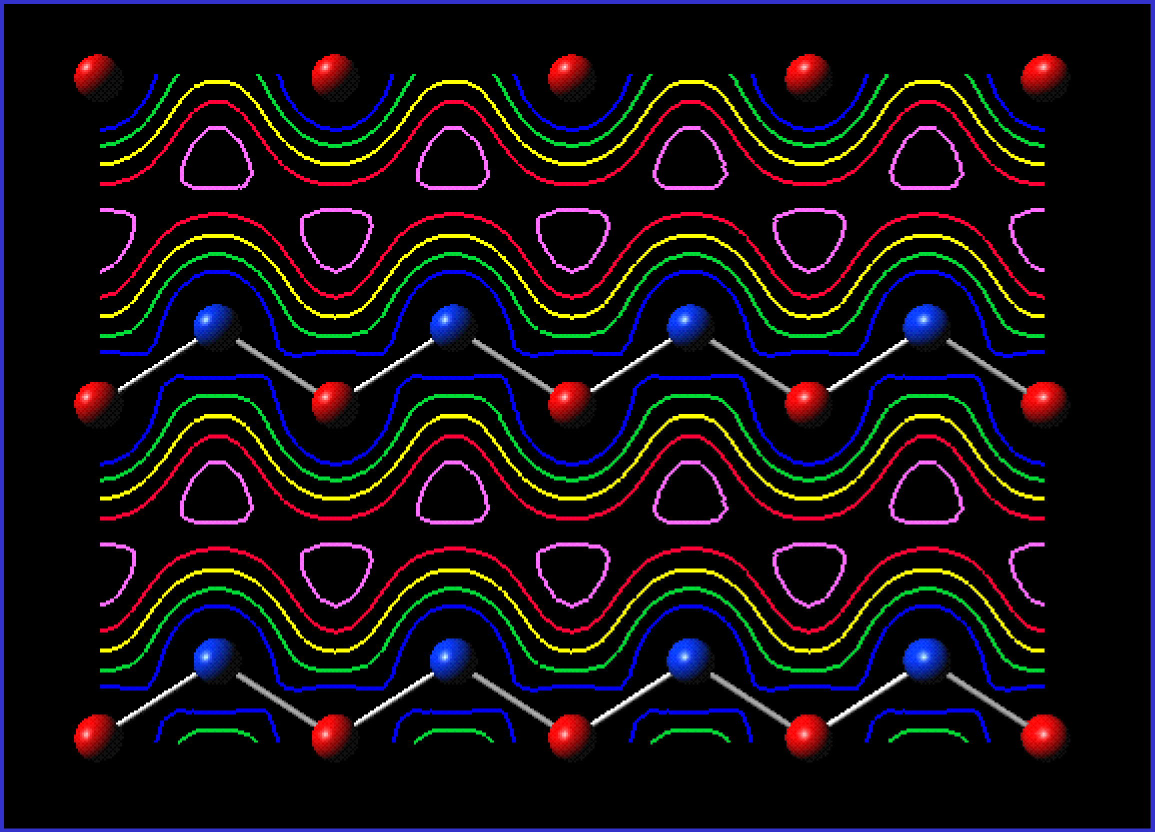
Positron in GaAs



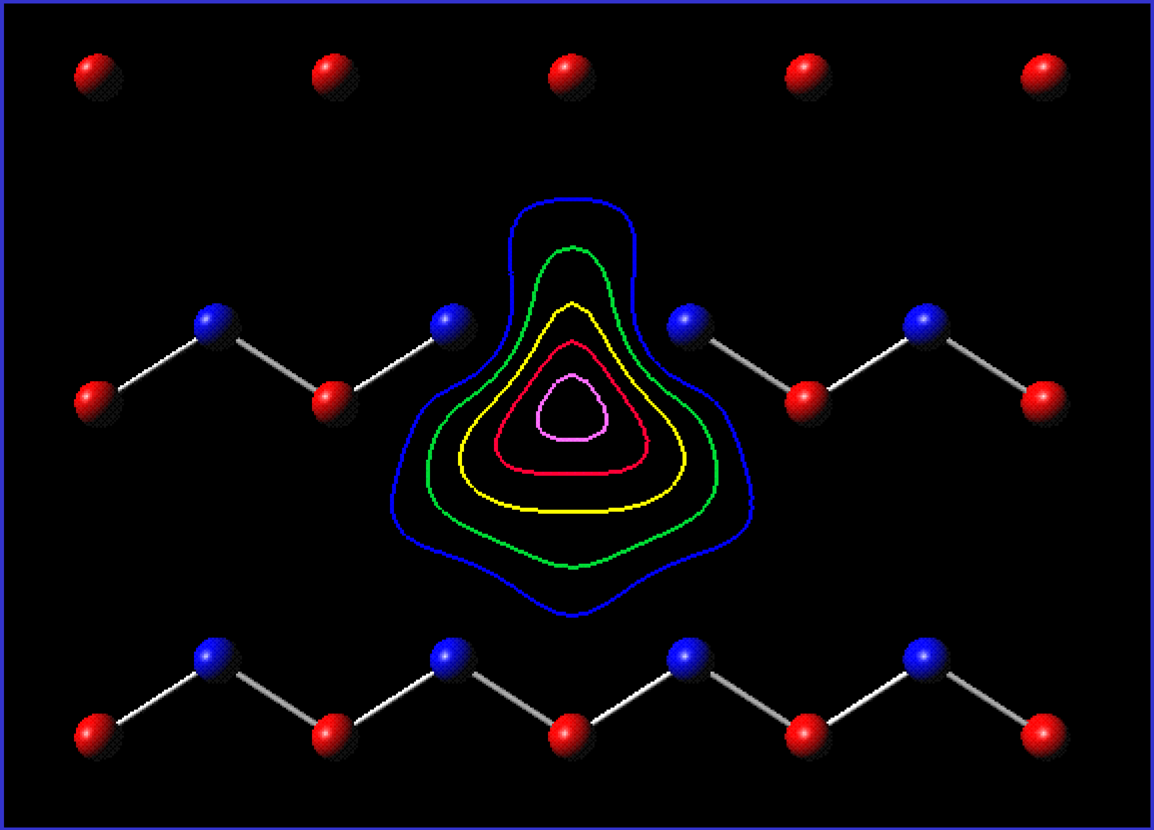
GaAs with B3 structure



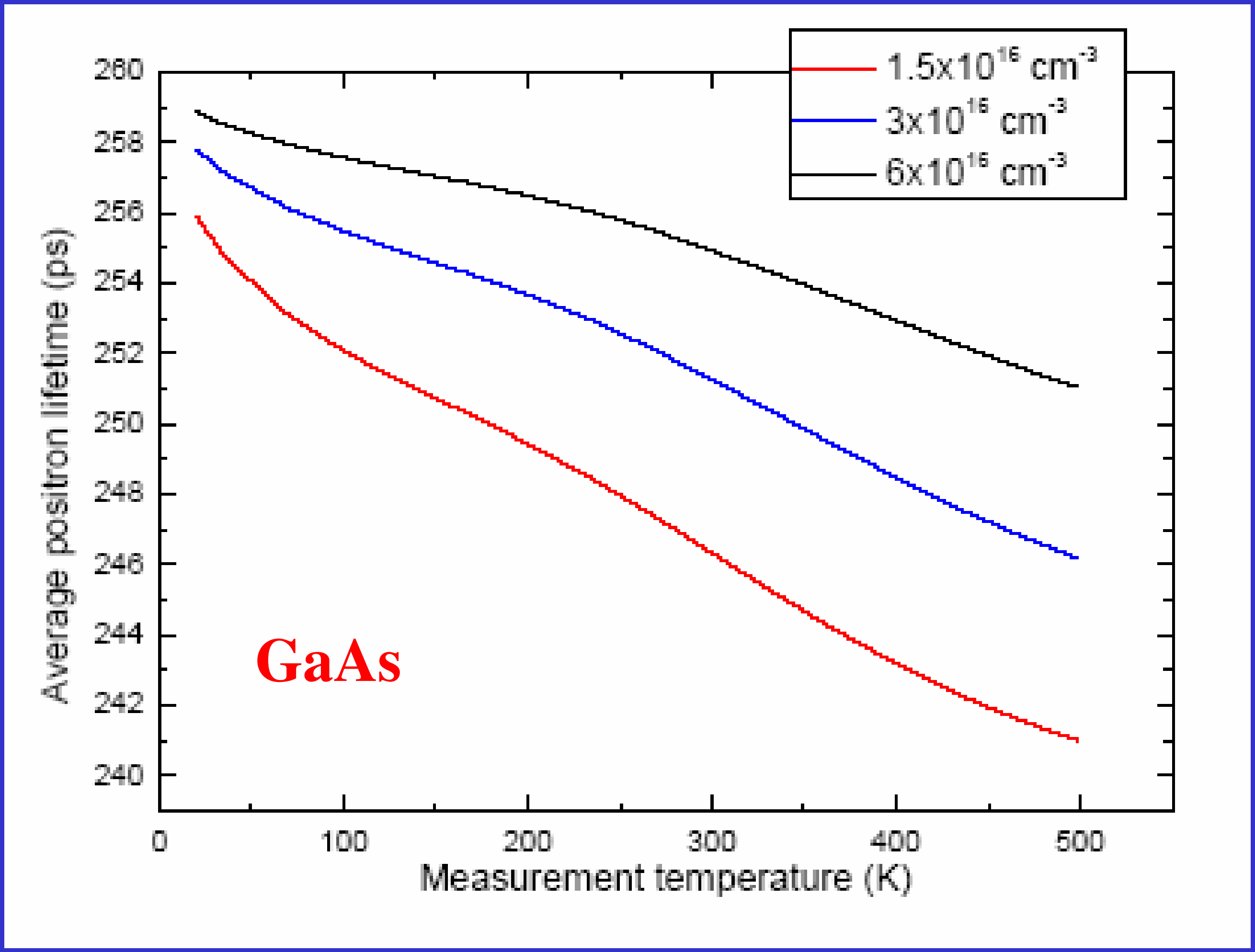
GaAs with B10 ctructure



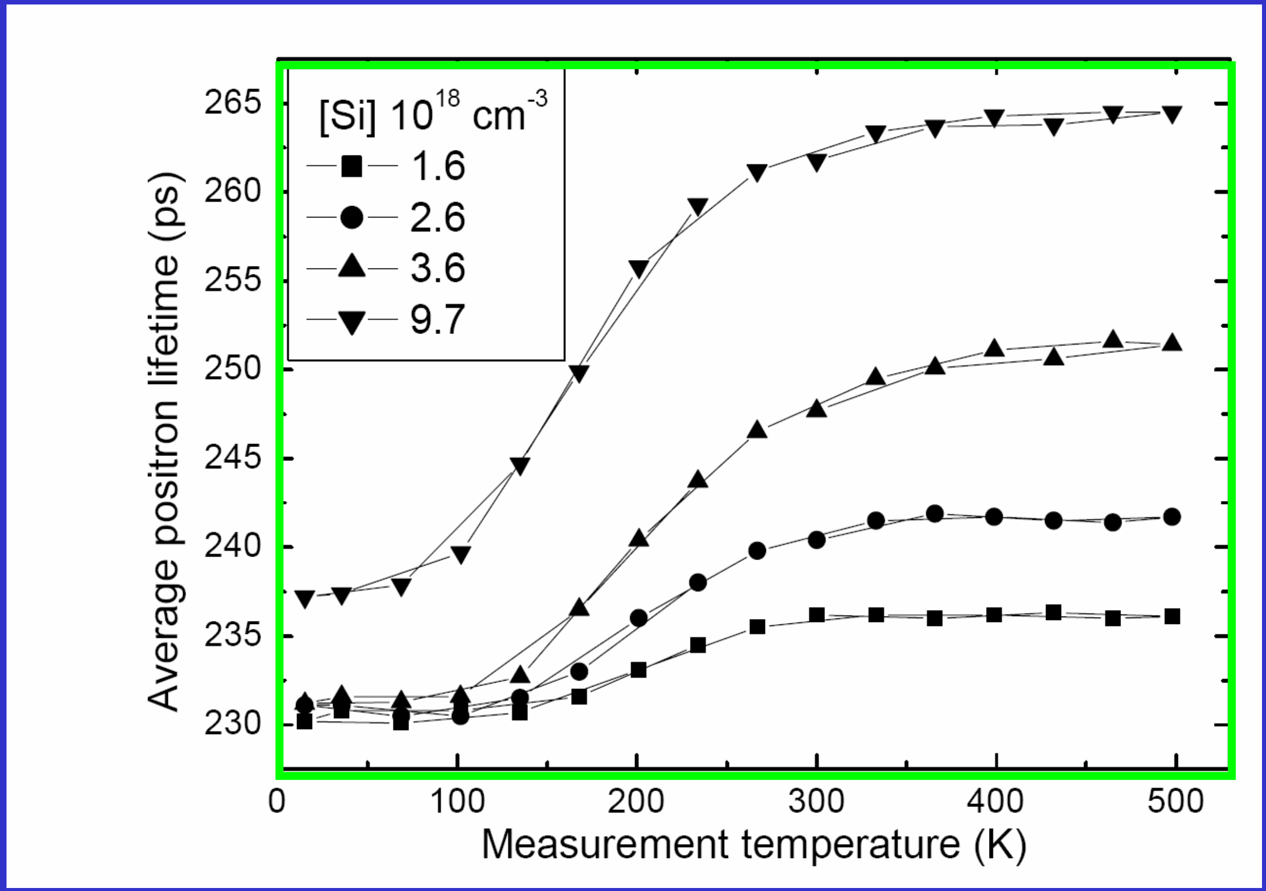
Positron density in a perfect GaAs lattice (110). The density value increases from the blue contours towards to the red ones. The positions of the Ga and As atoms are denoted by blue and red spheres, respectively.



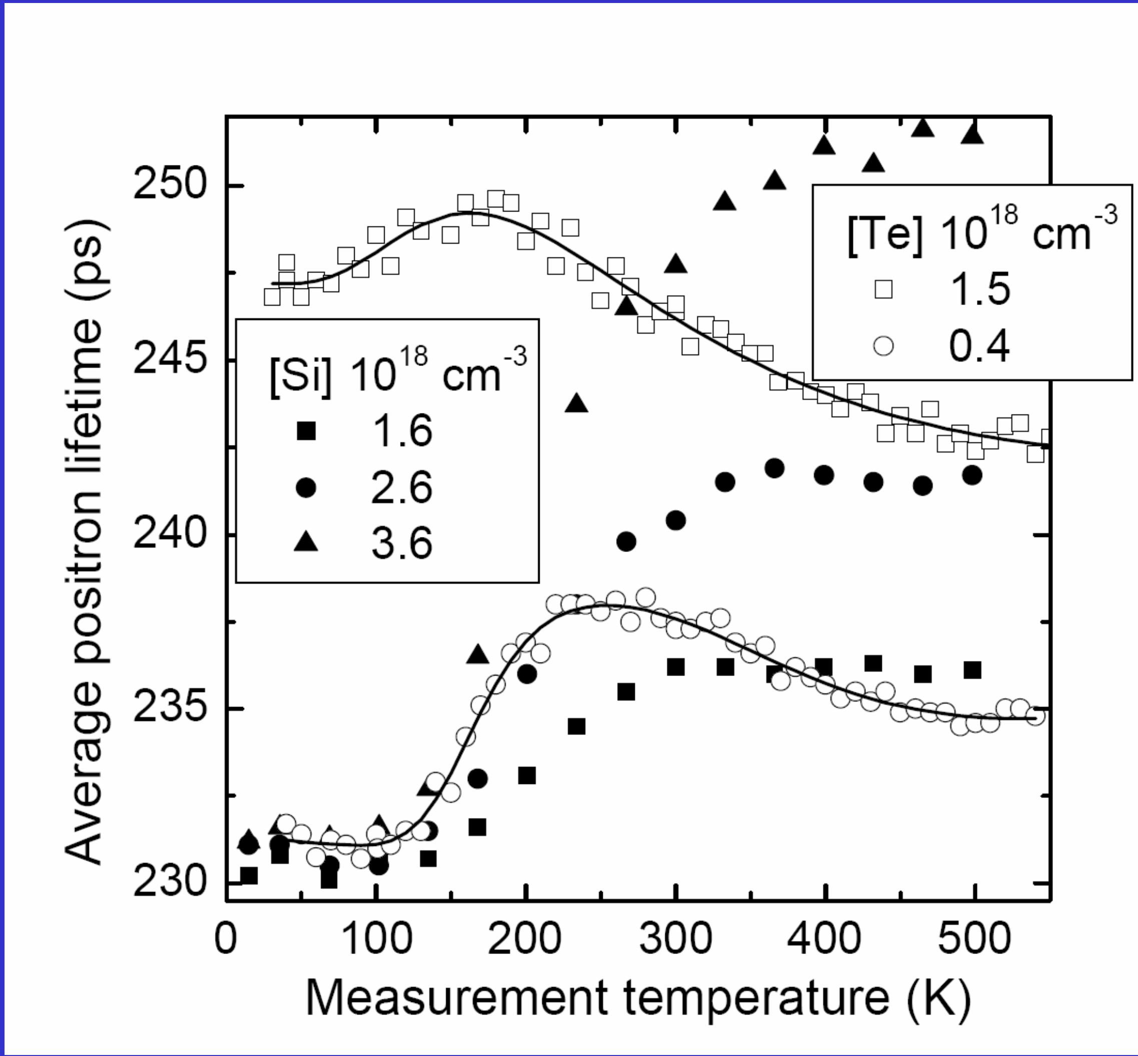
Positron density at an As vacancy in GaAs.



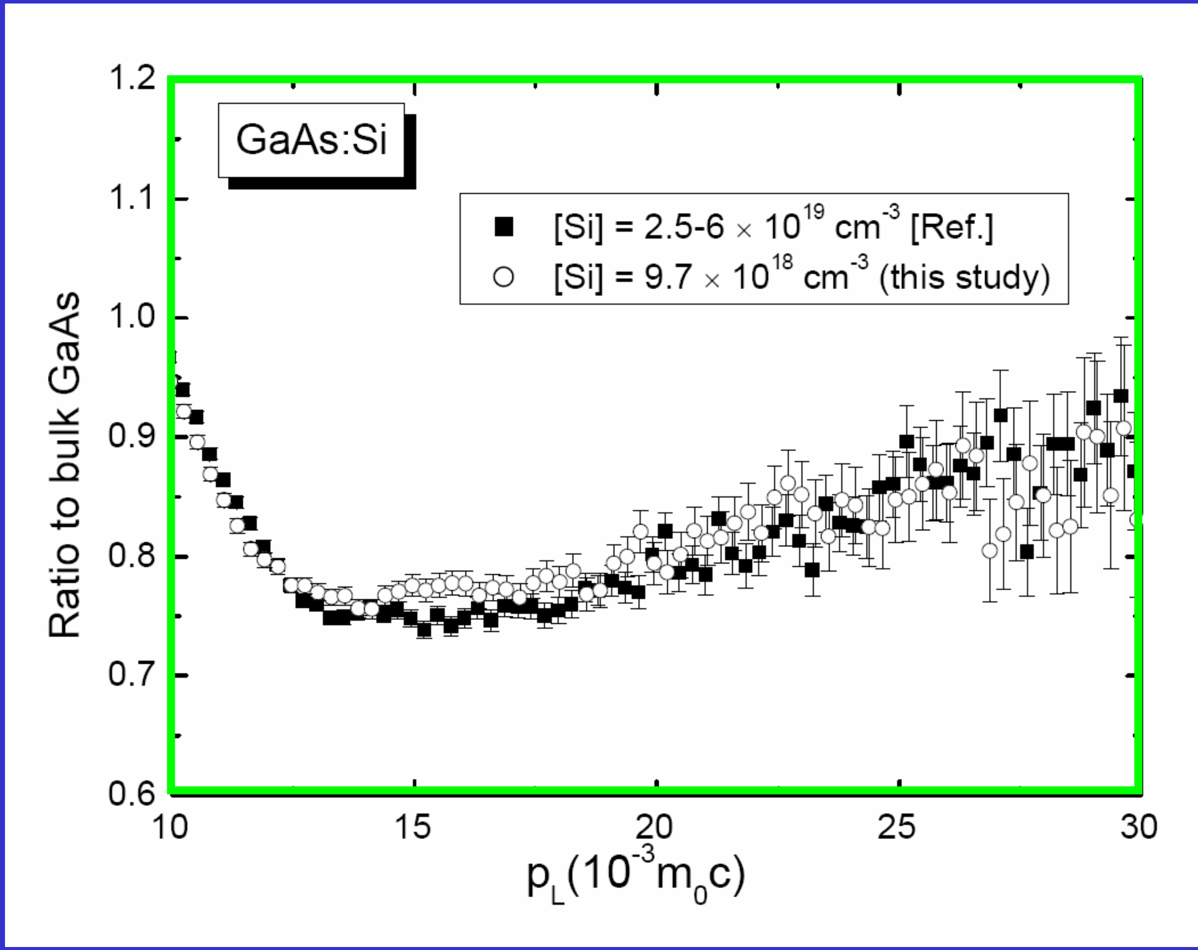
Average positron lifetime calculated as a function of temperature for different vacancy concentrations. One-defect trapping model was used. Trapping into a negative vacancy was assumed.



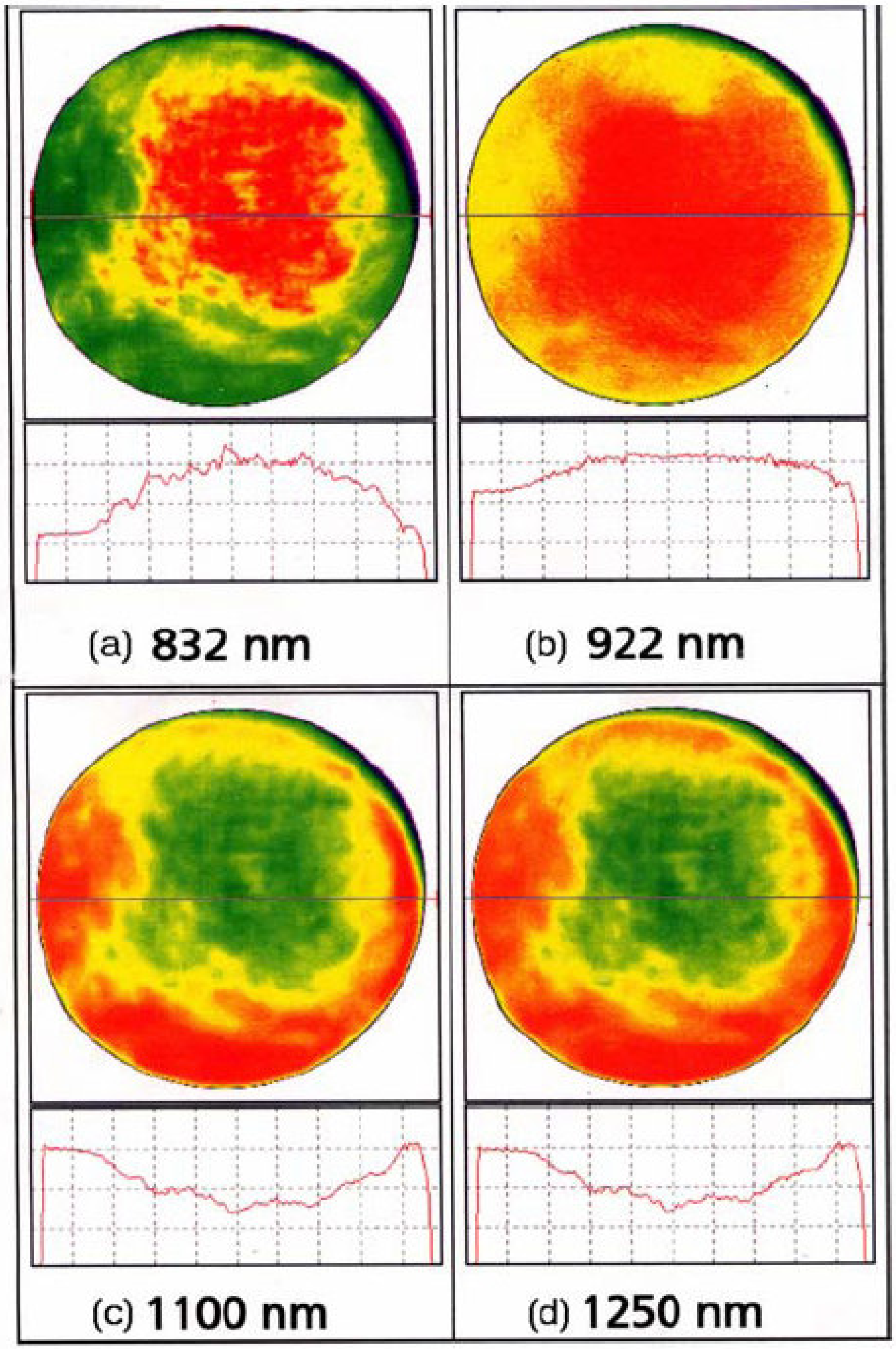
Average positron lifetime as a function of measurement temperature in highly Si-doped VGF-grown GaAs The concentrations of silicon dopants are indicated. The lines are to guide the eye.



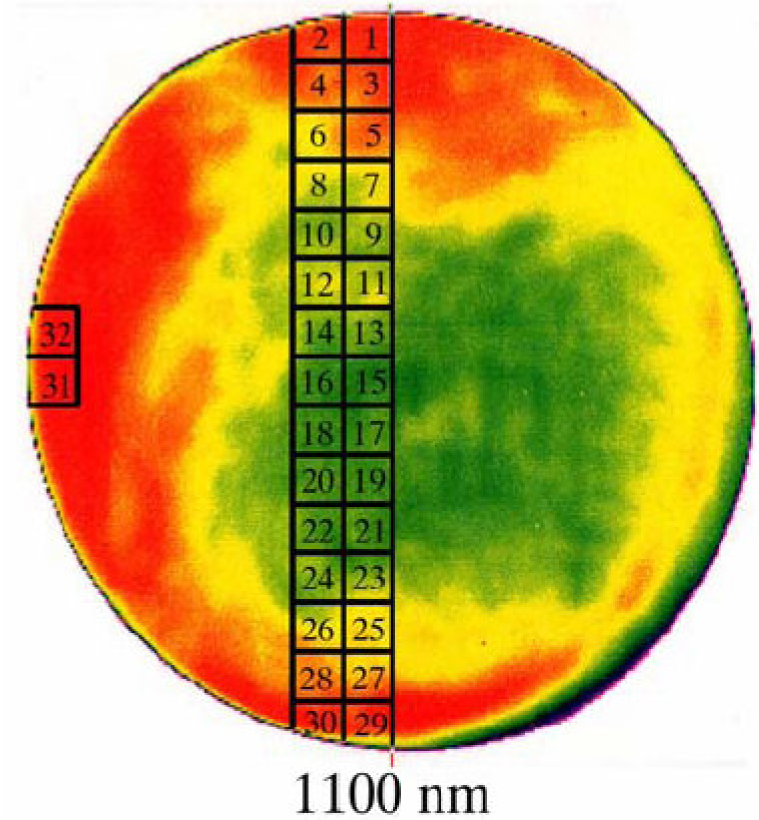
Average positron lifetime as a function of measurement temperature for as-grown Si- and Te-doped GaAs. The data for GaAs:Te are taken from (Gebauer et al. 2003).

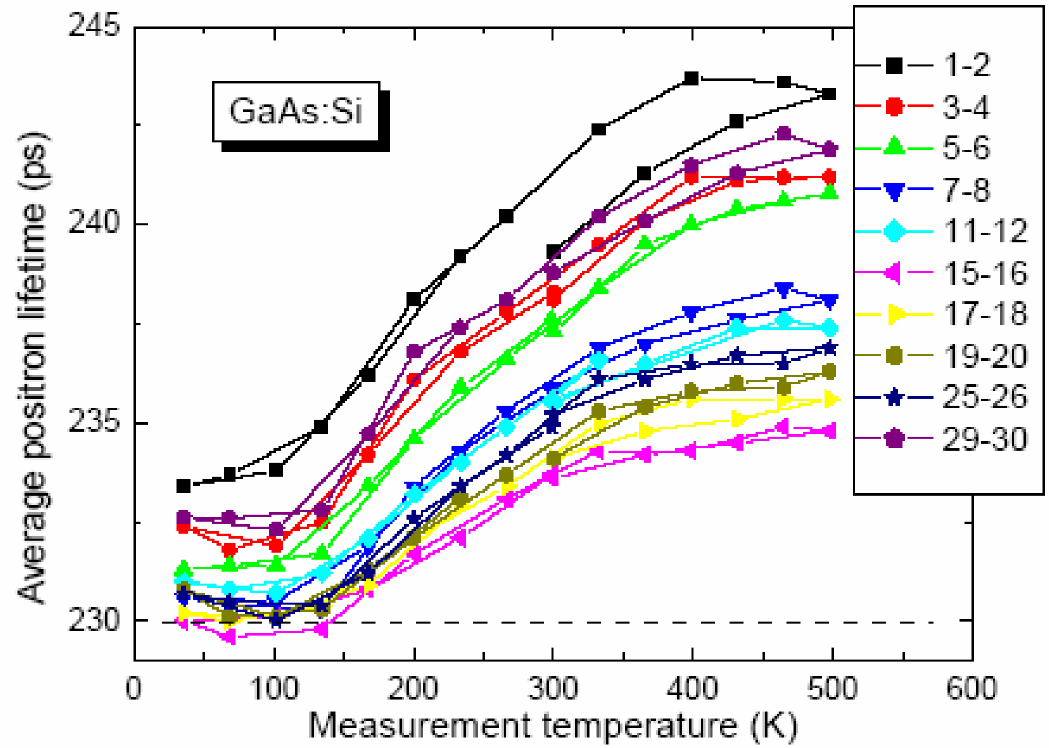


High momentum part of Doppler broadening peak normalized to the data of bulk GaAs. (■) corresponds to GaAs:Si studied by positron annihilation and STM spectroscopy (Gebauer et al. 1997); (○) this study.



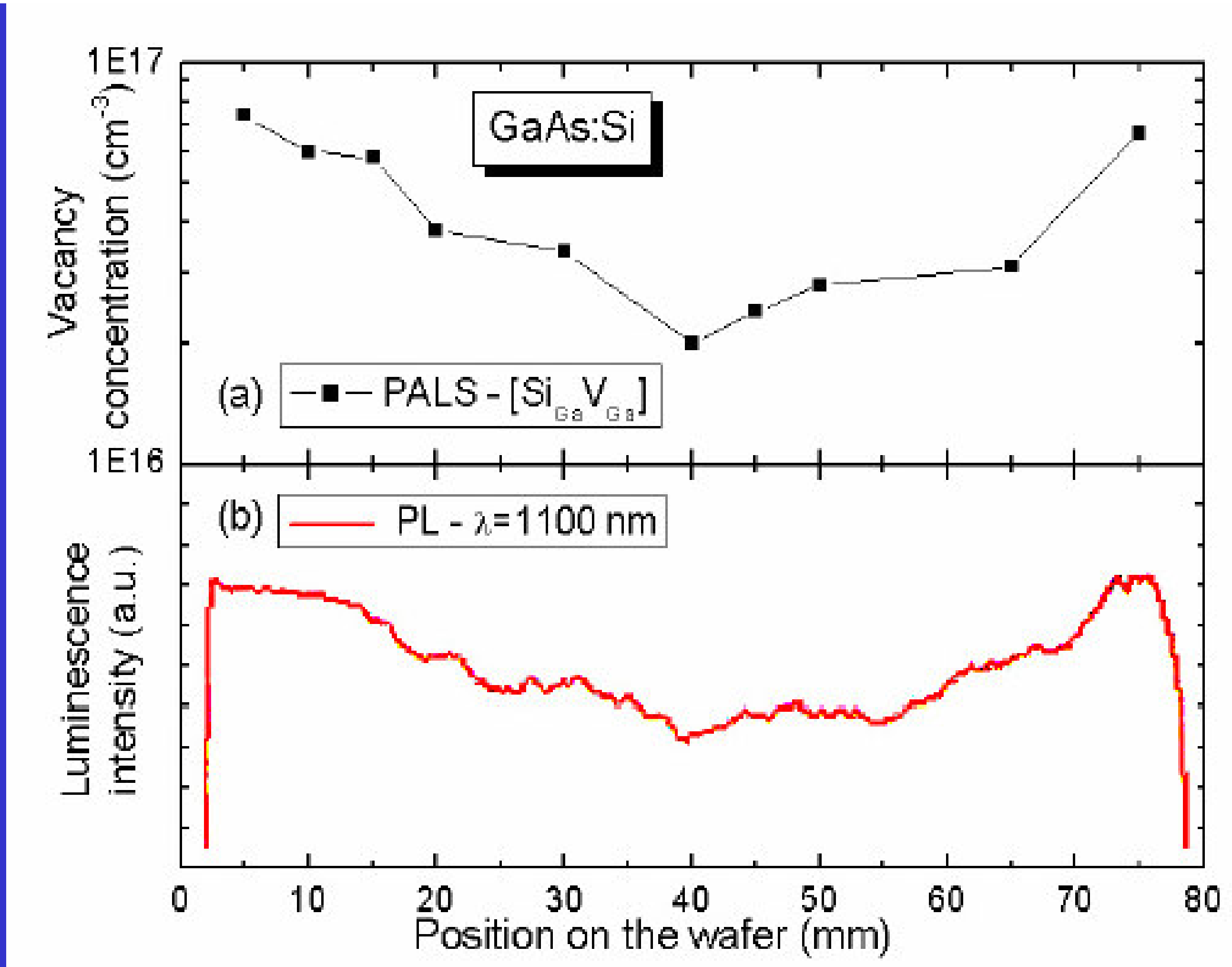
Photoluminescence topograms of wafer #1 measured for the four luminescence lines occurring in GaAs:Si.





Photoluminescence topogram image of wafer #1 recorded at the luminescence line of 1100 nm. Exact positions of the sample pares taken for PALS measurements are indicated. The area of each single sample equaled 5 ×5 mm.

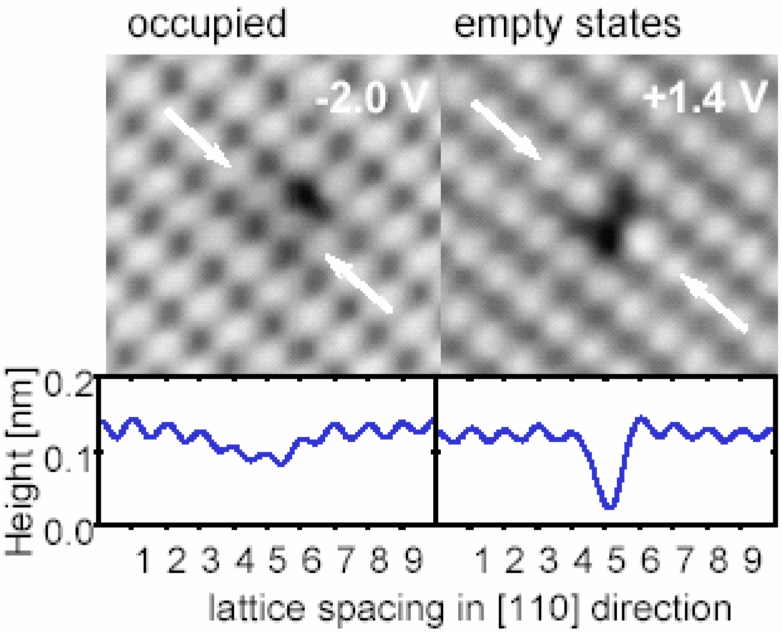
Average positron lifetime vs temperature measured across the wafer #1.

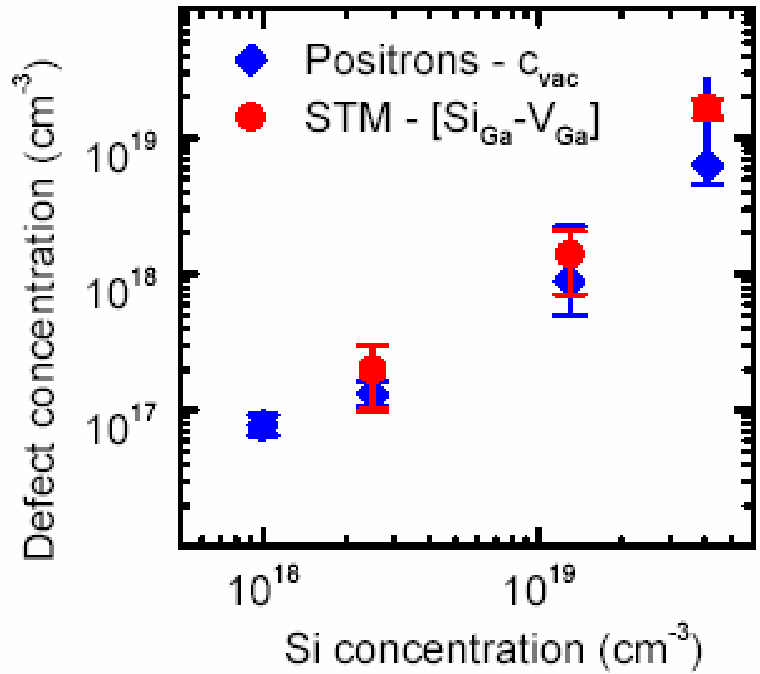


(a) The distribution of $Si_{Ga}V_{Ga}$ complexes across the wafer #1, as determined by PALS;

(b) intensity variation of the 1100 nm photoluminescence band, measured across wafer# 1.

Identification of V_{Ga}-Si_{Ga}-Complexes in GaAs:Si





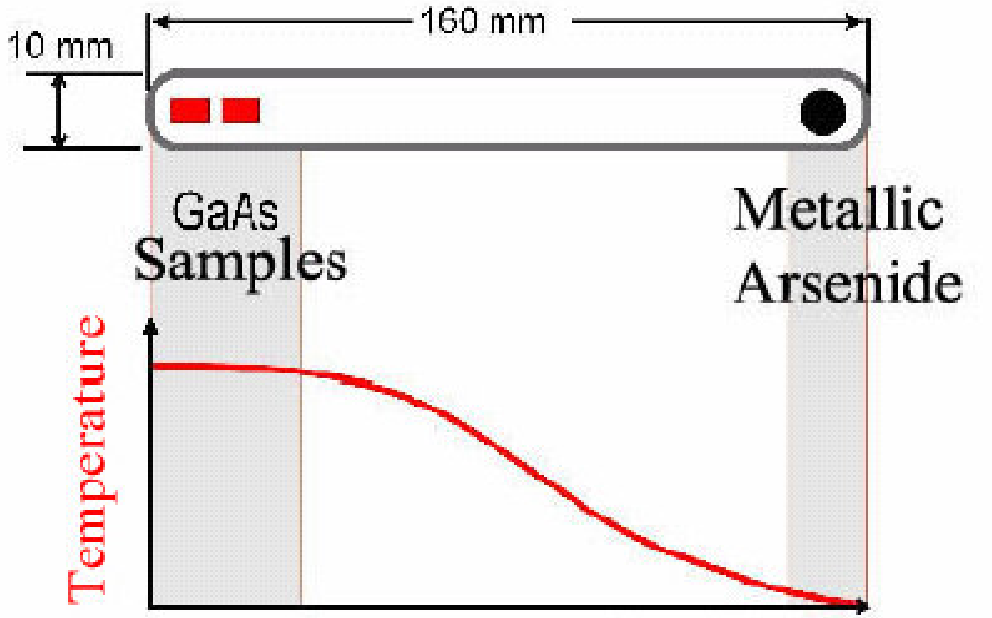
- Scanning tunneling microscopy at GaAs (110)-cleavages planes (by Ph. Ebert, Jülich)
- Defect complex identified as V_{Ga}-Si_{Ga}
- Quantification → Agreement

Mono-vacancies in GaAs:Si are V_{Ga}- Si_{Ga}-complexes

Gebauer et al., Phys. Rev. Lett. **78** (1997) 3334

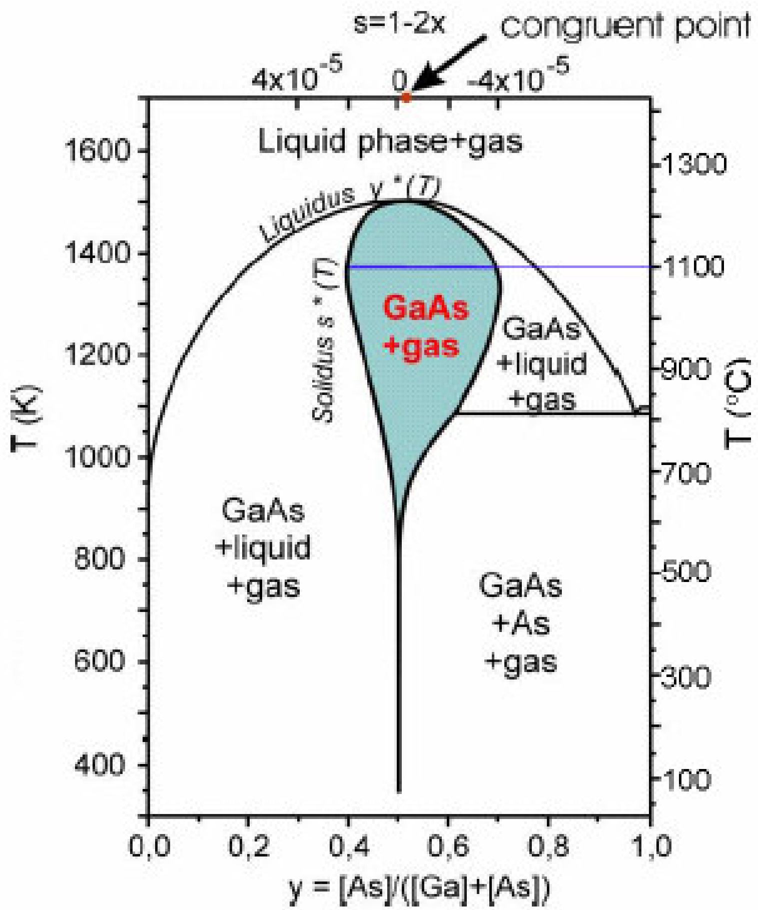
GaAs: annealing under defined As-partial pressure

- two-zone-furnace: Control of sample temperature **and** As partial pressure allows to navigate freely in phase diagram



T_{sample}: 1100° C

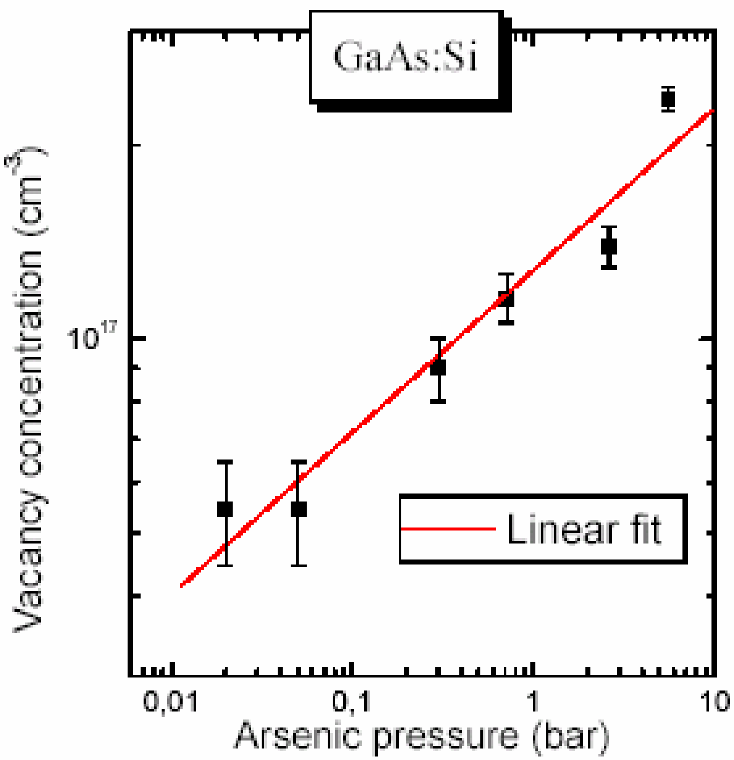
T_{As}: determines As-partial pressure



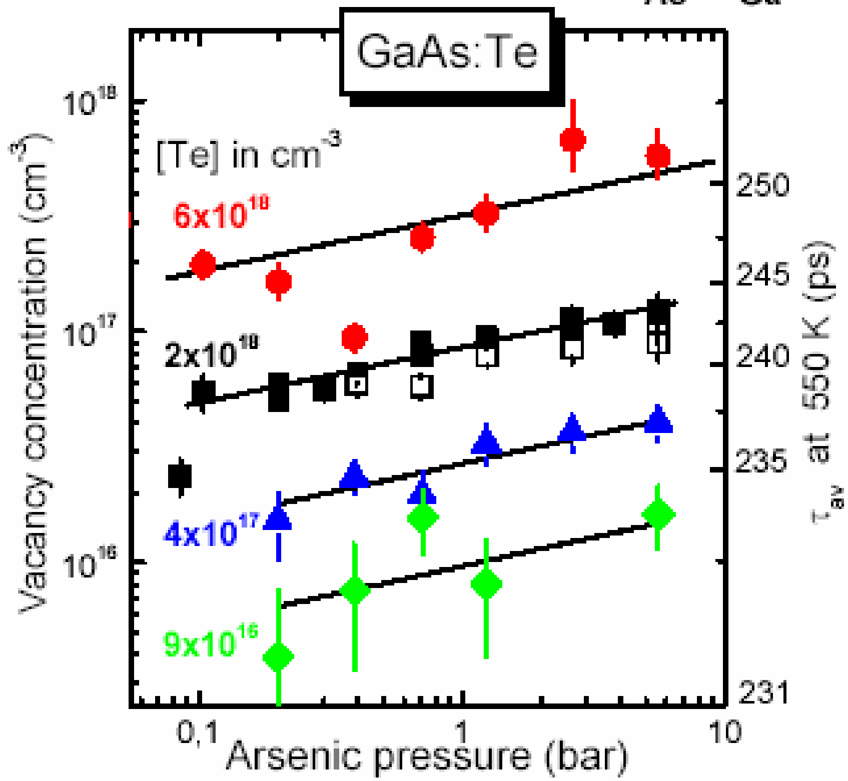
H. Wenzl et al., J. Cryst. Growth **109**, 191 (1991).

Experiments in n–GaAs

Si_{Ga}-V_{Ga}



Te_{As}-V_{Ga}



J. Gebauer et al., Physica B 273-274, 705 (1999)

Thermodynamic reaction:

$1/4\ As_4^{gas} \leftrightarrow As_{As} + V_{Ga}$

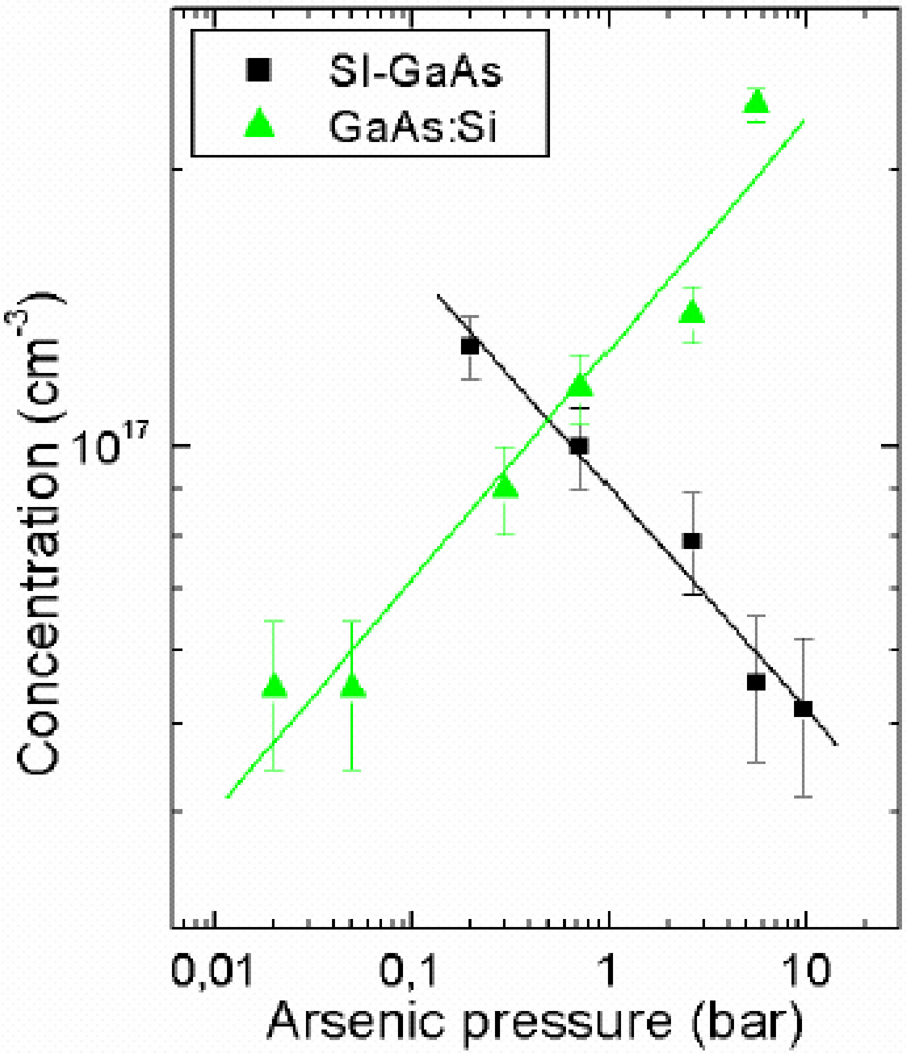
Mass action law:

$[V_{Ga}] = K_{VG} \times p_{As}^{1/4}$

Fit: $[V_{Ga}\text{-Dopant}] \sim p_{As}^{n}$

$\rightarrow n = 1/4$

Comparison of doped and undoped GaAs



Thermodynamic reaction:

$As_{As} \leftrightarrow V_{As} + 1/4As_4^{gas}$

Mass action law:

$[V_{As}] = K_{VAs} \times p_{As}^{-1/4}$

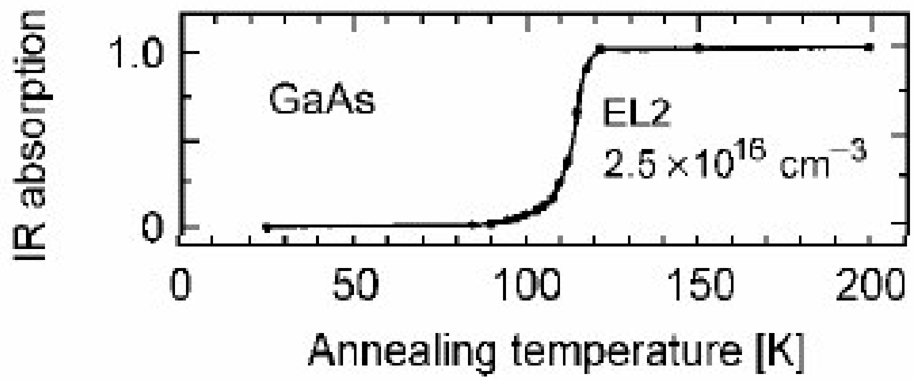
Fit: $[\text{V-complex}] \sim p_{As}^{n}$

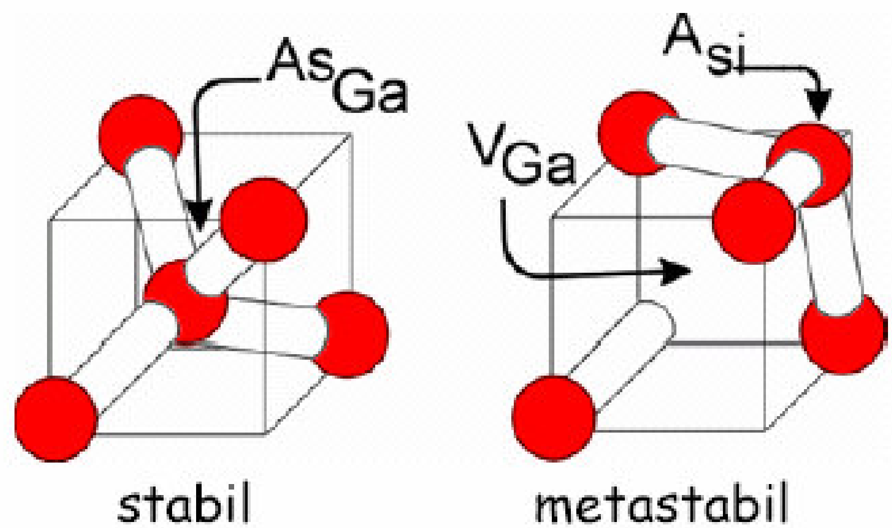
$\rightarrow n = -1/4$

As vacancy

The Nature of EL2 defect in GaAs

- one of the most frequently studied crystal lattice defects at all
- responsible for semi-insulating properties of GaAs: large technological importance
- is deep donor, compensates shallow acceptors, e.g. C^- impurities
- defect shows metastable state after illumination at low temperatures
- IR-absorption of defect disappears during illumination at T < 100 K
- ground state recovers during annealing at about 110 K
- many structural models proposed Dabrowski, Scheffler and Chadi, Chang (1988): simple As_{Ga}-antisite defect responsible
- must show a metastable structural change

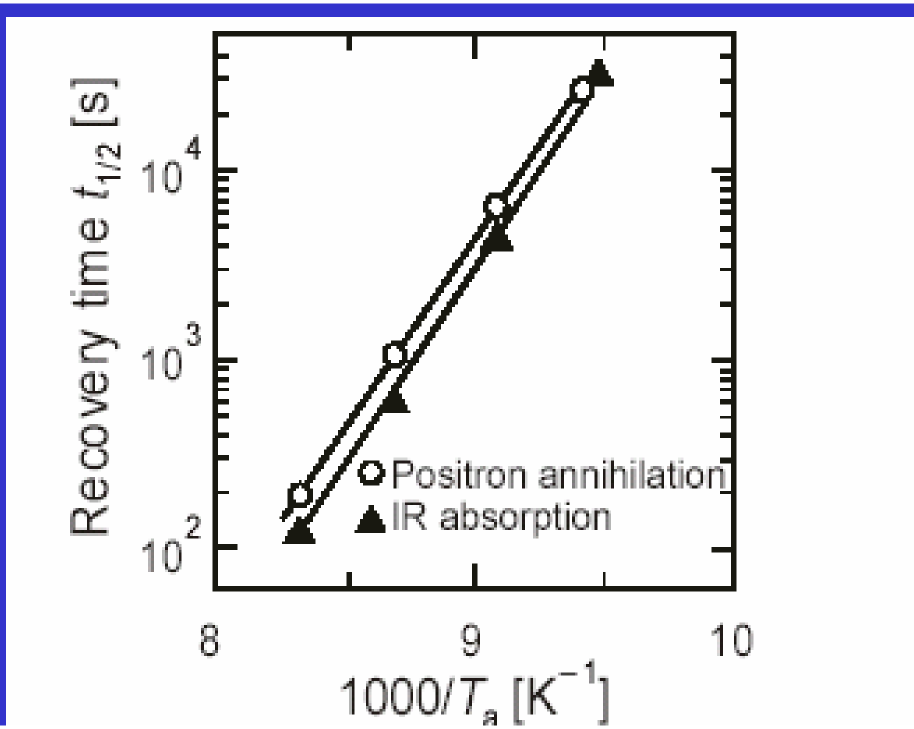


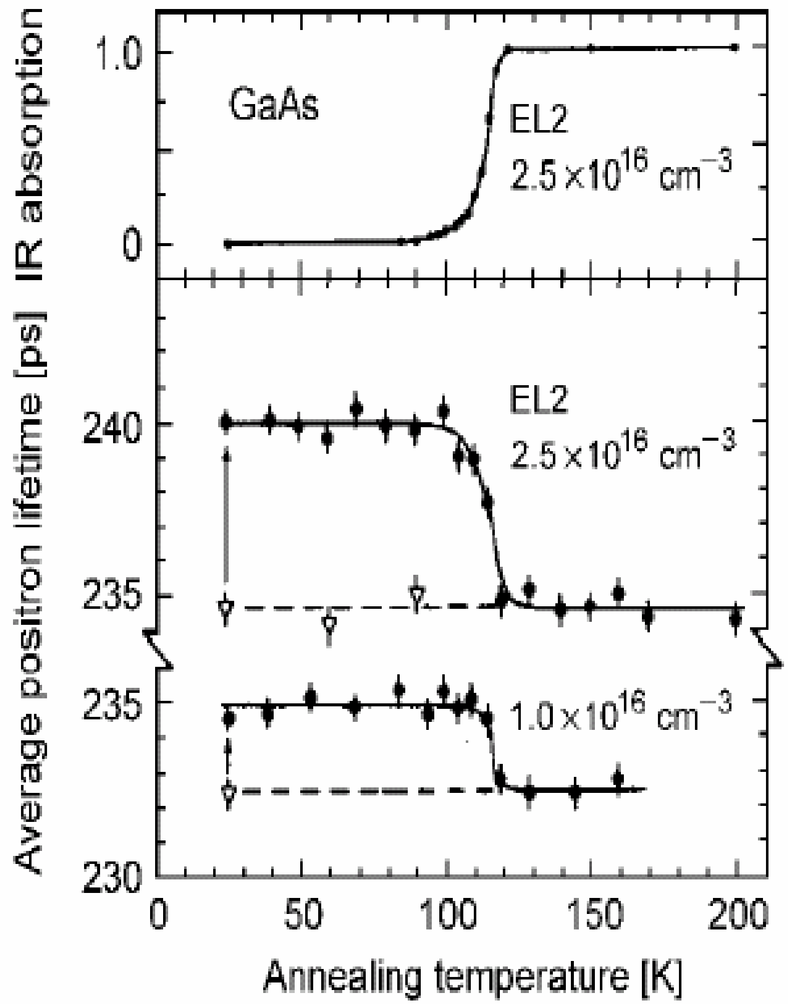


(Dabrowski 1988, Chadi 1988)

The Nature of EL2 defect in GaAs

- in metastable state at low temperature: Ga vacancy
- should disappear during annealing at about 110 K
- confirmed by positron lifetime measurements
- kinetics of recovery of ground state is identical for IR- und positron experiment: $E_A = (0.37 \pm 0.02)$ eV
- evidence of the vacancy in metastable state confirms the proposed structural model





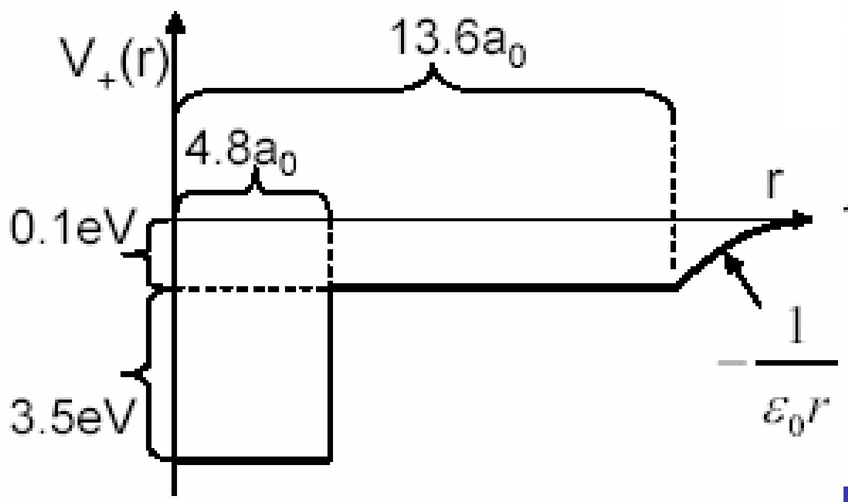
Krause et al., Phys. Rev. Lett. **65** (1990) 3329

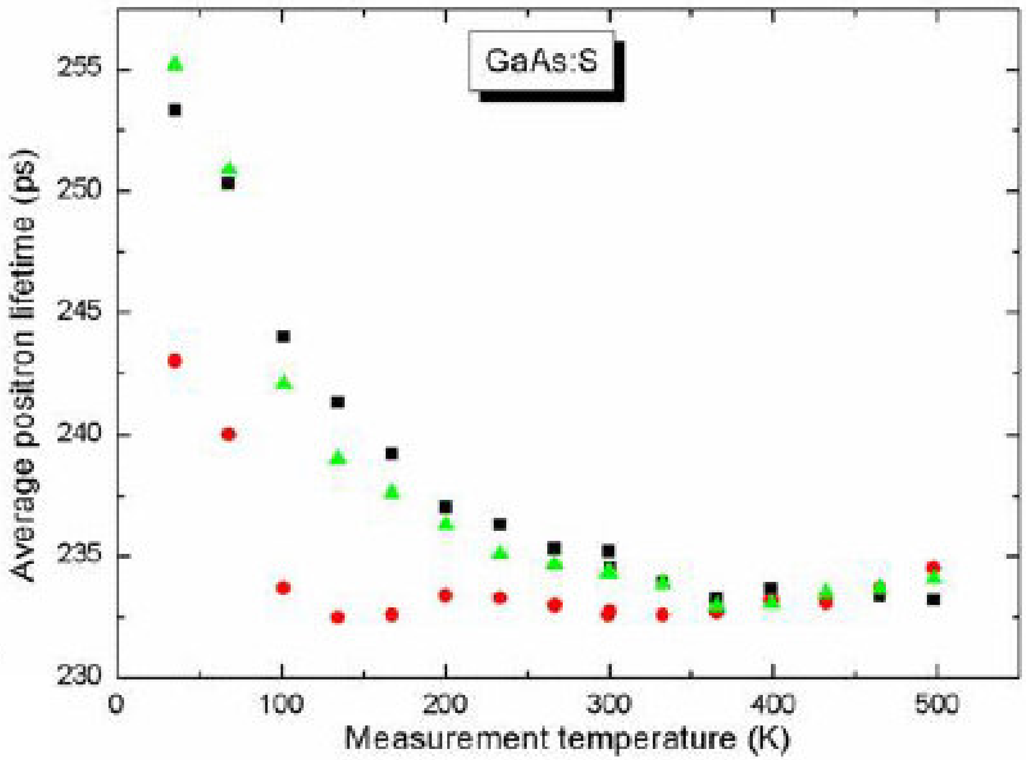
Temperature dependence of positron trapping

- Compensation in GaAs:S

• formation of S_{As}-V_{Ga} complex

• increase of τ_{av} to low T is due to the trapping into negative shallow Rydberg potential of the defect

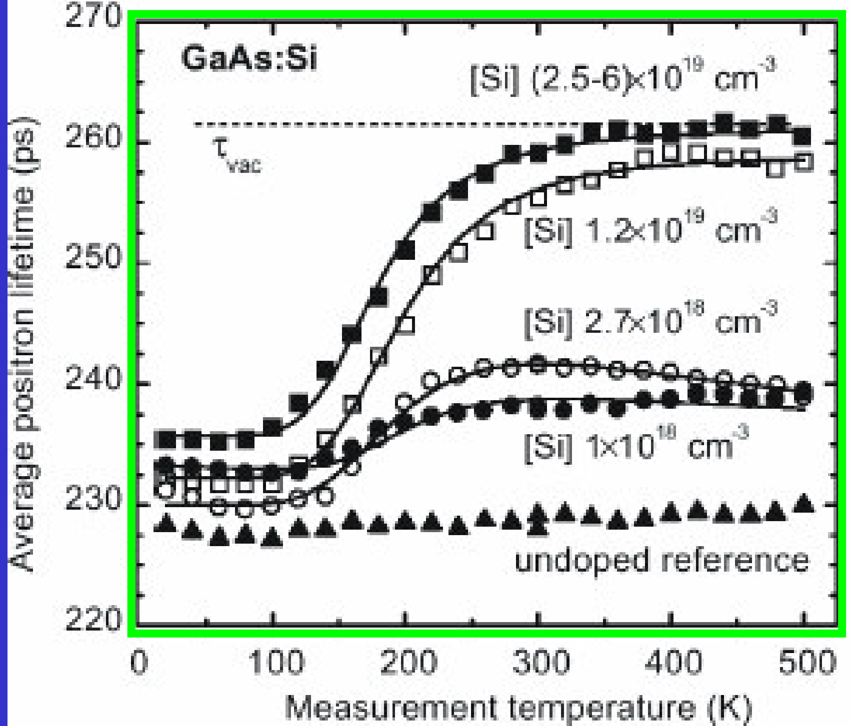


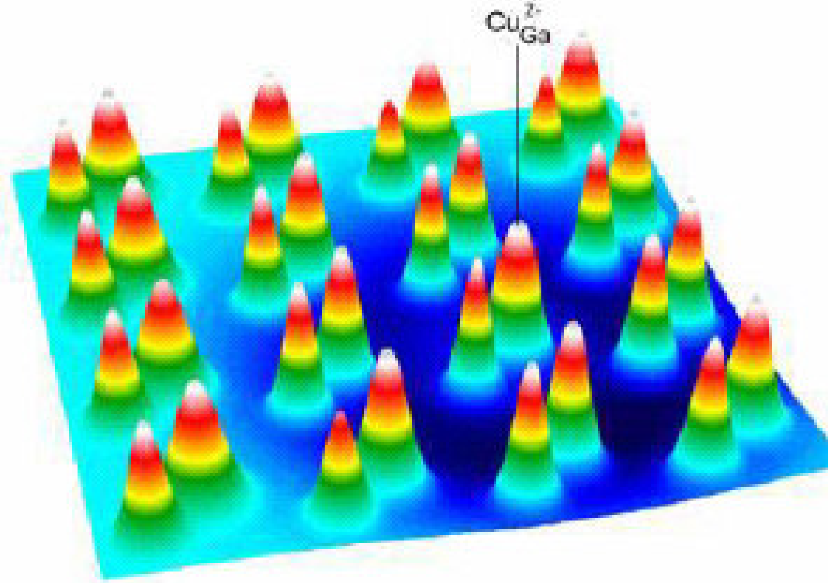


• observed S_{As}-V_{Ga} complex is *negatively* charged

Positron trapping – shallow traps

- negative ions are also positron trapping centers due to small negative Coulomb potential





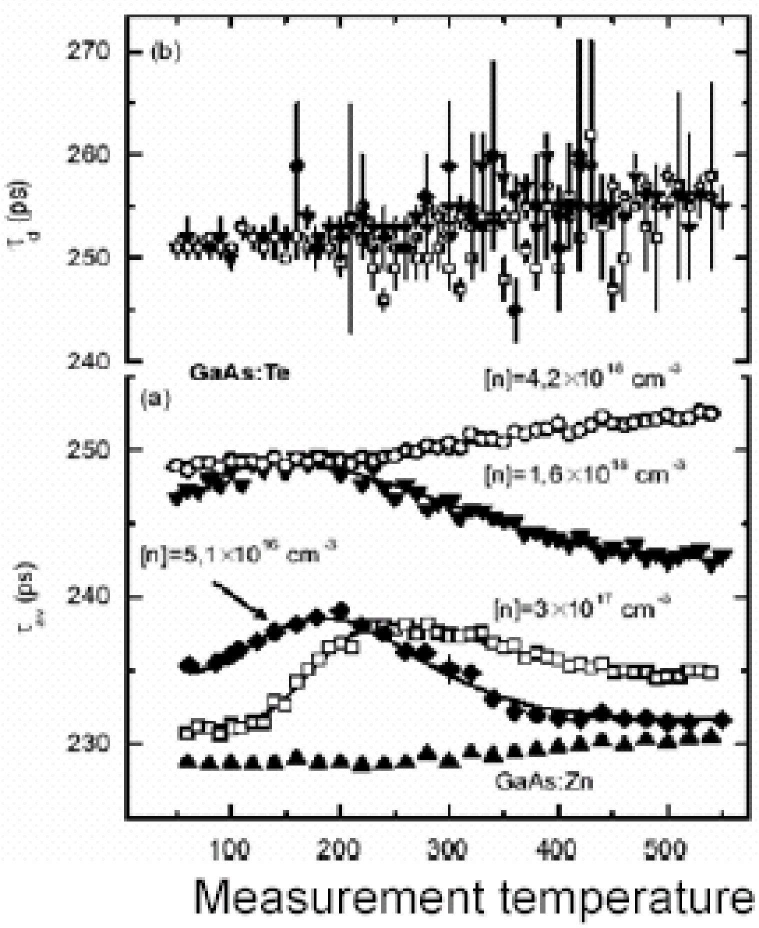
- term "shallow" relates to the positron bindi energy (few meV).
- therefore the trapping is significant at low temperatures only
- the electron density is not reduced:

$$\tau_{st} = \tau_b$$

PRL, V78,17, J.Gebauer

Nature of vacancy complexes in Si and Te doped GaAs

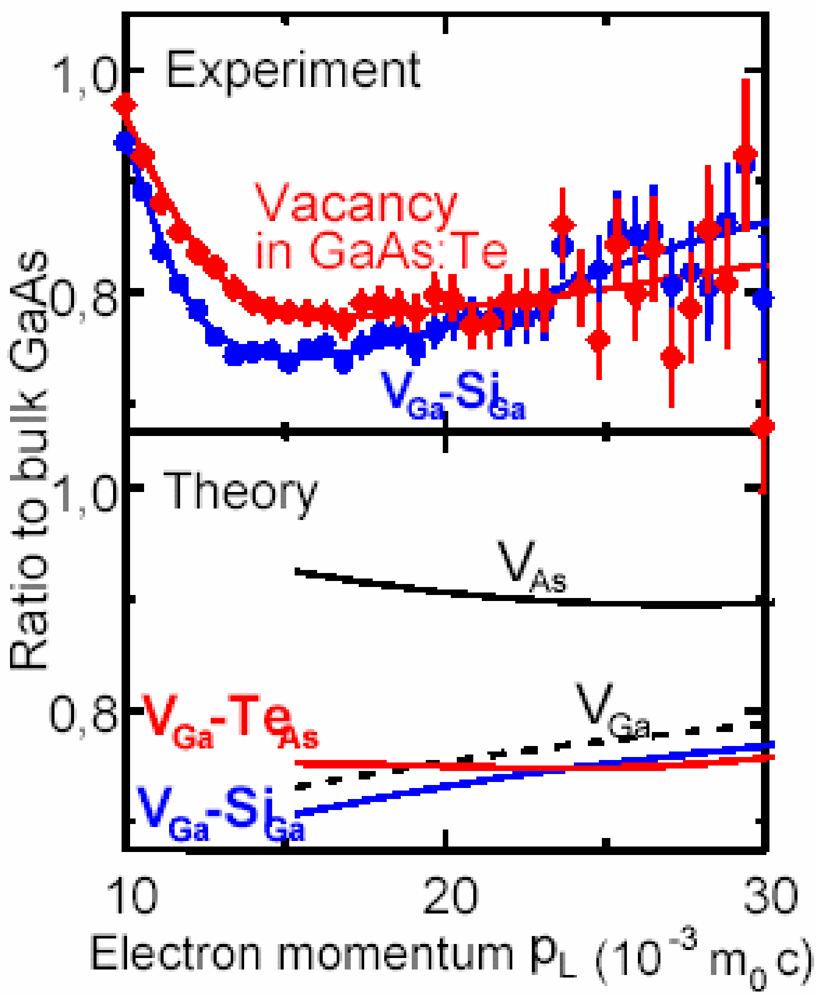
- positron lifetime spectroscopy



V_{Ga}-Si_{Ga} in GaAs:Si τ_2 = 260 ps

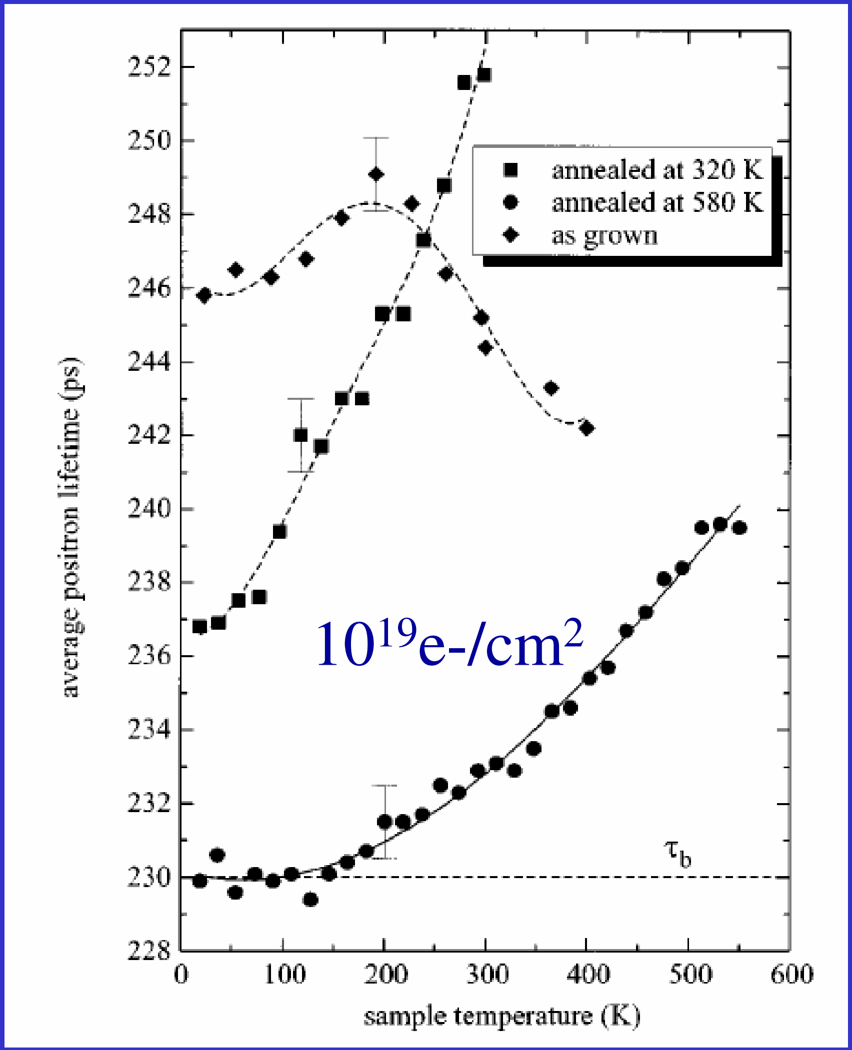
V_{Ga}-Te_{As} in GaAs:Te τ_2 = 253 ps

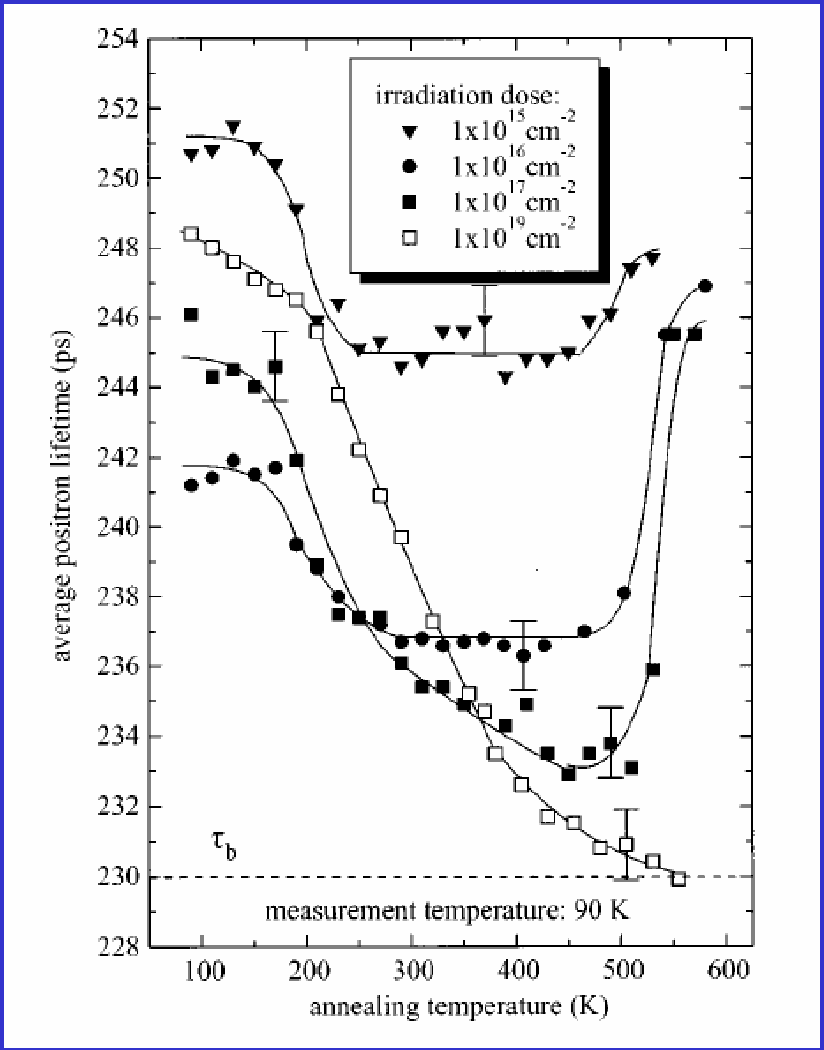
- Doppler coincidence



J. Gebauer et al., Phys. Rev. B ***60****, 1464 (1999)*

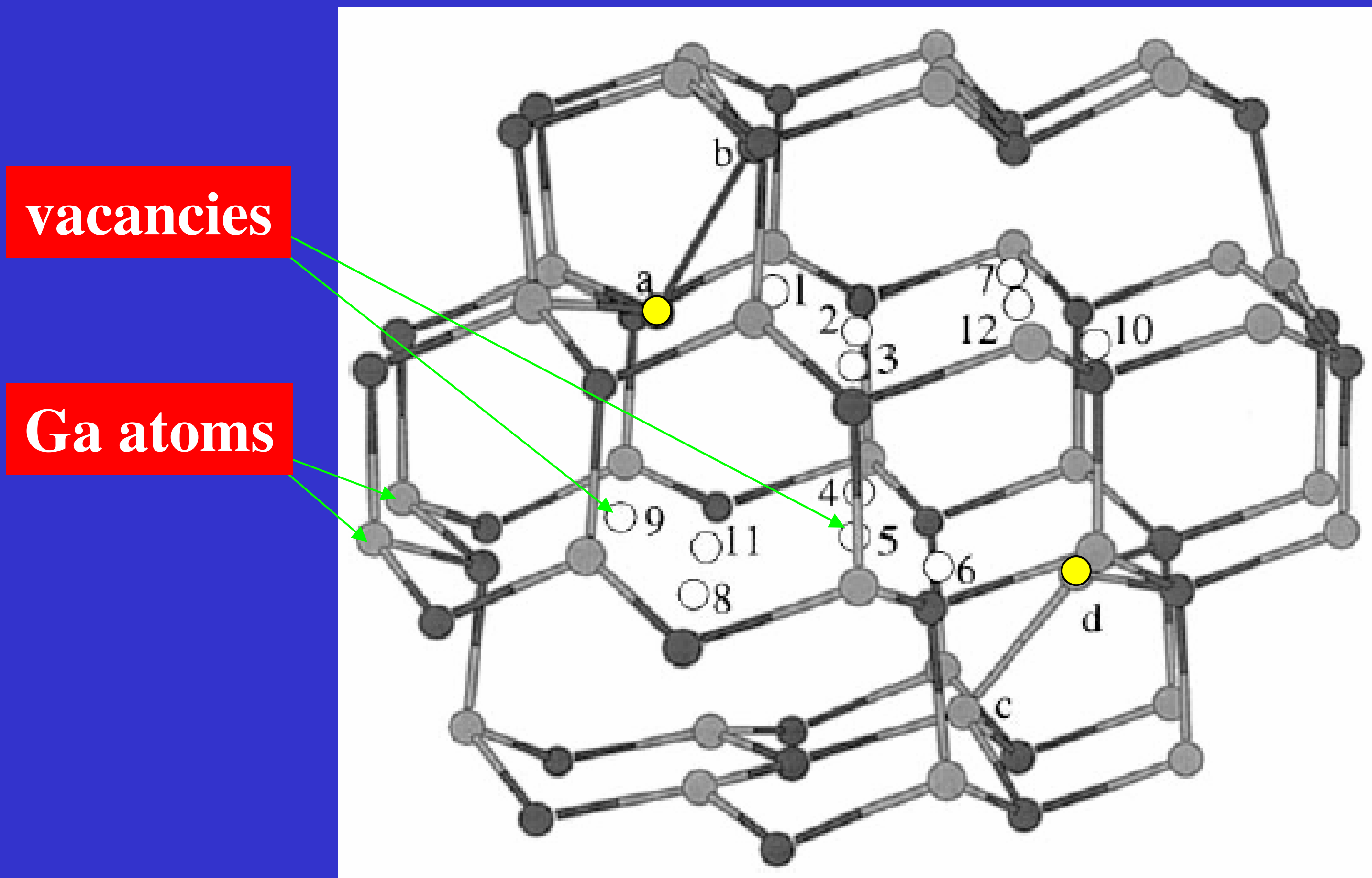
Electron-irradiation GaAs:Te



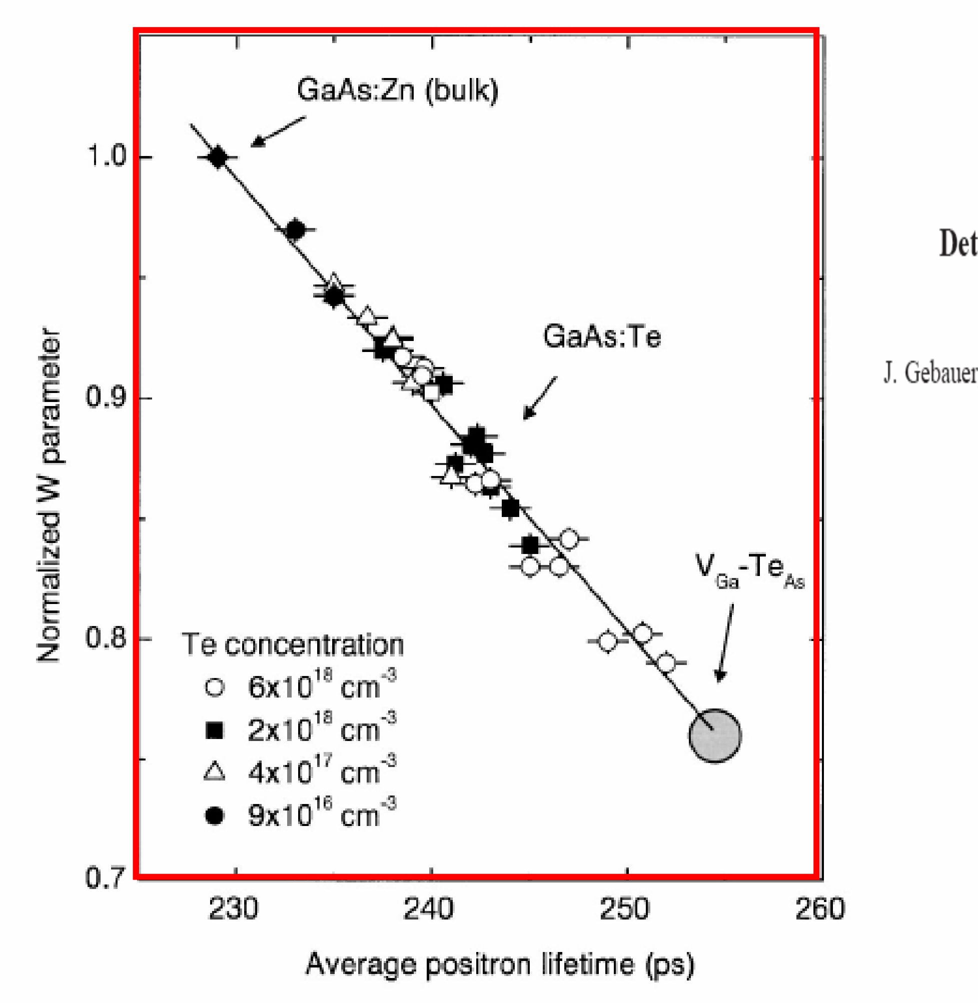


高剂量辐照

低剂量辐照



Structure in GaAs consisting of 12 vacancies.
Atoms a and d are removed to get V14.



PHYSICAL REVIEW B **67**, 235207 (2003)

Determination of the Gibbs free energy of formation of Ga vacancies in GaAs by positron annihilation

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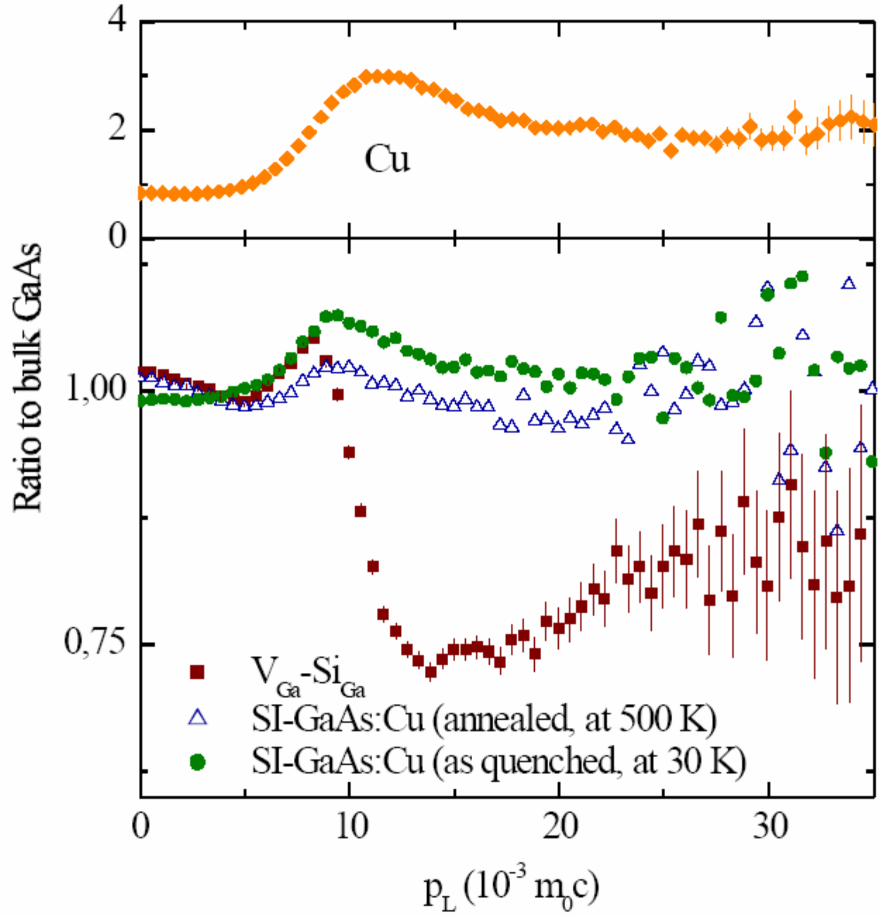
Average positron lifetime vs *W* parameter for differently high-Te-doped GaAs. The *W* parameter is normalized to the value found in GaAs:Zn. All samples were annealed at 1100 ° C . The solid line is a linear fit to the data, showing that all samples contain the same defect type. The defect is identified to be a $V_{Ga\text{-}}Te_{As}$ complex.

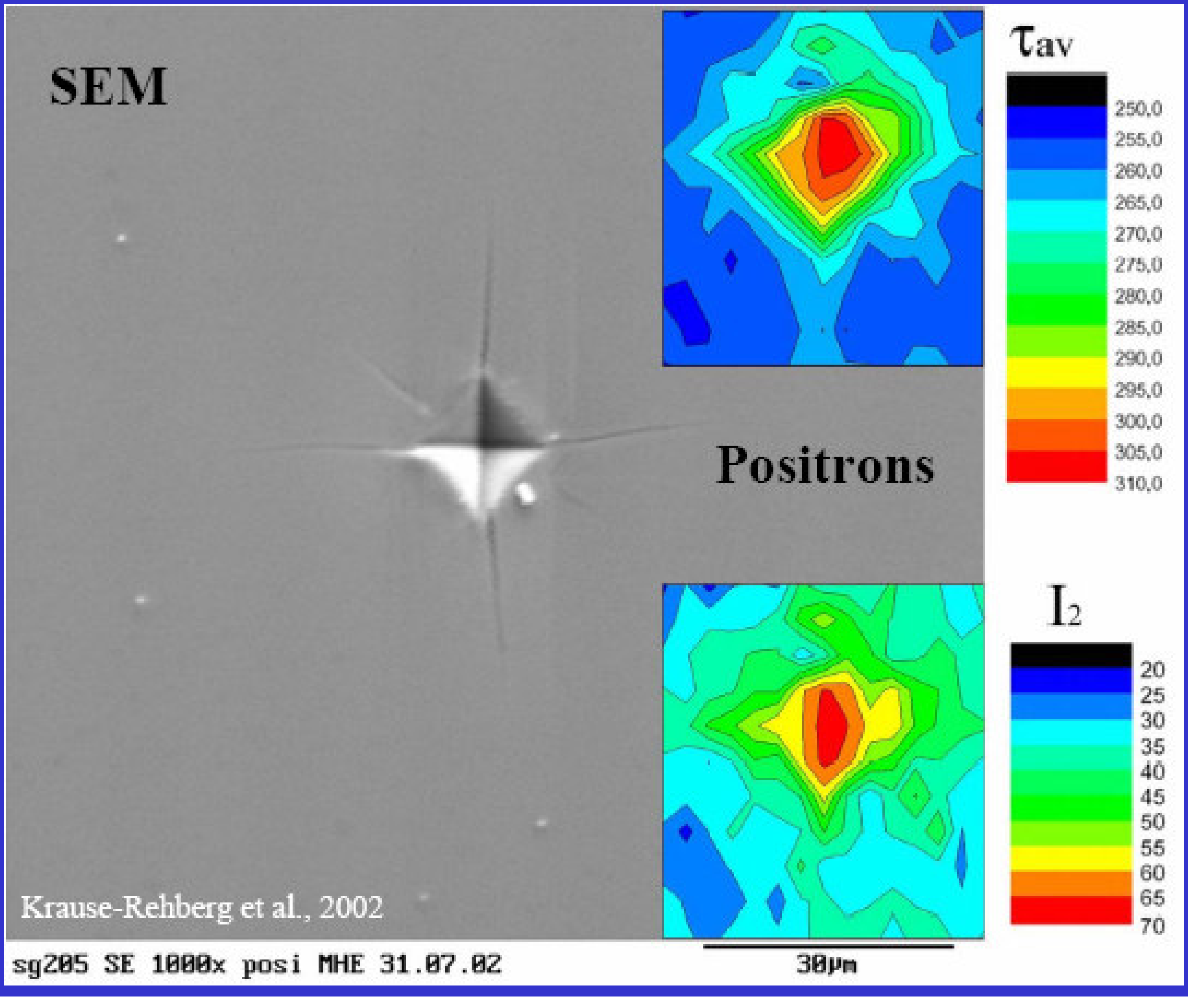
Cu diffusion in GaAs



High-momentum part of the positron annihilation momentum distribution, normalized by taking the ratio to a GaAs:Zn reference

Microhardness indentation in GaAs

Comparison of SEM and Munich Positron Scanning Microscope



The lifetime of bulk and vacancy in GaAs

	Positron annihilation characteristics		Dissolution
	Lifetime [ps]	τ_d/τ_b	temperature [K]
Bulk lifetime	228 to 232[a,b,c,d]	—	—
As monovacancies	295[e,f]	1.28	750[b]
	255 to 295[b,g]	1.11 to 1.28	
Ga monovacancies	255[h]	1.11	300[s]
	260 to 270[i]	1.13 to 1.17	
$V_{Ga}Te_{As}$	251 to 257[j,k]	1.09 to 1.12	> 1000[k]
$V_{Ga}Si_{Ga}$	262[d]	1.14	
$V_{As}Cr_{Ga}$	250 to 260[l,e]	1.09 to 1.13	
EL2*	255[m]	1.11	
	245[n]		
Dislocation-bound	300 to 320[o]	1.30 to 1.39	
vacancies	270[p]	1.17	
Voids	460 to 500[q]	2 to 2.17	700 to 900[q]
	590[r]	2.56	

τ_d is the defect-related positron lifetime, τ_b the positron lifetime in the defect-free bulk.

Appl. Phys. A 66, 599–614 (1998)

Review of defect investigations by means of positron annihilation in II – VI compound semiconductors

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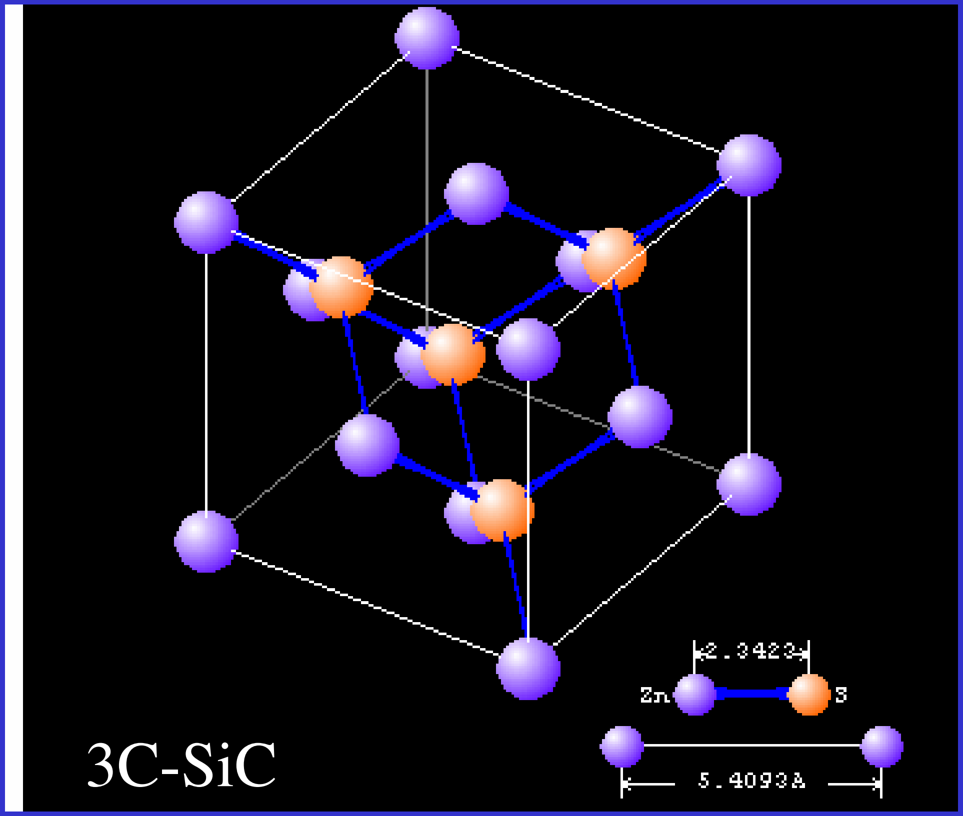
Received: 19 November 1997/Accepted: 20 November 1997

Material	Bulk lifetime/ps		Cation-vacancy lifetime /ps		Anion-vacancy lifetime /ps	
	Cal.	Exp.	Cal.	Exp.	Cal.	Exp.
CdTe	286	291 [104] 281 [68] 283 ± 1 [44] 285 ± 1 [45, 46] 280 ± 1 [52]	298	320 ± 5 [45, 46] 330 ± 15 [44, 52, 68]	312	–
HgTe	274	274 [68]	285	–	300	–
$Hg_{0.8}Cd_{0.2}Te$	–	274 [68] 286 [69] 275 [54] 278 [70] 282 [97]	–	309 [69] 305 [54, 70] 319 [97]	–	325 ± 5 [93]
ZnO	–	169 ± 2 [88] 183 ± 4 [86, 87]	–	255 ± 16 [86, 87] 211 ± 6 [102]	–	–
ZnS	225	230 [78, 80]	240	290 [80]	237	–
ZnSe	240	240 [79]	253	–	260	–
ZnTe	260	266 [78]	266	–	297	–

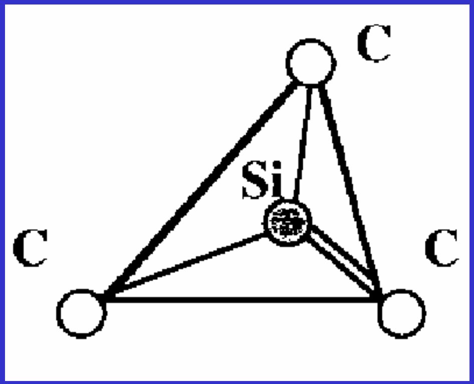
Positron in SiC

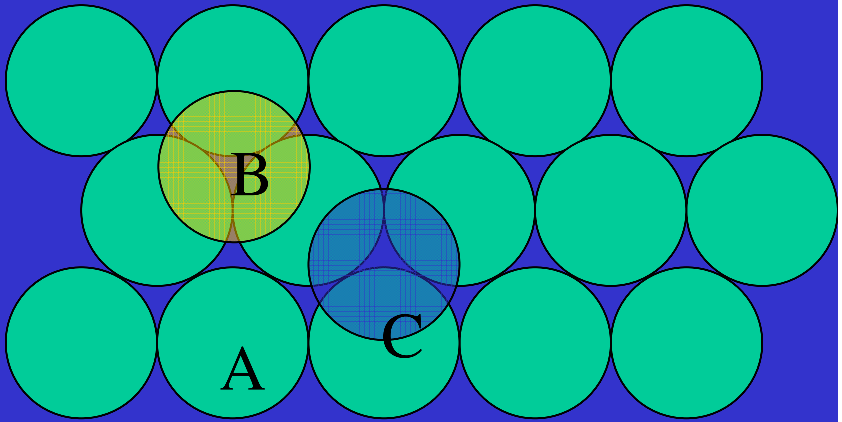


物理量	3C-SiC	4H-SiC	6H-SiC	GaAs	Si	特　性
宽带隙(eV)	2.3	3.26	3.03	1.43	1.12	高温及短波蓝光发射。SiC：最高工作温度近 1000K；Si：不能超过 500K。
击穿电场 (V/cm, 100V 下操作)	4.0×10^6	2.2×10^6	2.4×10^6	3.0×10^5	2.5×10^5	比 GaAs 或 Si 高约一个量级。制作高电压、高功率器件。
热导率 (W/cm.K@RT)	4.9	4.9	4.9	0.5	1.5	有利于提高集成密度,减少冷却系统，使器件更小型化，提高器件的运行功率。
饱和电子漂移率 (cm/sec, E@2×10^5V/cm)	2.5×10^7	2.0×10^7	2.0×10^7	1×10^7	1×10^7	有利于高频使用，对提高逻辑器件的运算速率有重要意义。
键结合能	~5eV					抗腐蚀、辐射，高机械强度和化学稳定。

SiC Atomic structure

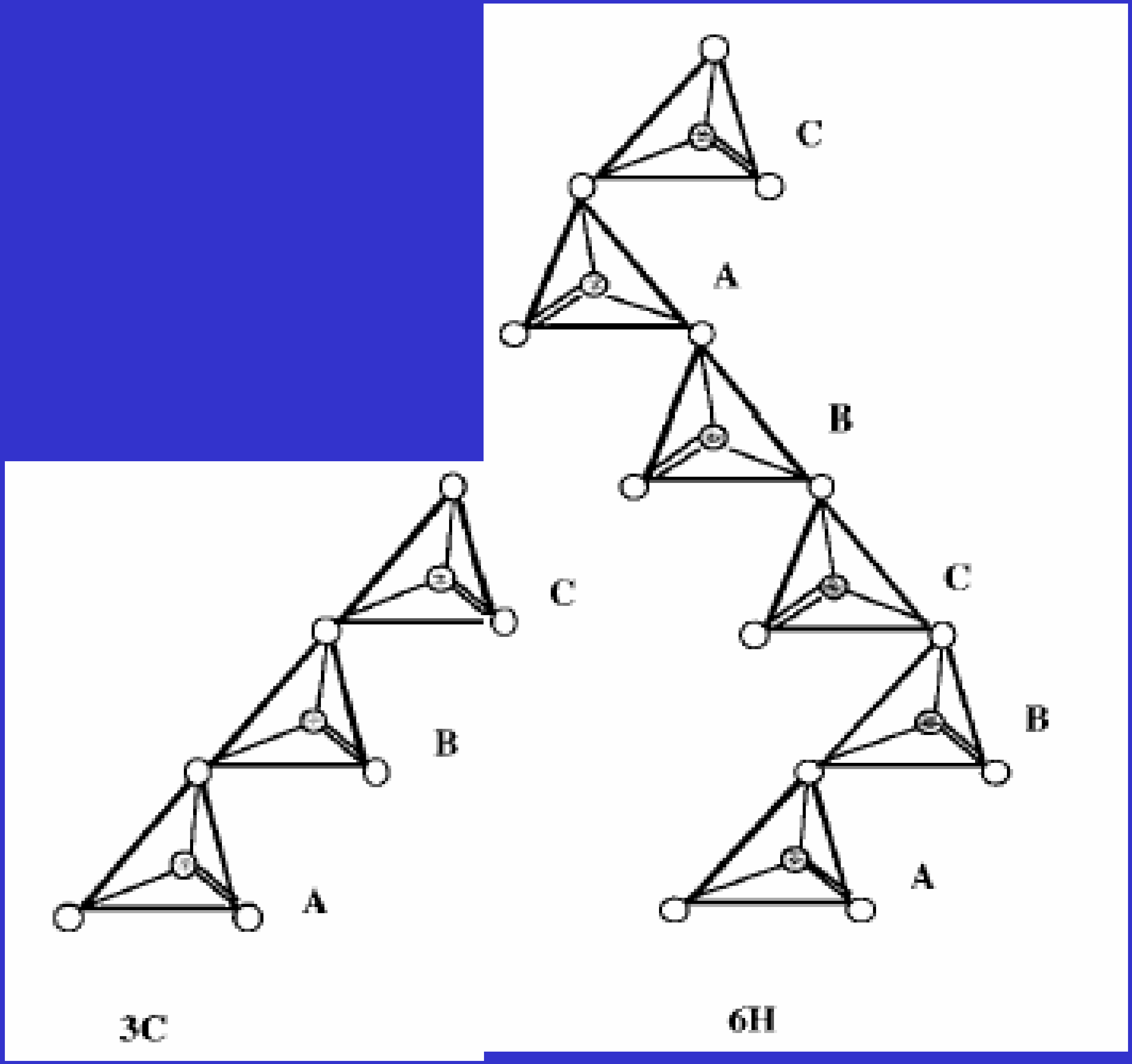
- Silicon Carbide has more than 200 polytype
- Polytype refers to a family of material which has common stoichiometric composition but not common crystal structure
- SiC are made by arrangement of covalently bonded tetrahedral Si and C atoms





Possible stacking sequence for SiC tetrahedral structure

Edited from C. Kittle, 1996 and Mehregany et al., 2000



Stacking order of 3C-SiC and 6H-SiC

3 commonly used polytypes

3C-SiC:

Cubic structure, Zinc-blend, ABCABC….

4H-SiC:

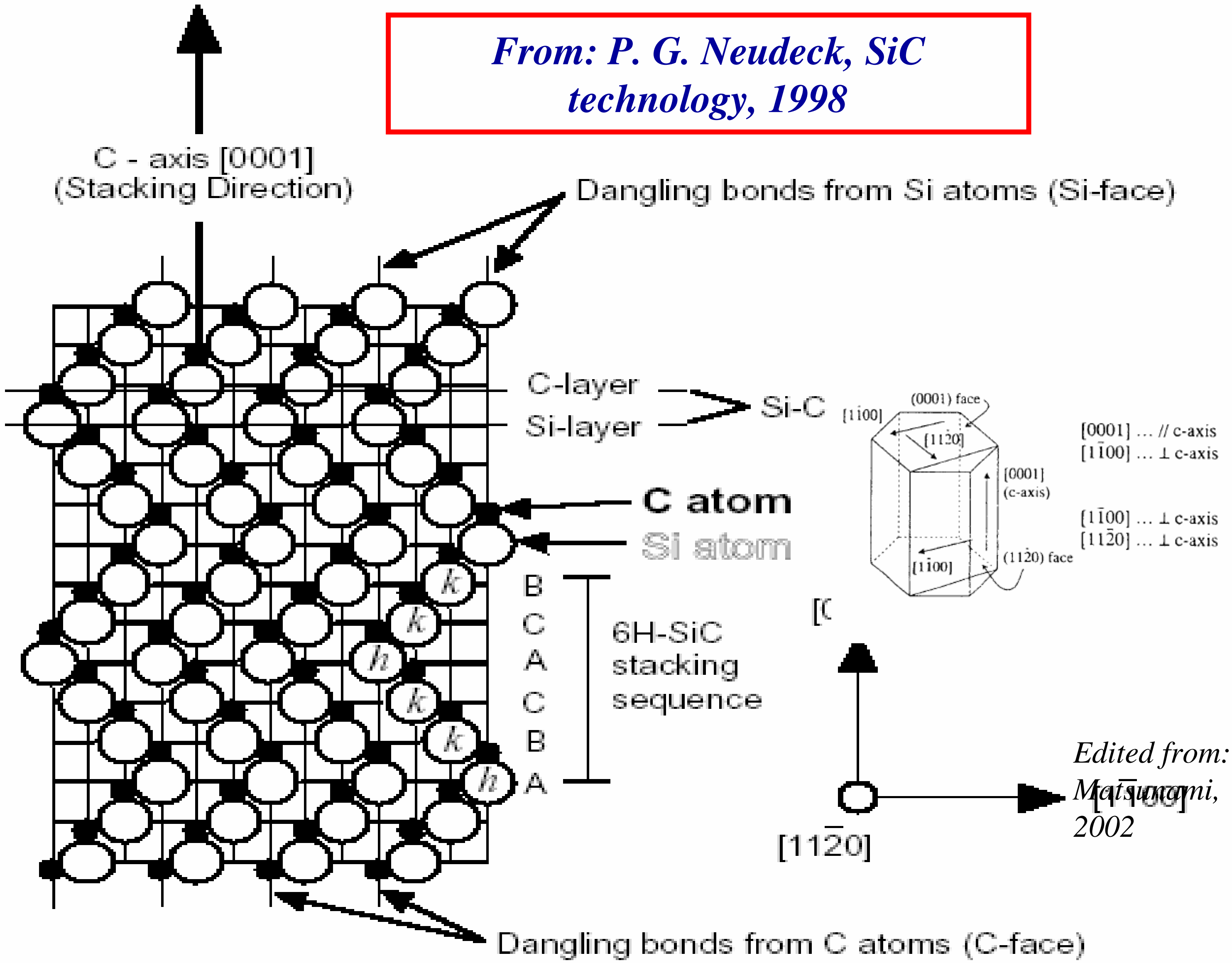
Hexagonal close packed, ABCBABCB…

6H-SiC:

Hexagonal close packed, ABCACBABCAC…

Atomic structure of 6H-SiC

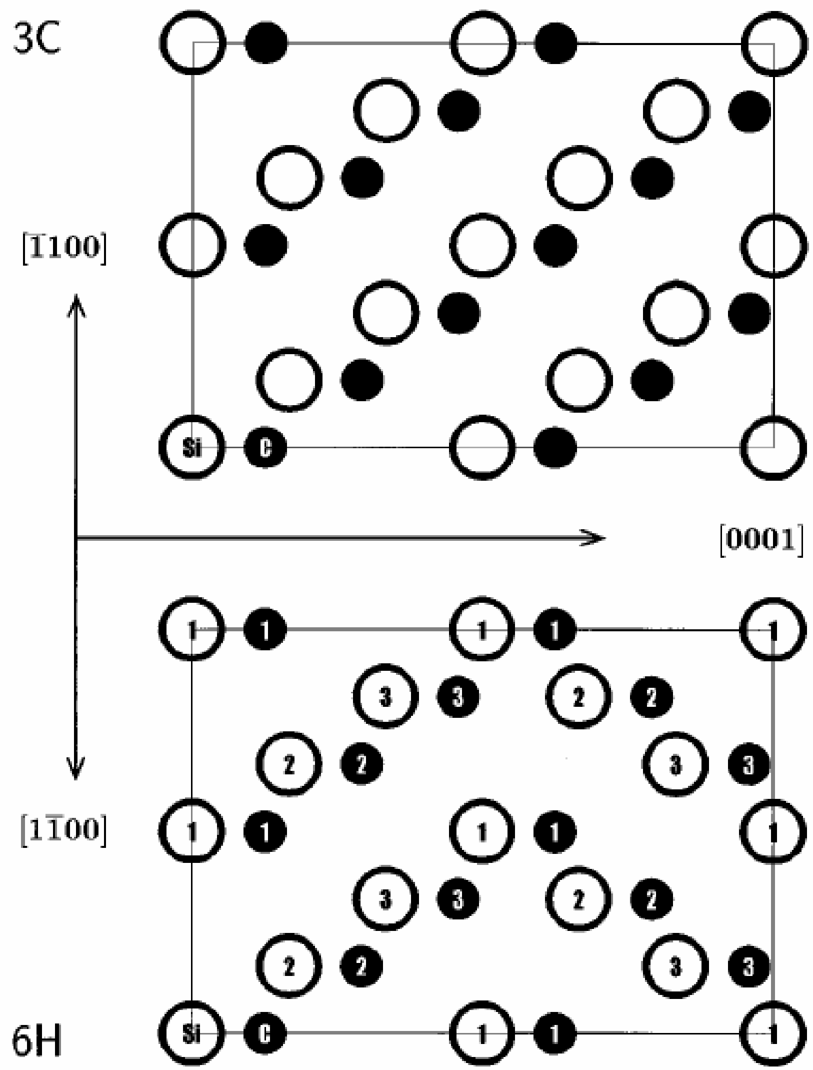
From: P. G. Neudeck, SiC technology, 1998



Edited from: Matsunami, 2002

Positron in SiC

Host	a [a.u.]	c [a.u.]	τ_{LDA} [ps]
3C-SiC	8.24	-	141
2H-SiC	5.81	9.54	142
6H-SiC	5.81	28.50	141



Atomic positions for 3C-SiC and6H-SiC.

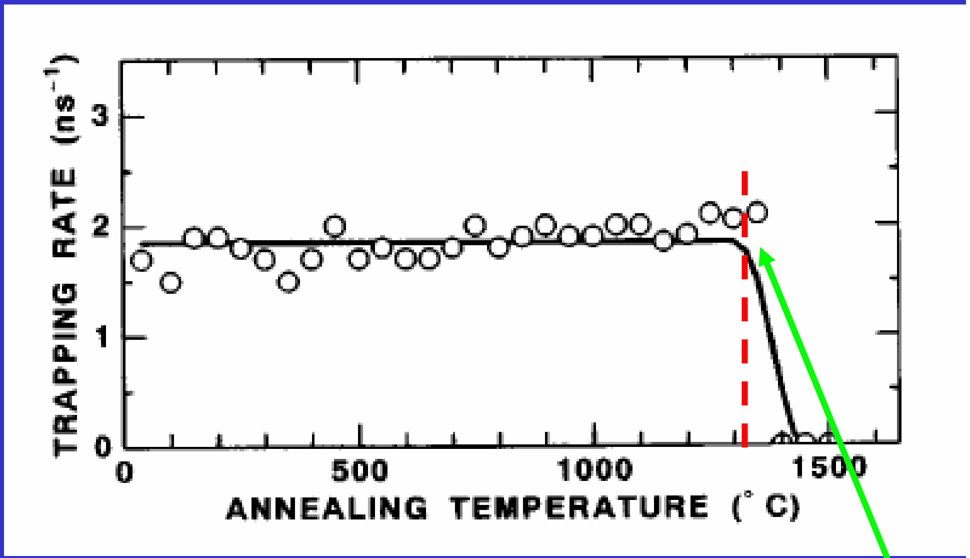
TABLE II. Calculated positron lifetimes τ_d in different types of neutral and unrelaxed vacancy-type defects in three SiC polytypes. The defect configuration n-$V_{Si}V_C$ (n=1,2,3,4) indicates a vacancy agglomerate with n divacancies. E_b indicates the binding energy of the positron in the corresponding defect.

Defect	3C-SiC		2H-SiC		6H-SiC	
	τ_d [ps]	E_b [eV]	τ_d [ps]	E_b [eV]	τ_d (ps)	E_b (eV)
V_C	150	0.28	151	0.26	150	0.28
V_{Si}	185	1.69	184	1.67	183	1.73
1-$V_{Si}V_C$	216	2.39	216	2.40	214	2.44
2-$V_{Si}V_C$	254	3.48	-	-	-	-
3-$V_{Si}V_C$	286	4.27	-	-	-	-
4-$V_{Si}V_C$	321	4.94	-	-	-	-

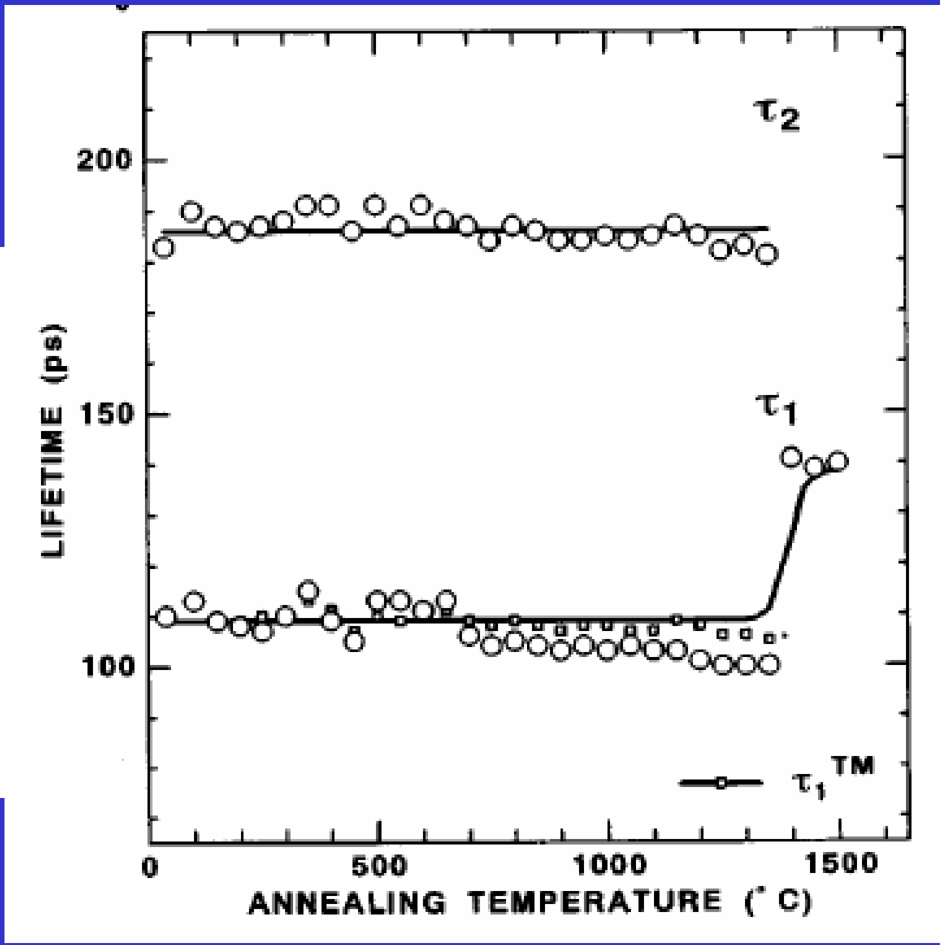
两种SiC的正电子寿命,结合能和亲和势

Positron state	τ (ps)	E_b (eV)	A_+ (eV)
	3C-SiC		
bulk	138(141)		−5.57
C vacancy	153(150)	+1.05(+0.28)	−4.39
Si vacancy	191(185)	+2.66(+1.69)	−8.22
Si+C divacancy	212(216)	+3.17(+2.39)	−8.18
Si+Si divacancy	194	+2.69	−8.93
C+C divacancy	160	+1.29	−4.92
Si vacancy+N	191	+2.73	−8.56
	6H-SiC		
bulk	141(141)		−5.91
C vacancy (1)	153(150)	+0.26(+0.28)	−4.30
Si vacancy (1)	194(183)	+2.46(+1.73)	−8.27
Si vacancy (2)	192	+2.30	−8.17
Si vacancy (3)	192	+2.32	−8.16
Si+C divacancy	214(214)	+2.95(+2.44)	−8.10
Si+Si divacancy	196	+2.64	−8.91
C+C divacancy	161	+0.58	−4.72
Si vacancy+N	194	+2.52	−8.75

6H-SiC



空位型缺陷消失

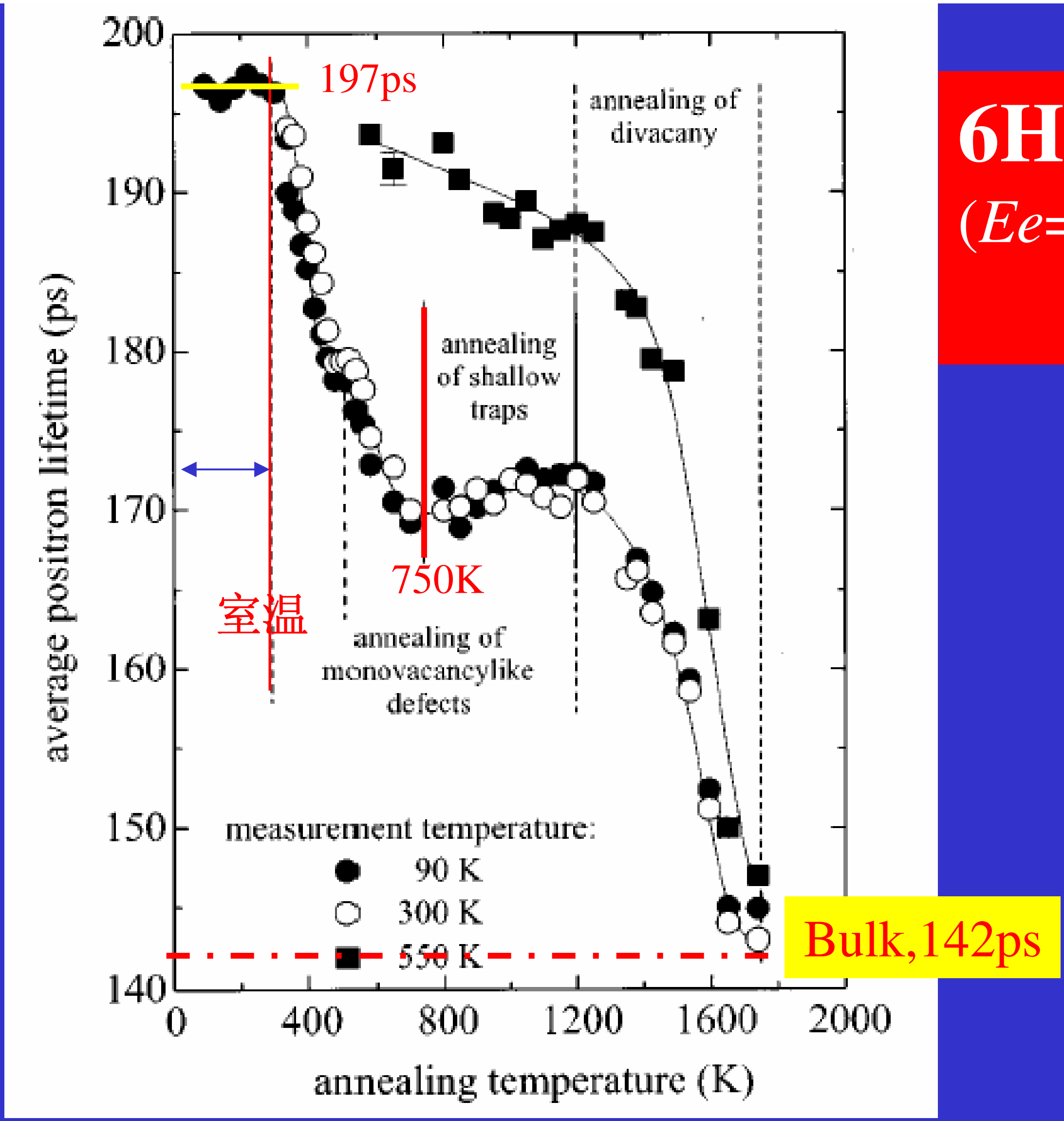


正电子捕获率随等时退火温度的变化.

正电子寿命 τ_1 和τ_2 , 以及强度I_2 随退火温度变化.

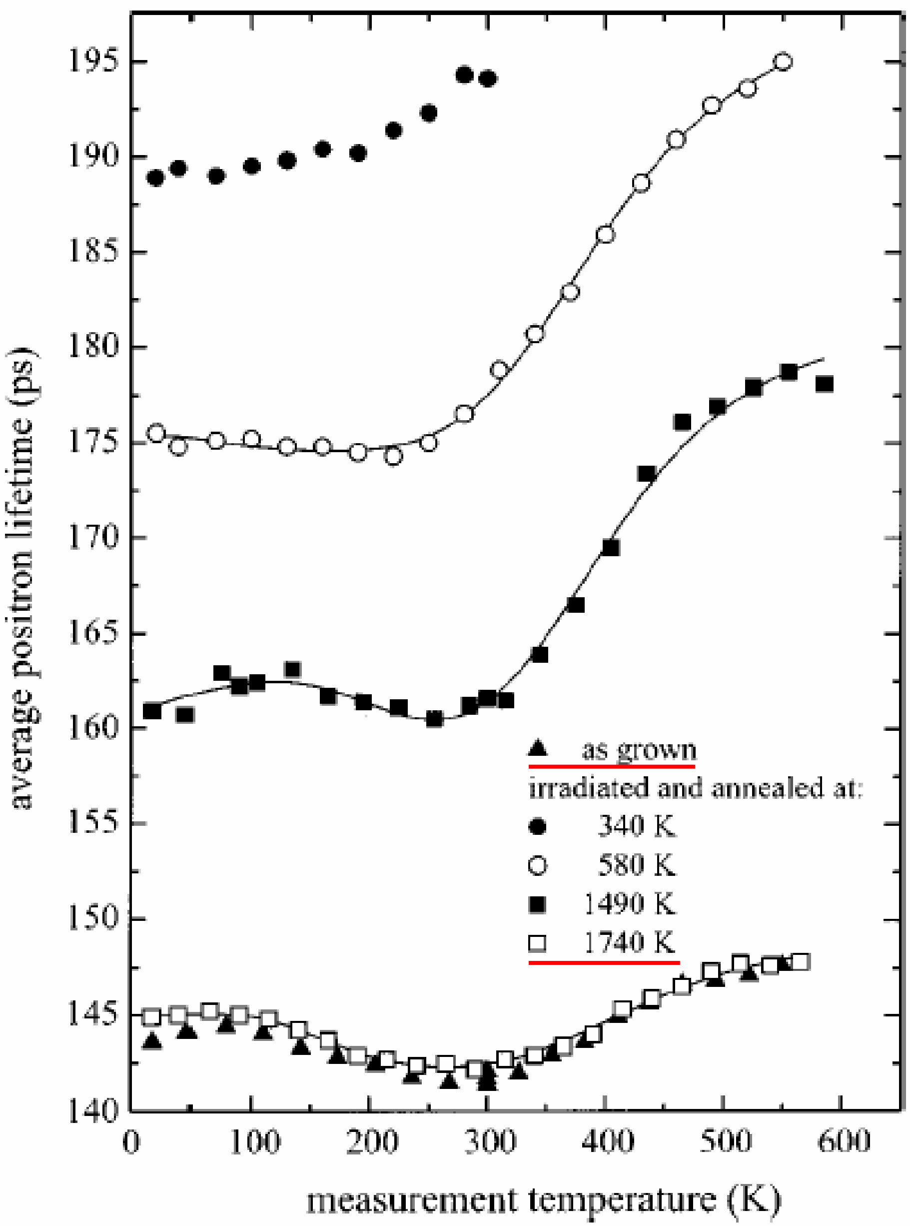
6H-SiC(电子辐照)

(*Ee*=2 MeV, $\Phi=10^{18}$ cm^{-2}, *T*=4 K)



6H-SiC
(未辐照和辐照)

(Ee=2 MeV, $\Phi=10^{18}$ cm^{-2}, T=4 K)



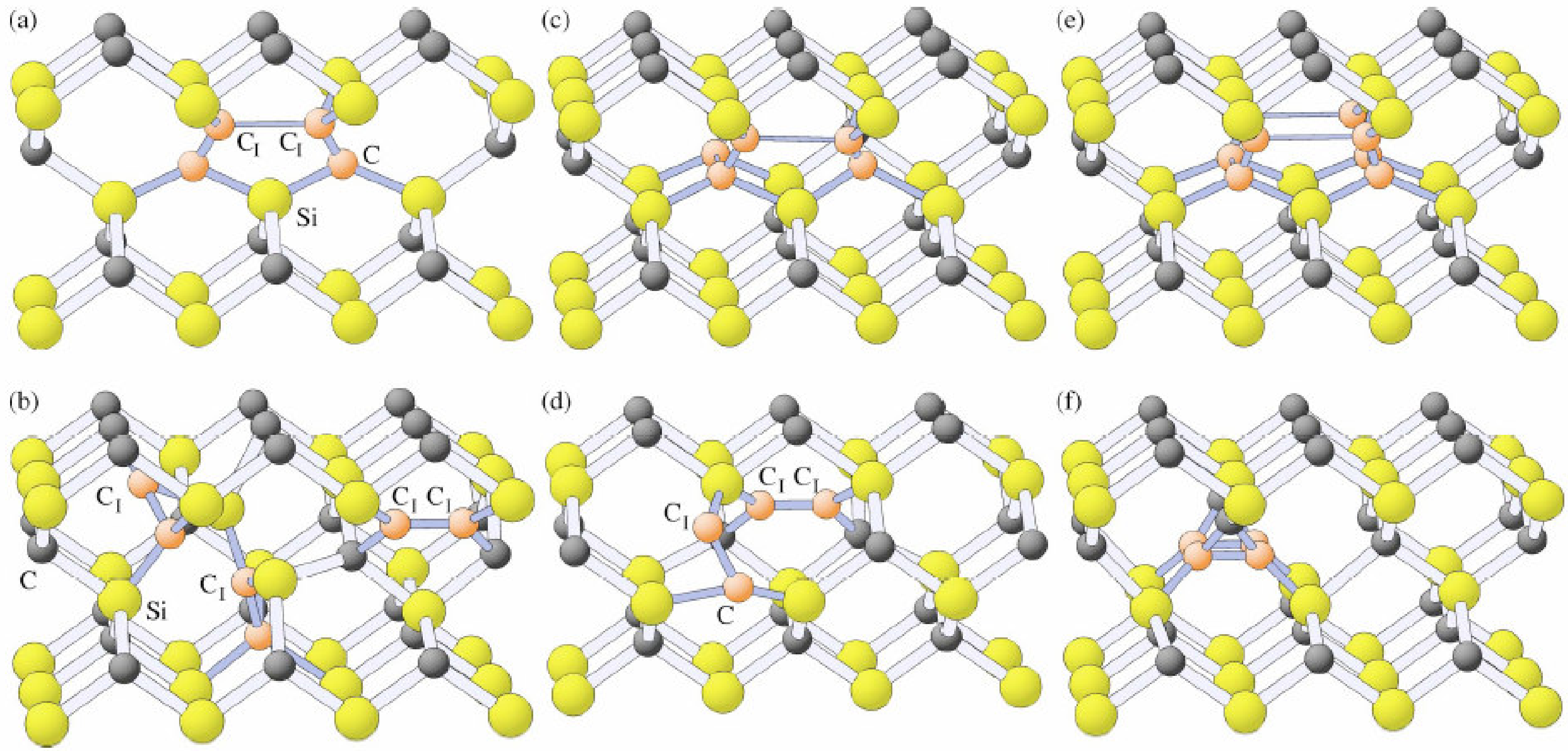
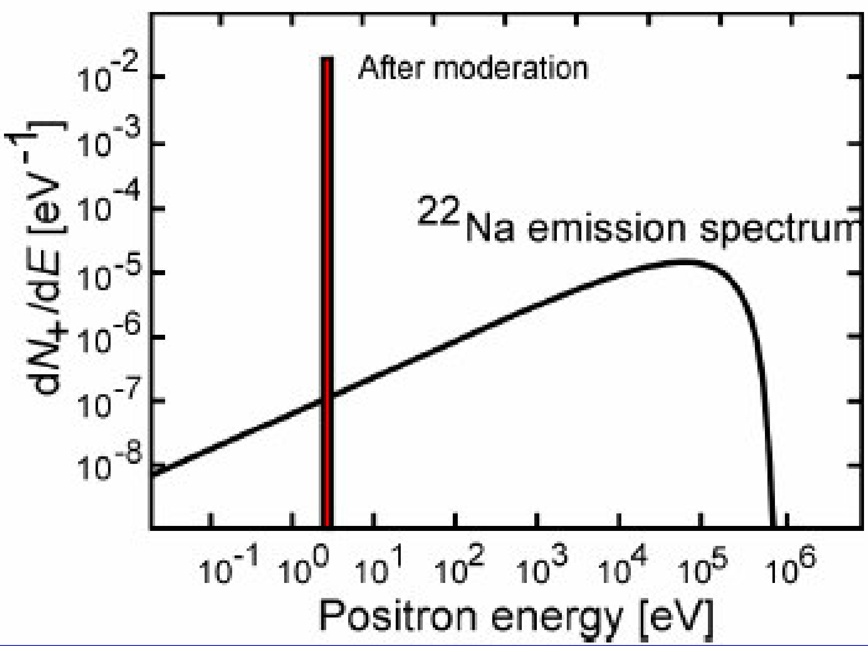


FIG. 3. Carbon interstitial clusters in 3C-SiC. Di-interstitials: (a) $(C_{sp})_2$, (b) $(C_{sp})_{2,tilted}$, and $(C_2)_{Hex}$. Tri-interstitials: (c) $(C_{sp})_3$ and (d) $(C_2)_{Hex}$-C_{sp}. Tetrainterstitials: (e) $(C_{sp})_4$ and (f) $[(C_2)_{Hex}]_2$.

Slow positron beam

- semiconductor technology: thin layers (epitaxy, ion implantation)
- broad energy distribution due to β^+ decay
- some surfaces: negative workfunction ⇒ moderation (but rather inefficient)

Energy distribution after β^+ decay



Effect of moderation

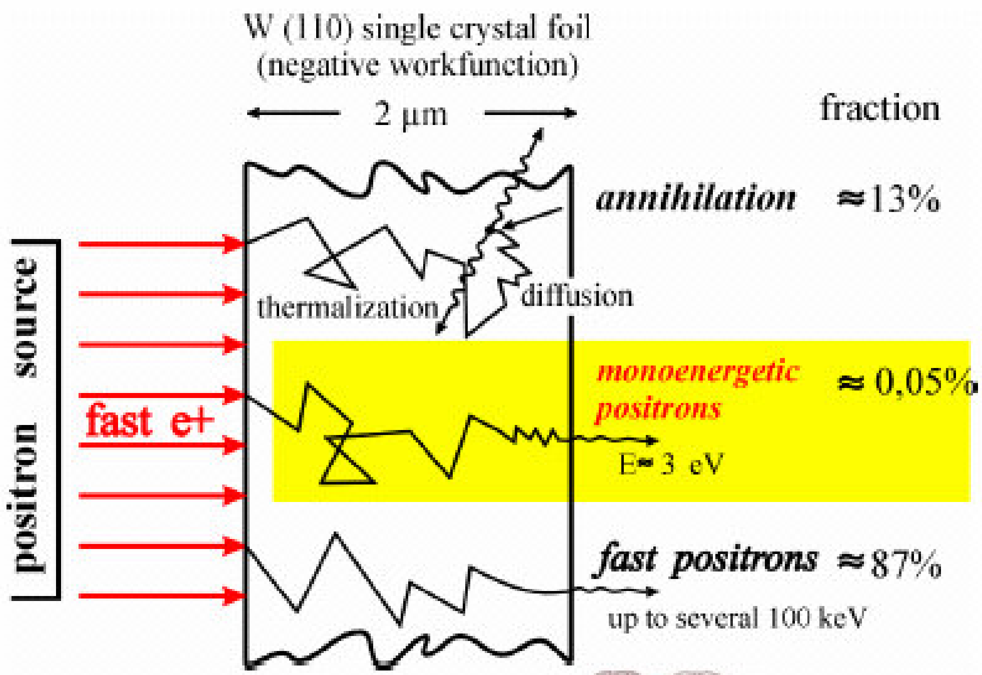


TABLE I. Experimental results for S_{expt} and W_{expt} (obtained at room temperature) ordered according to increasing r_s values, i.e., with decreasing valence-electron density. S_{val} is the calculated S parameter for valence electrons using the core fractions f_c from Puska *et al.*'s data (Ref. 3). The second-last column lists the ratio between the "Fermi" momentum for the valence electrons and the momentum for the outermost core electrons. The last column summarizes the nature of the investigated samples. *Uncertainties in W_{expt} and S_{expt} large due to the large backing contribution. †Average values for S- or Zn-doped GaP (S_{expt}=0.4806 and 0.4925, respectively, and W_{expt}=0.0397 and 0.0372, respectively). ††Average values. 1 Ω cm: S_{expt}=0.5013, W_{expt}=0.0375; 50 Ω cm: S_{expt}=0.5023, W_{expt}=0.0373.

Material	Band gap (eV)	r_s (Å)	f_c (%)	W_{expt} ±0.0003	S_{expt} ±0.0005	S_{val}	p_F/p_n^{core}	Comments
C	5.5	0.70	1.20	0.0660	0.4071	0.4099	0.43	synthetic, type I_b
SiC	3.0	0.85	2.65	0.0450	0.4376	0.4441	0.44	n type, N doped
GaN	3.4	0.88	14.0	0.053±0.003*	0.455 ±0.005*	0.4913	0.43	12-μm-thick film on sapphire
Si	1.1	1.06	2.25	0.0230	0.5098	0.5158	0.41	Fz-Si, undoped
GaP	2.2	1.07	6.87	0.0385†	0.4865†	0.5057	0.38	p type, n type
Ge	0.7	1.11	6.80	0.0374††	0.5018††	0.5261	0.32	n type: 1 Ω cm and 50 Ω cm
GaAs	1.4	1.11	7.80	0.0385	0.4970	0.5230	0.33	semi-insulating
InP	1.3	1.15	8.33	0.0357	0.5034	0.5298	0.37	semi-insulating
InAs	0.36	1.18	8.79	0.0377	0.5132	0.5435	0.33	n type, undoped
GaSb	0.67	1.19	7.38	0.0345	0.5183	0.5451	0.30	n type, Te doped
InSb	0.17	1.27	7.92	0.0346	0.5277	0.5567	0.30	n type, undoped

TABLE III. Characteristic S and W parameters calculated for the perfect bulk lattice and for the ideal vacancy clusters in Si. The momentum component p_z is along the [111] direction. Before calculating the S and W parameters the theoretical Doppler spectra have been convoluted with a Gaussian with FWHM of 4.7 $\times 10^{-3} m_0 c$. S_{val} and $S_{B,val}$ have been calculated using the valence electron momentum distributions instead of the total distribution.

System	S/S_B	$S_{val}/S_{B,val}$	W/W_B
Bulk	$S_B = 0.5344$	$S_B = 0.5410$	$W_B = 0.01701$
V	1.018	1.014	0.86
V_2	1.045	1.038	0.72
V_3	1.053	1.045	0.68
V_4	1.067	1.058	0.64
V_5	1.081	1.072	0.59

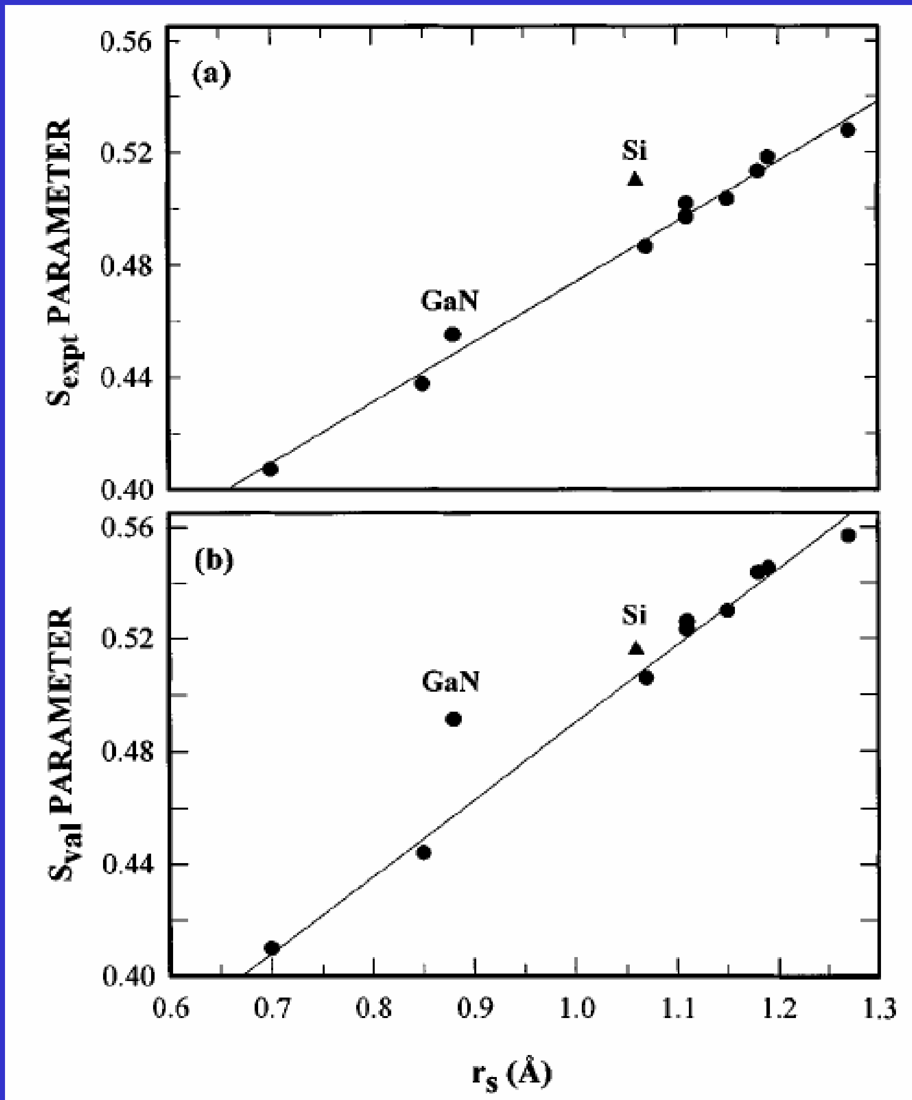


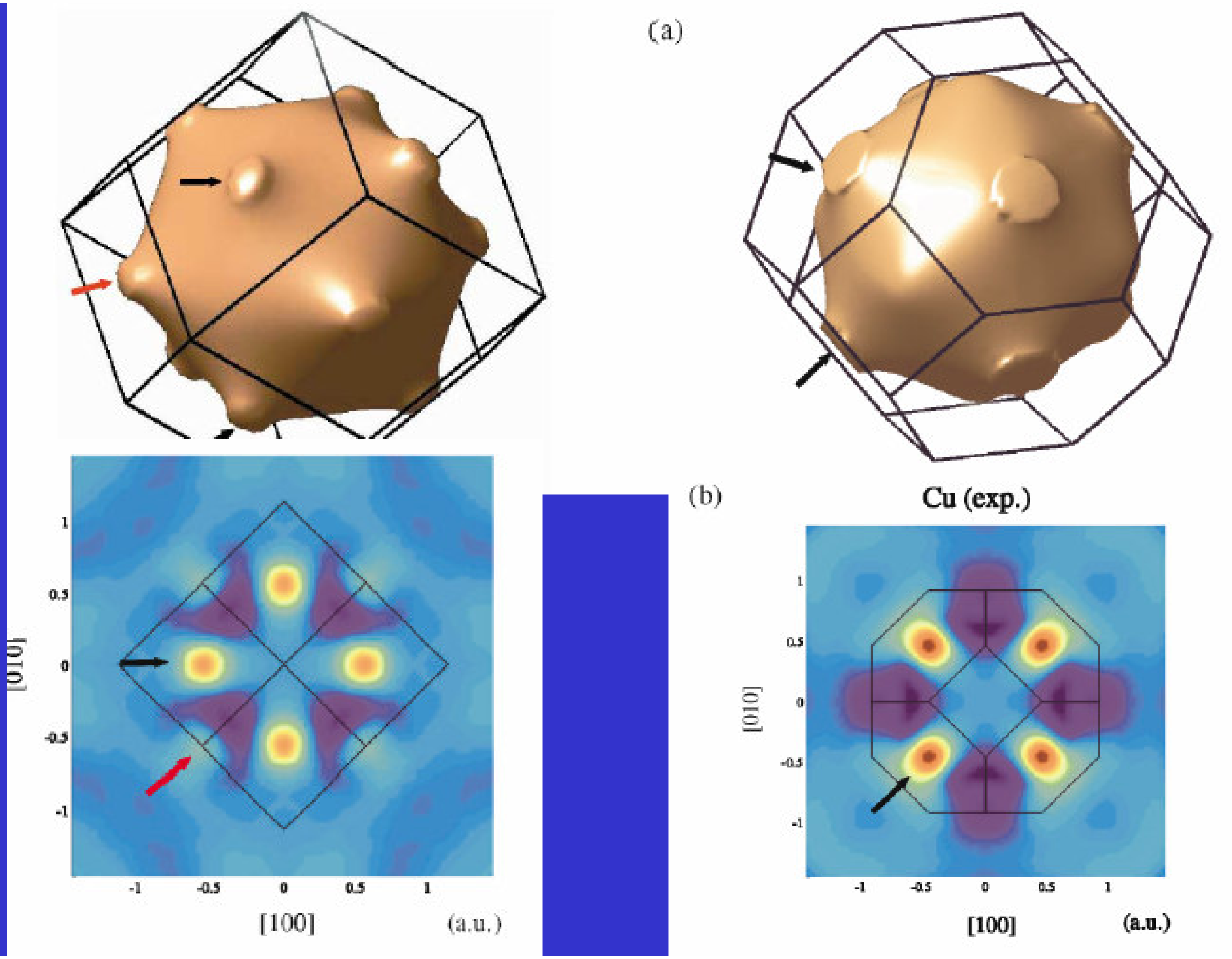
FIG. 1. (a) Experimentally obtained S_{expt} values as a function of r_s. All measurements were made at room temperature. (b) Calculated S_{val} values for valence electrons. The large value for GaN arises because of an uncharacteristically large calculated core contribution.

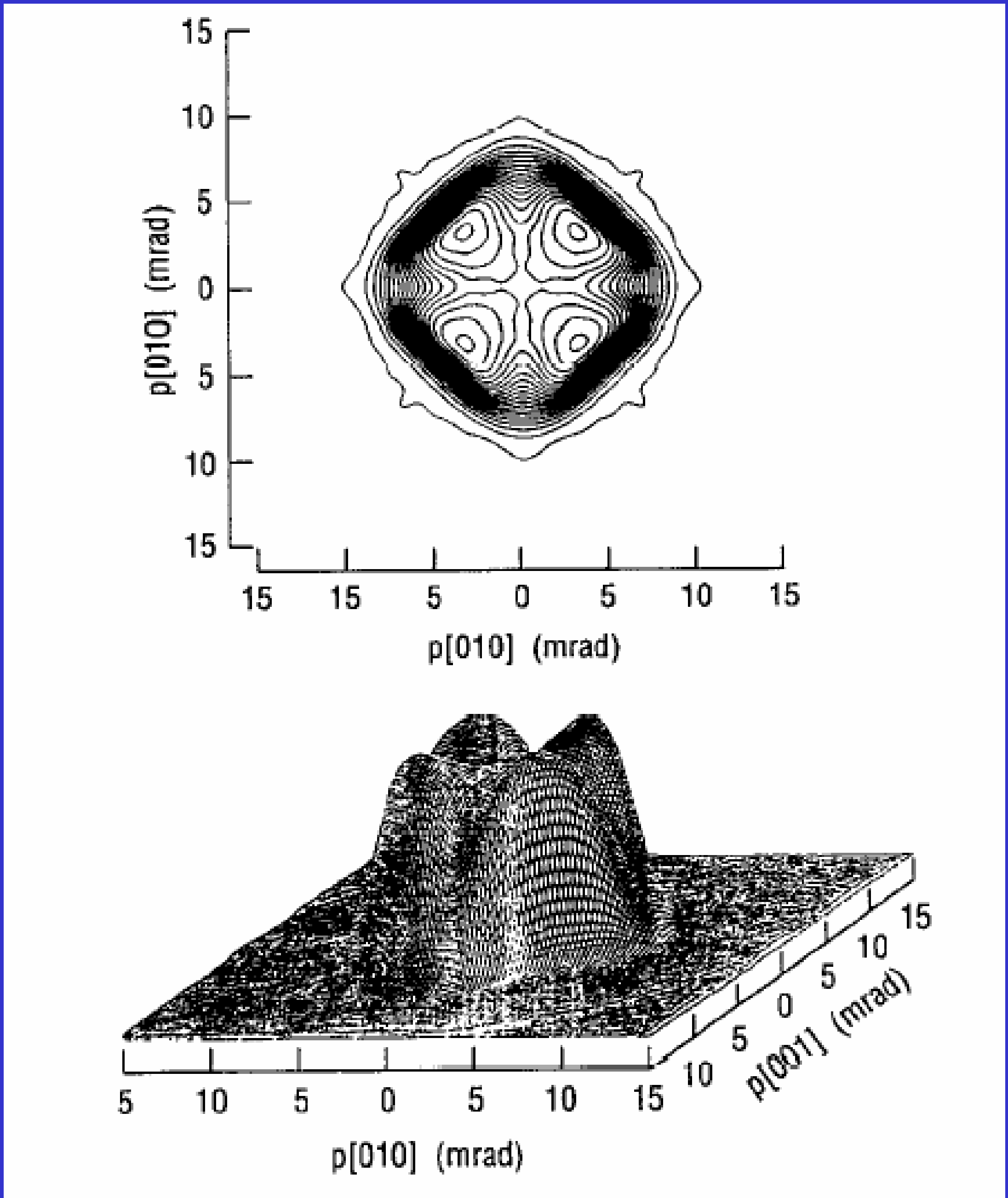
$$\frac{4\pi}{3} r_s^3 = n_{val}^{-1},$$

where n_{val} is the density of valence electrons

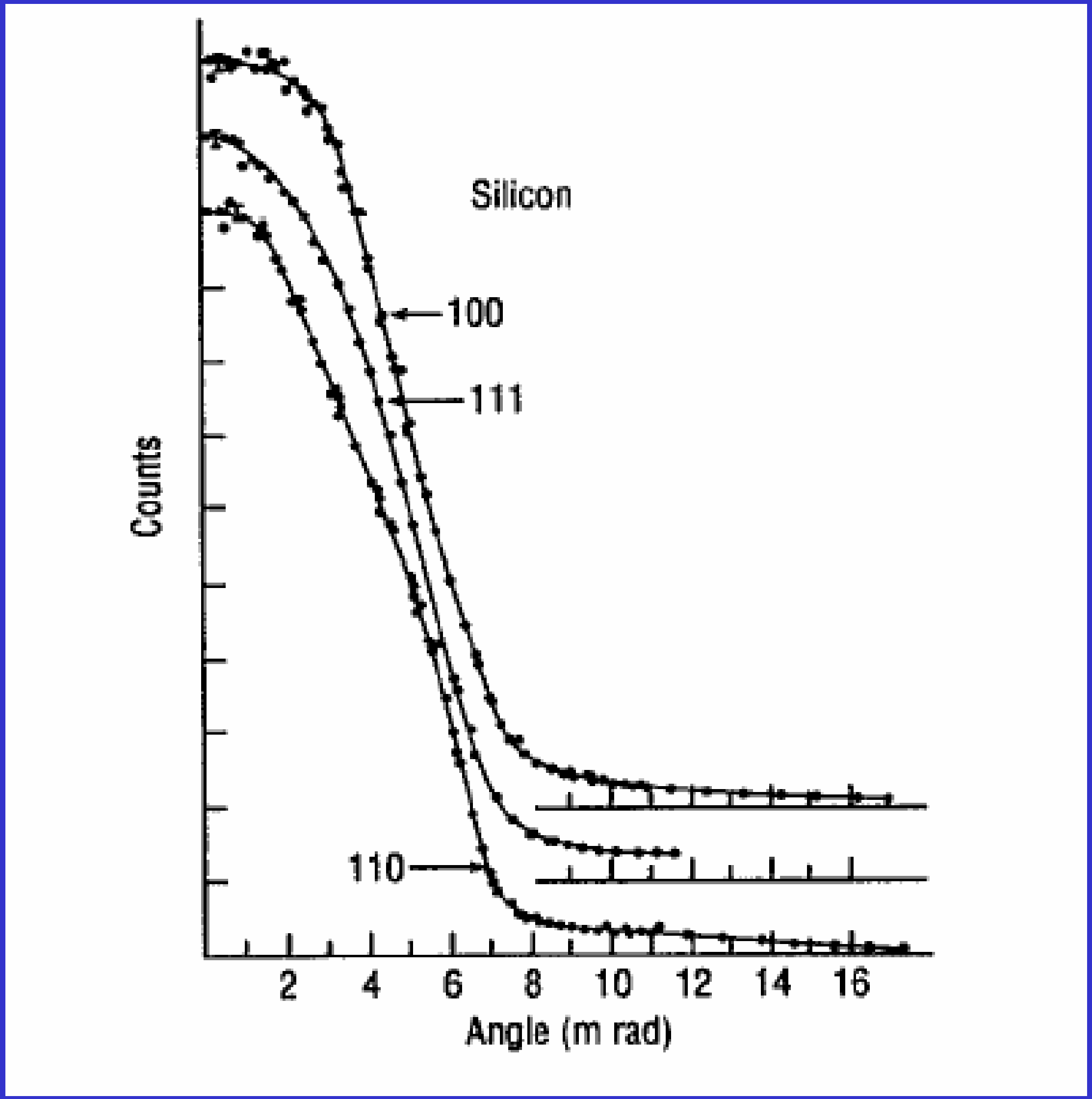
电子结构

Fermi Surface of Nanocrystalline Embedded Particles in Materials: bcc Cu in Fe

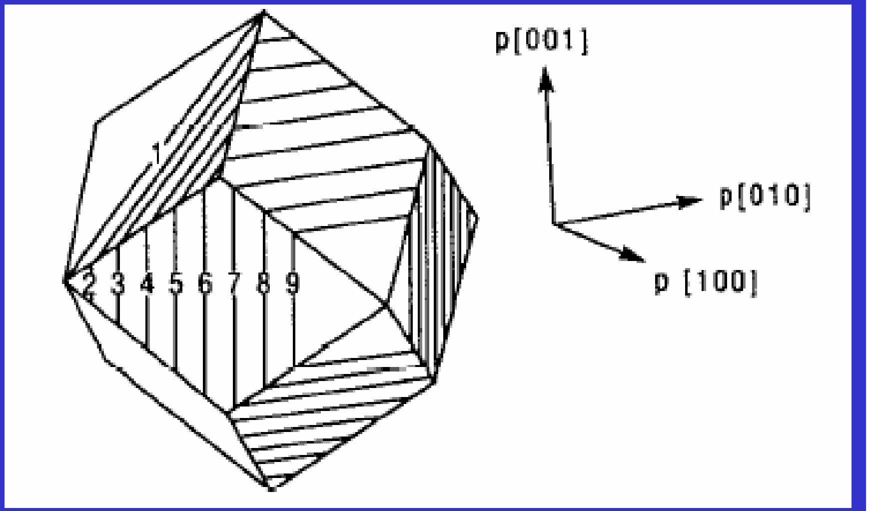


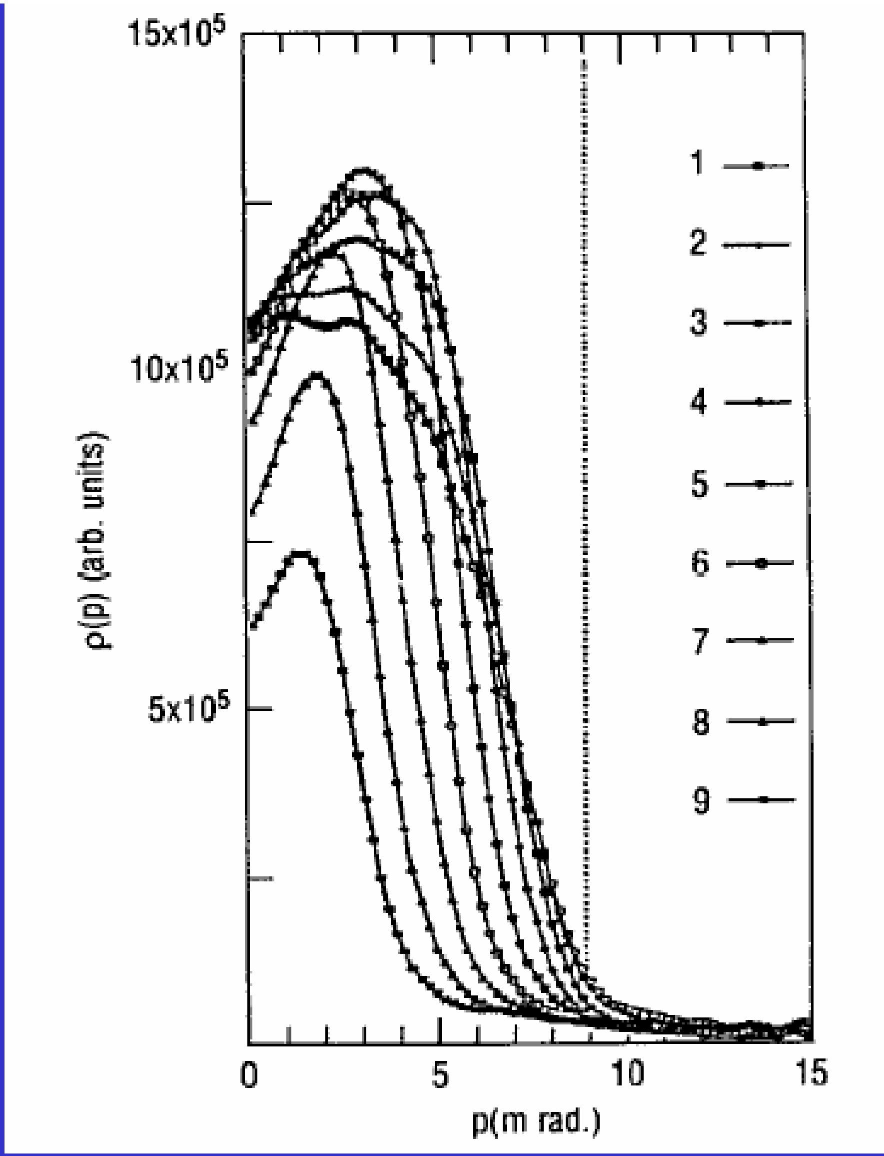


- 用2D-ACAR测量得到的 Si的动量分布.

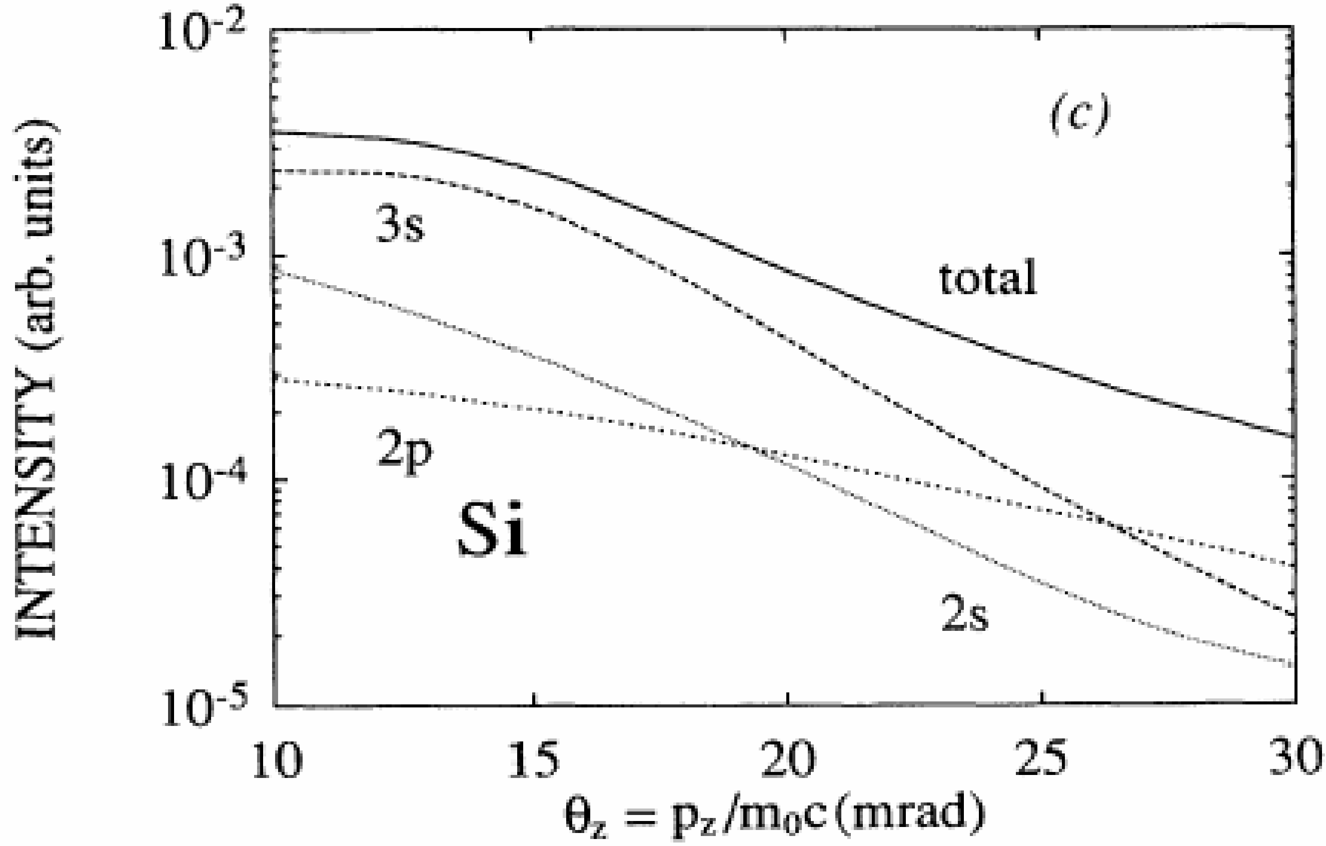


- **Experimental angular distribution of annihilation y-rays from in Si oriented along [100], [111], and [110] directions.**

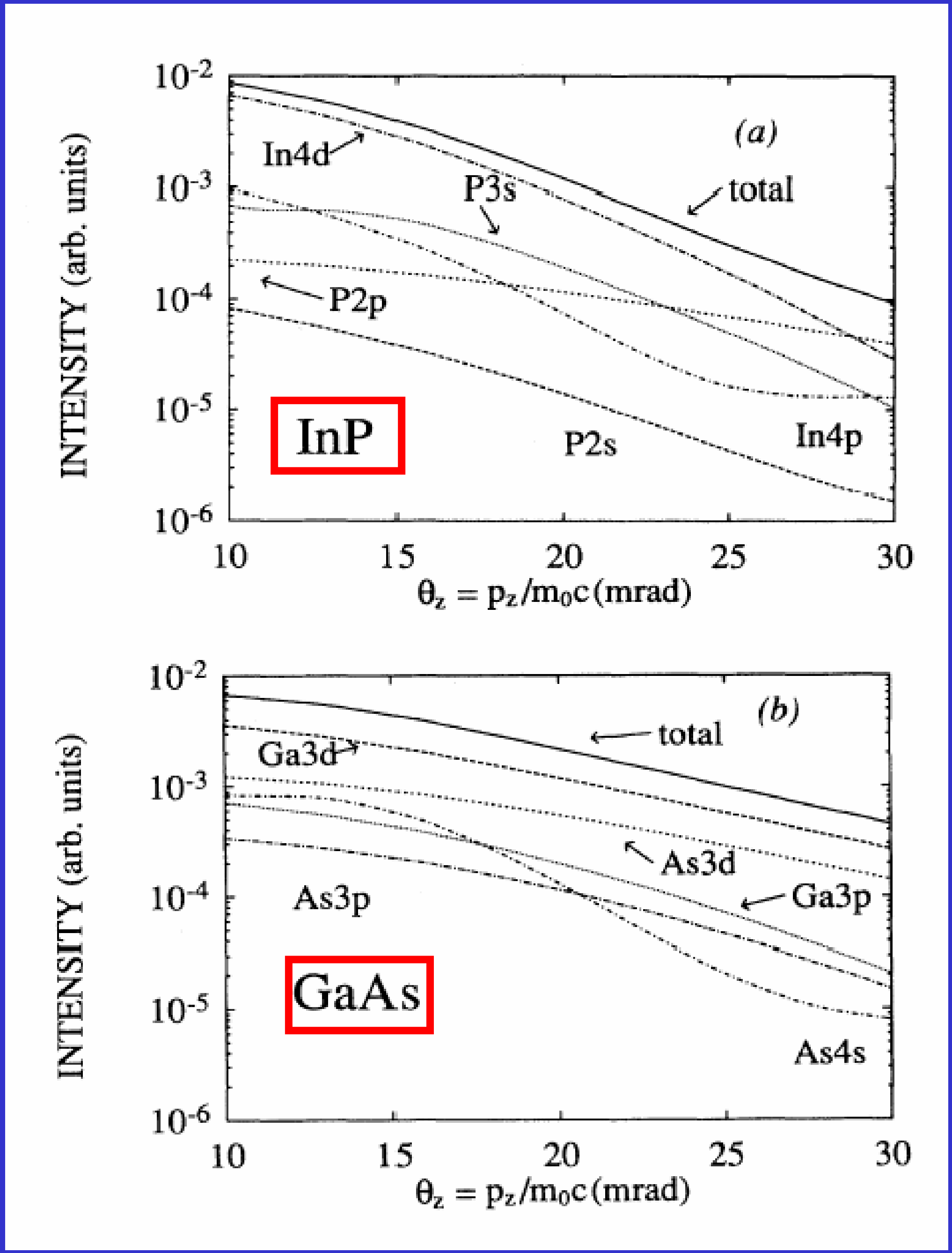




- **The electron momentum density in Si in several cross-sections corresponding to the reference Jones zone as shown.**



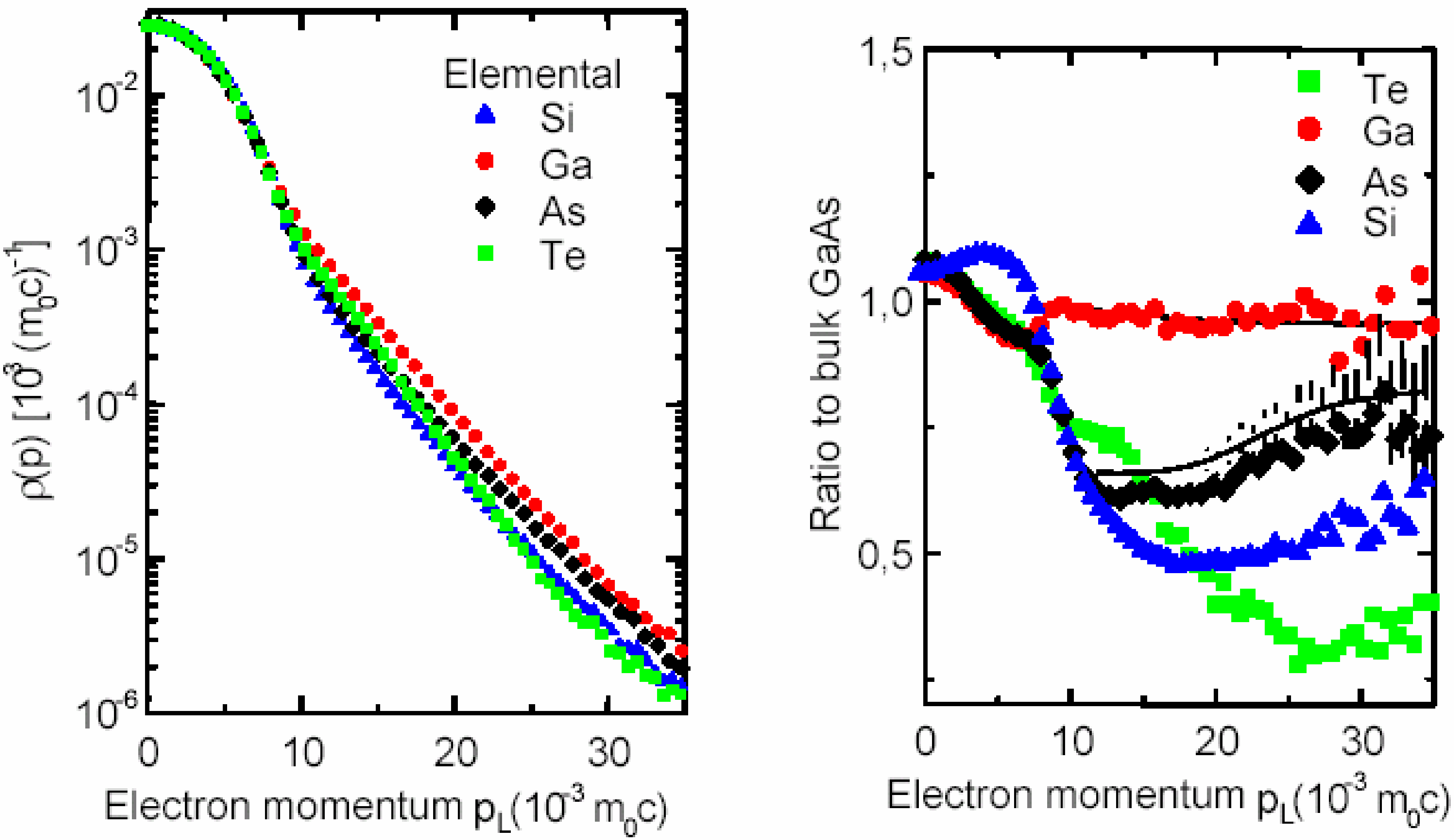
INTENSITY (arb. units)
10-2
10-3
10-4
10-5
(c)
3s
total
2p
Si
2s
10
15
20
25
30
θz = pz/m0c (mrad)



(a)
INTENSITY (arb. units)
In4d
P3s
total
P2p
InP
P2s
In4p
$\theta_z = p_z/m_0c$ (mrad)
(b)
total
Ga3d
As3d
Ga3p
As3p
GaAs
As4s

Doppler coincidence spectroscopy

- chemical sensitivity of energy spectra



PHYSICAL REVIEW B VOLUME 51, NUMBER 7 15 FEBRUARY 1995-I

Identification of vacancy defects in compound semiconductors by core-electron annihilation: Application to InP

M. Alatalo, H. Kauppinen, K. Saarinen, M. J. Puska, J. Mäkinen, P. Hautojärvi, and R. M. Nieminen
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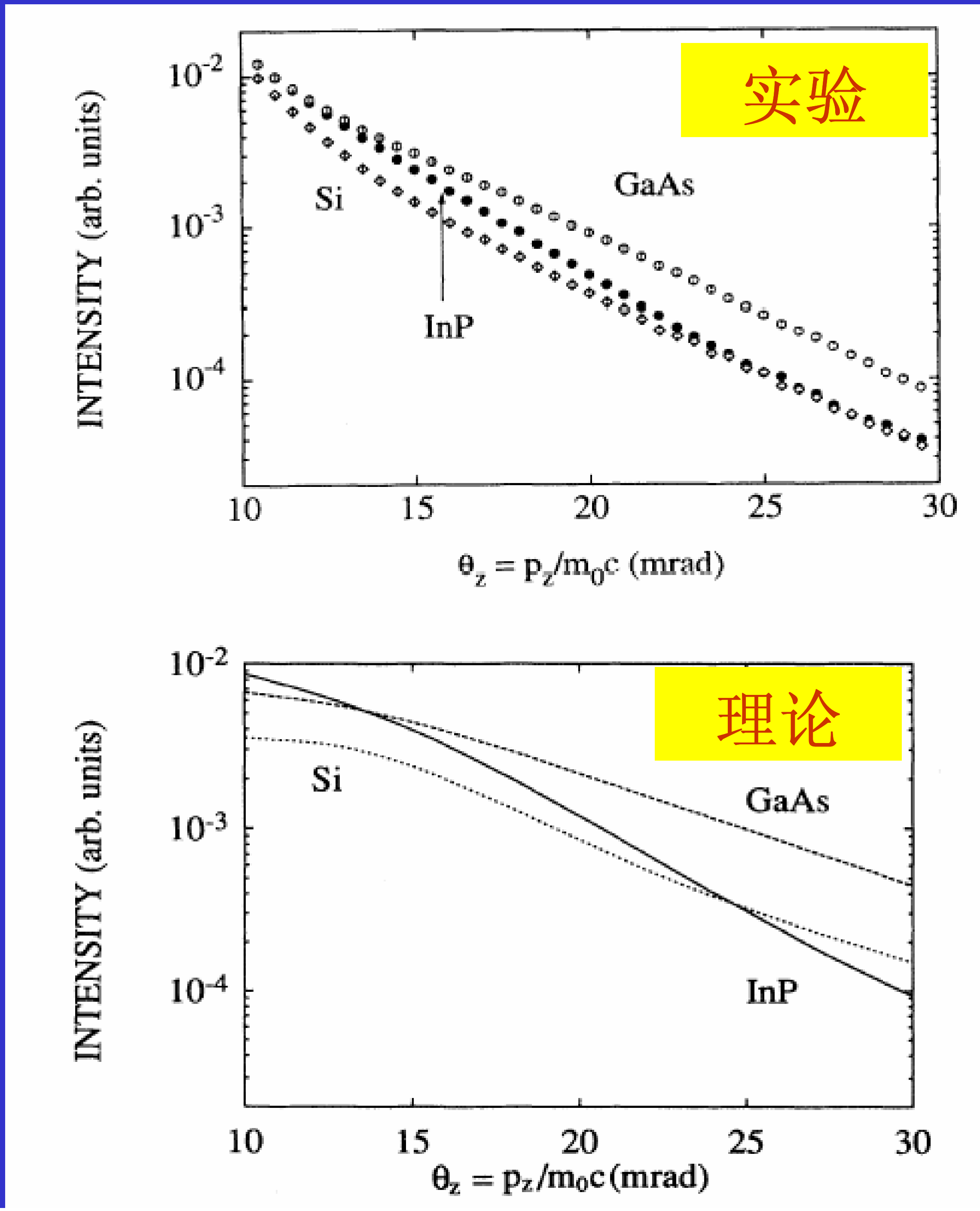
(Received 21 June 1994)


实验
INTENSITY (arb. units)
10-2
10-3
10-4
Si
GaAs
InP
10
15
20
25
30
θz = pz/m0c (mrad)
理论
INTENSITY (arb. units)
10-2
10-3
10-4
Si
GaAs
InP
10
15
20
25
30
θz = pz/m0c (mrad)

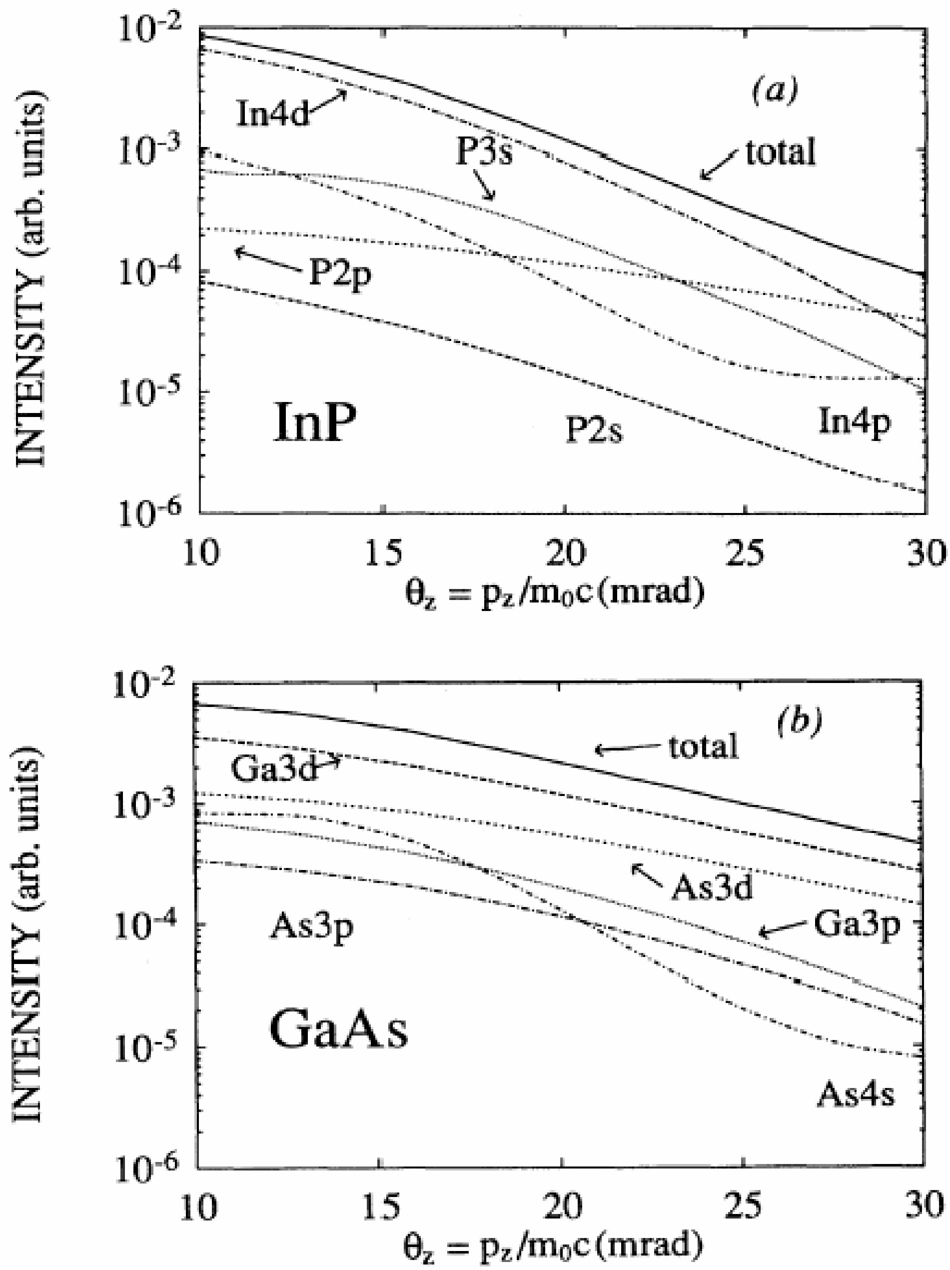
多普勒展宽

TABLE II. Annihilation rates λ_i (in ns^{-1}) for different core shells in bulk Si and GaAs.

Core shell	λ^i
Si 2*s*	0.034
Si 2*p*	0.106
Ga 3*d*	0.320
Ga 3*p*	0.061
As 4*s*	0.577
As 3*d*	0.116
As 3*p*	0.030

TABLE III. Annihilation rates λ_i (in ns^{-1}) for different core shells in bulk InP, V_P, and V_{In}. V_P is relaxed outwards by 3% of the bulk bond length, V_{In} is assumed ideal.

	λ^i_{bulk}	$\lambda^i_{V_P}$	$\lambda^i_{V_{In}}$
In 4*d*	0.504	0.489	0.256
In 4*p*	0.077	0.071	0.037
P 3*s*	0.511	0.355	0.574
P 2*p*	0.022	0.014	0.019
P 2*s*	0.008	0.005	0.007


INTENSITY (arb. units)
10-2
10-3
10-4
10-5
10-6
(a)
In4d
P3s
total
P2p
InP
P2s
In4p
10
15
20
25
30
θz = pz/m0c (mrad)
INTENSITY (arb. units)
10-2
10-3
10-4
10-5
10-6
(b)
total
Ga3d
As3d
Ga3p
As3p
GaAs
As4s
10
15
20
25
30
θz = pz/m0c (mrad)

Thank you!