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Extended defects in semiconductors studied by positron annihilation

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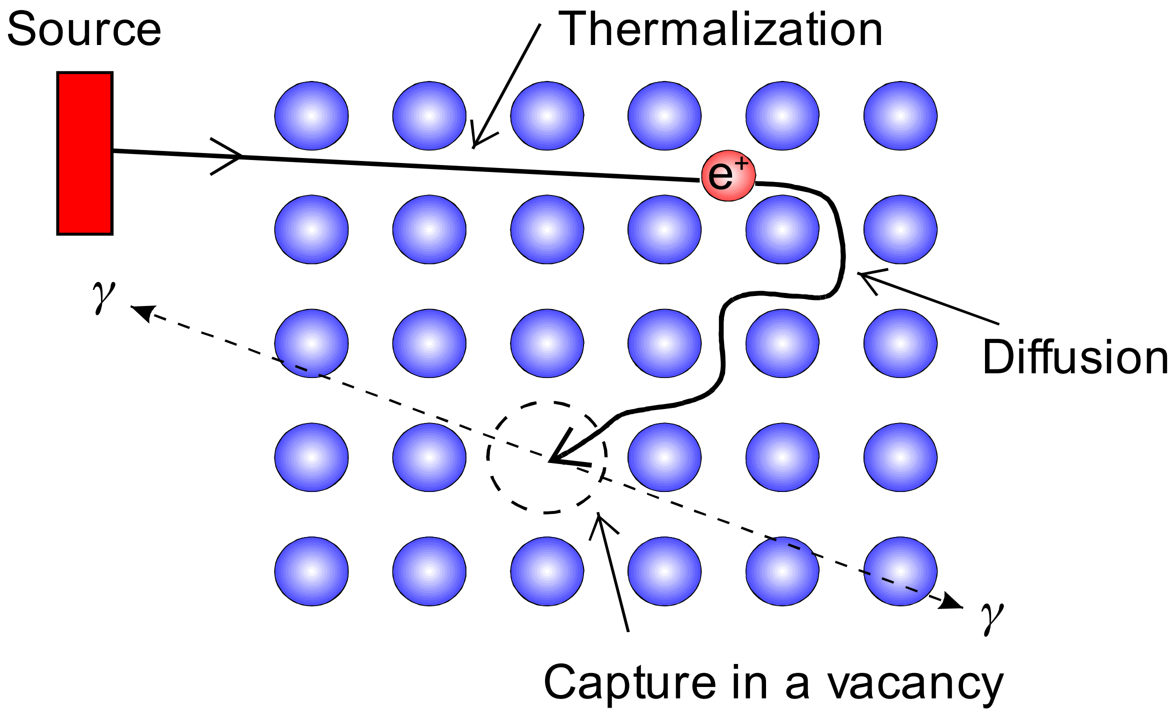
Overview

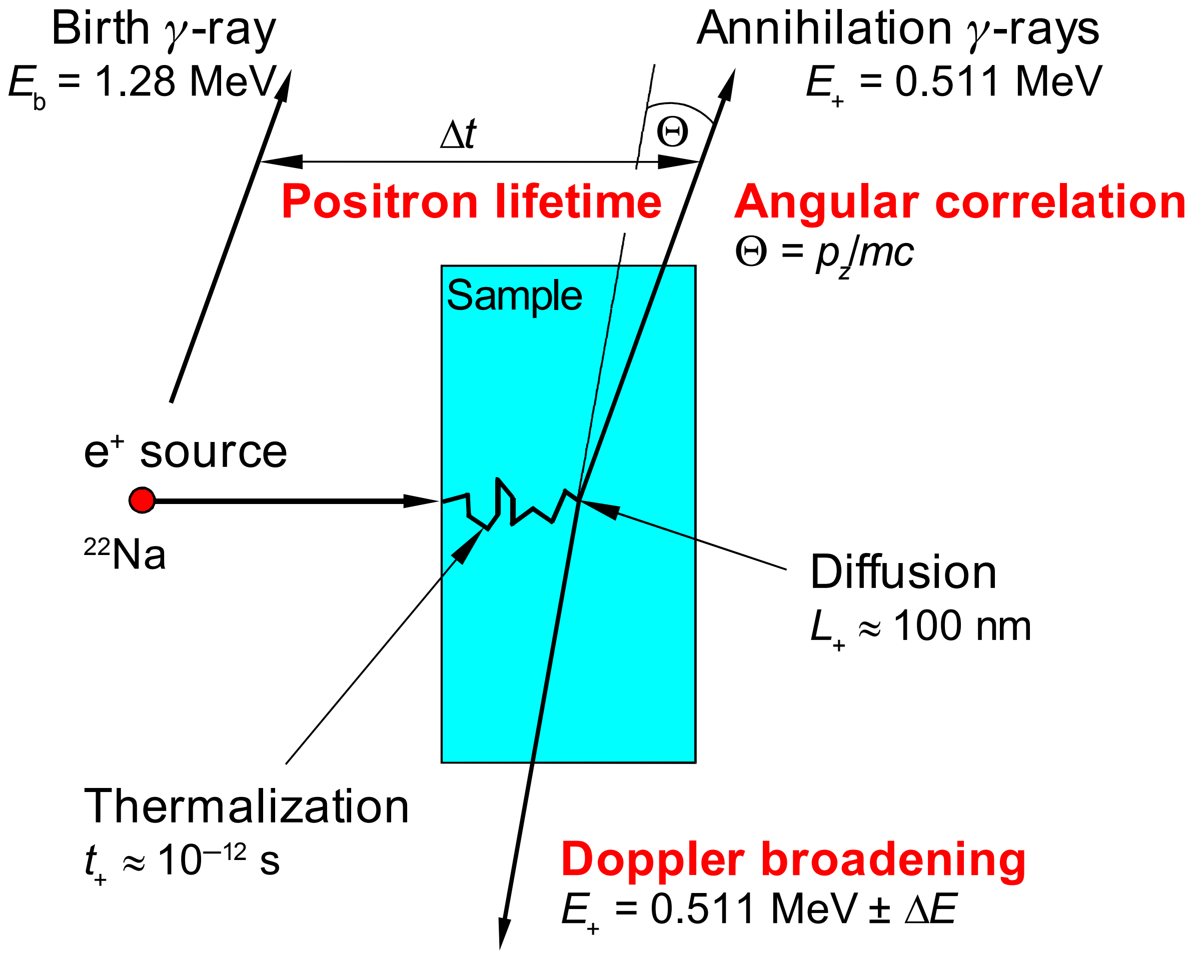
- Positron techniques
- Point defect generation during plastic deformation
- What we can learn from positron annihilation about defect structures?
- Calculations of vacancy clusters
- Low temperature – high temperature deformation
- Modell of point defect generation
- Implantation-induced defects

Positron annihilation

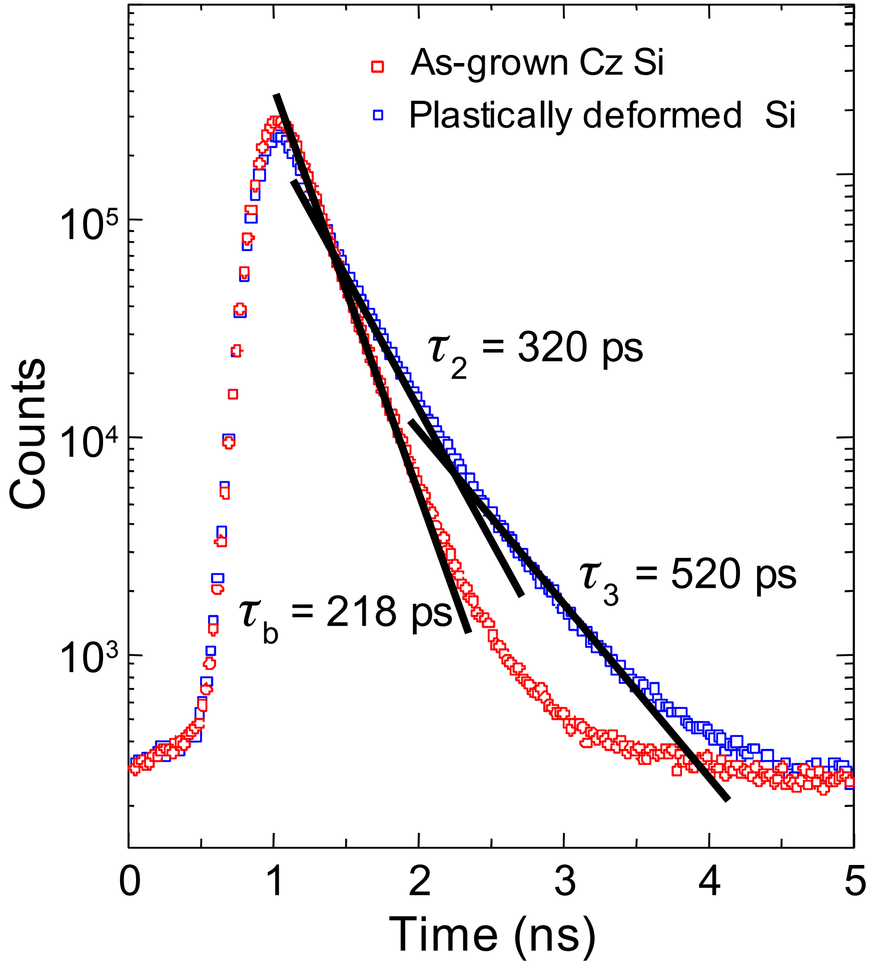


- Positrons may be captured during their diffusion in lattice defects.
- Annihilation rate (reciprocal lifetime) depends on the local electron concentration at the annihilation site.

Positron annihilation techniques



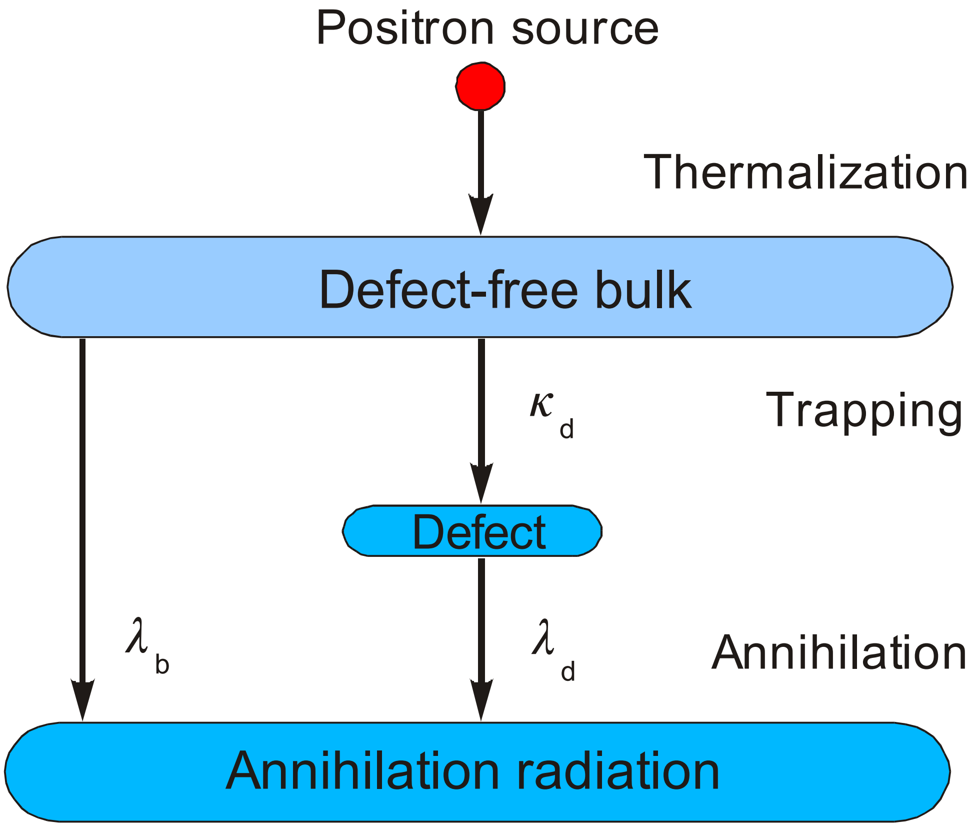
Positron lifetime spectrum



Decomposition of the experimental positron lifetime spectra

- Undeformed Czochralski Si:
  one component, $\tau_b = 218$ ps
- Plastically deformed Si:
  (3 %, 1050 K)
  three components
  $\tau_1 = 120$ ps (not shown),
  $\tau_2 = 320$ ps, $\tau_3 = 520$ ps

Trapping model



Positron source

Thermalization

Defect-free bulk

κ_d Trapping

Defect

λ_b

λ_d Annihilation

Annihilation radiation

- Quantitative analysis of positron trapping by a set of rate equations
- Solution (lifetime spectrum):

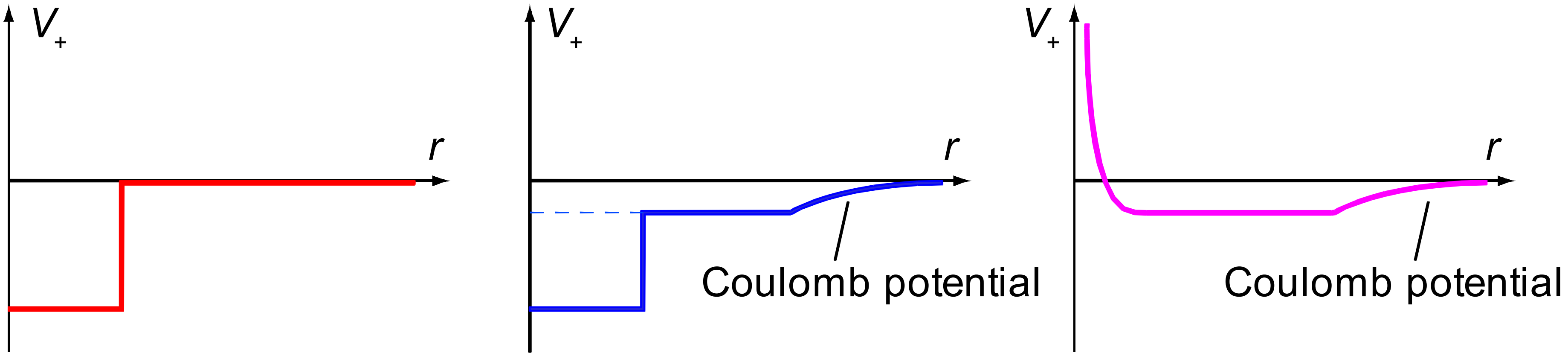
$$\sum_i \frac{I_i}{\tau_i} \exp\left(-\frac{t}{\tau_i}\right)$$

Trapping rate: $\kappa_{di} = \mu C_{di}$

$$\tau_1 = 1/(\lambda_d + \kappa_d), \quad \tau_2 = 1/\lambda_d$$

Average positron lifetime: $\bar{\tau} = \sum_i I_i \tau_i$

Positron capture in defects

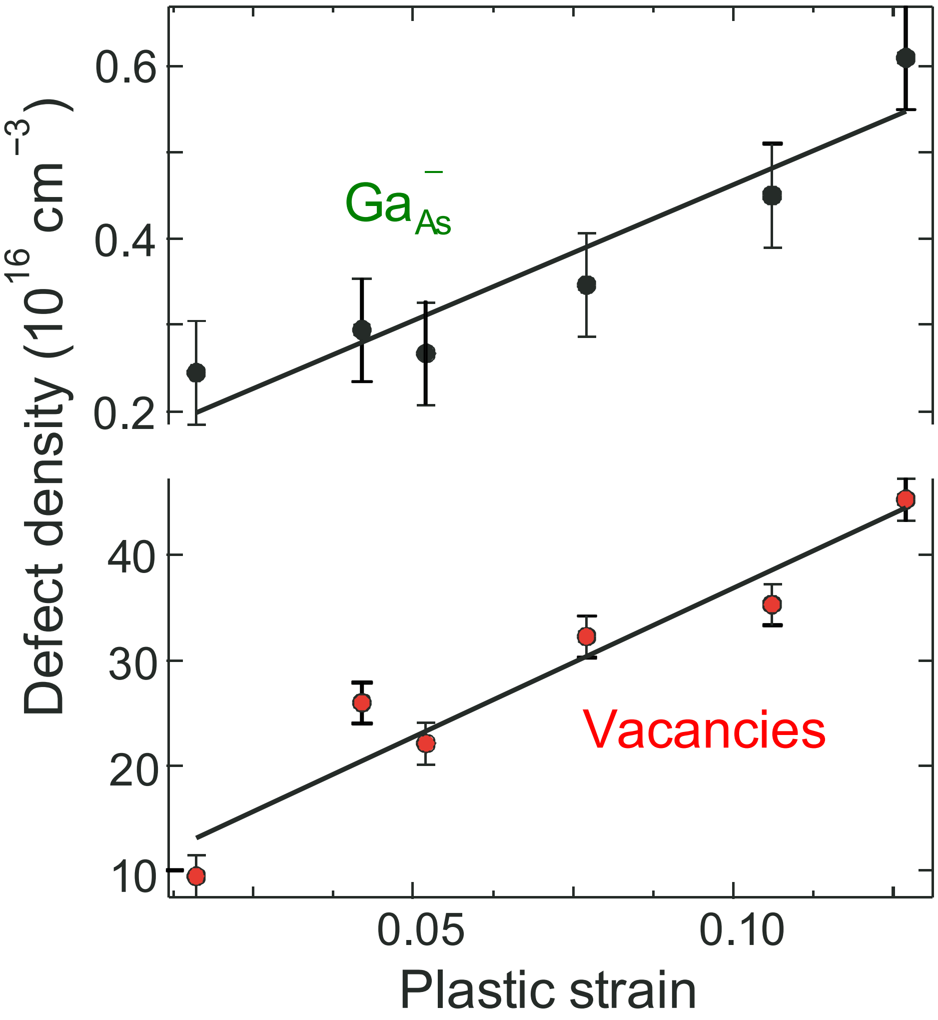


$\lambda \propto$ open volume

$\lambda \approx \lambda_b$

Positron potential $V_+(r)$ of a neutral and a negatively charged vacancy. The potential of a negatively charged acceptor acting as a shallow positron trap is shown on the right. λ is the annihilation rate (inverse positron lifetime). The trapping rate κ is constant for neutral defects and a function of temperature for charged defects.

Point defect density as a function of deformation conditions (i)

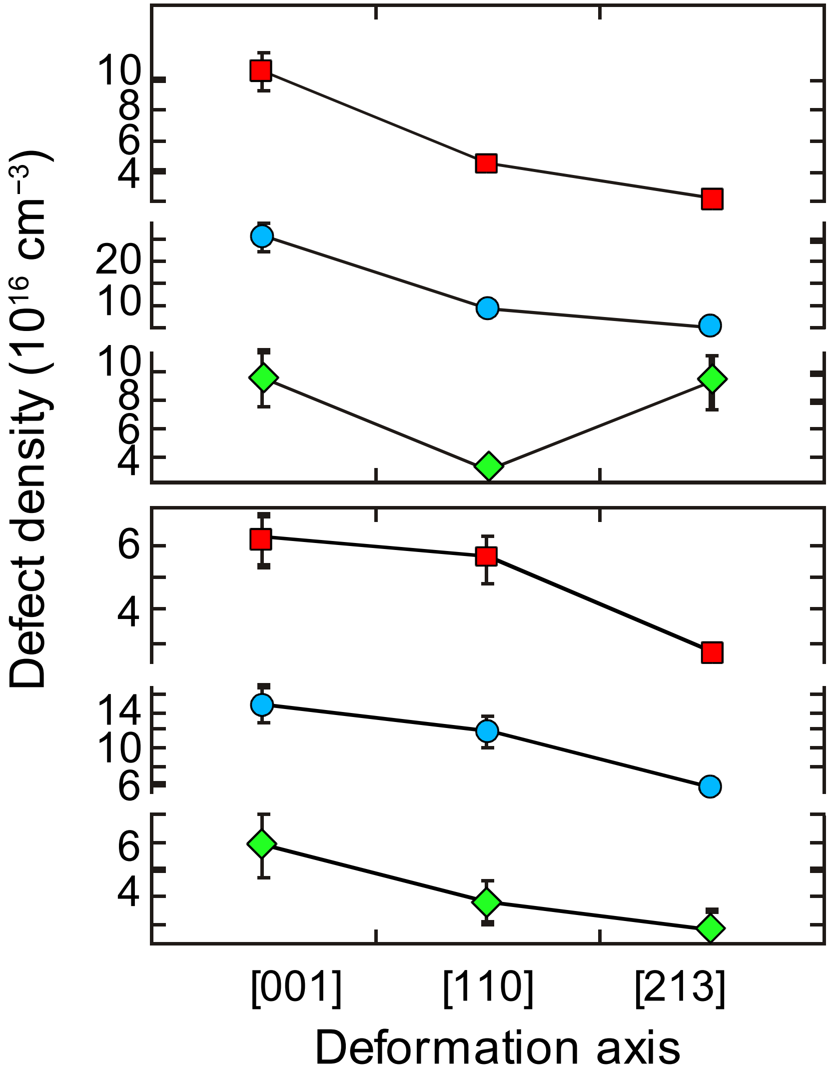


Density of vacancies and antisite defects as a function of the strain. Result of measurements by positron annihilation in plastically deformed GaAs. Uniaxial compression in [110] direction at 773 K, strain rate 1×10^{-3} s^{-1}.

Relation between density of excess vacancies and strain

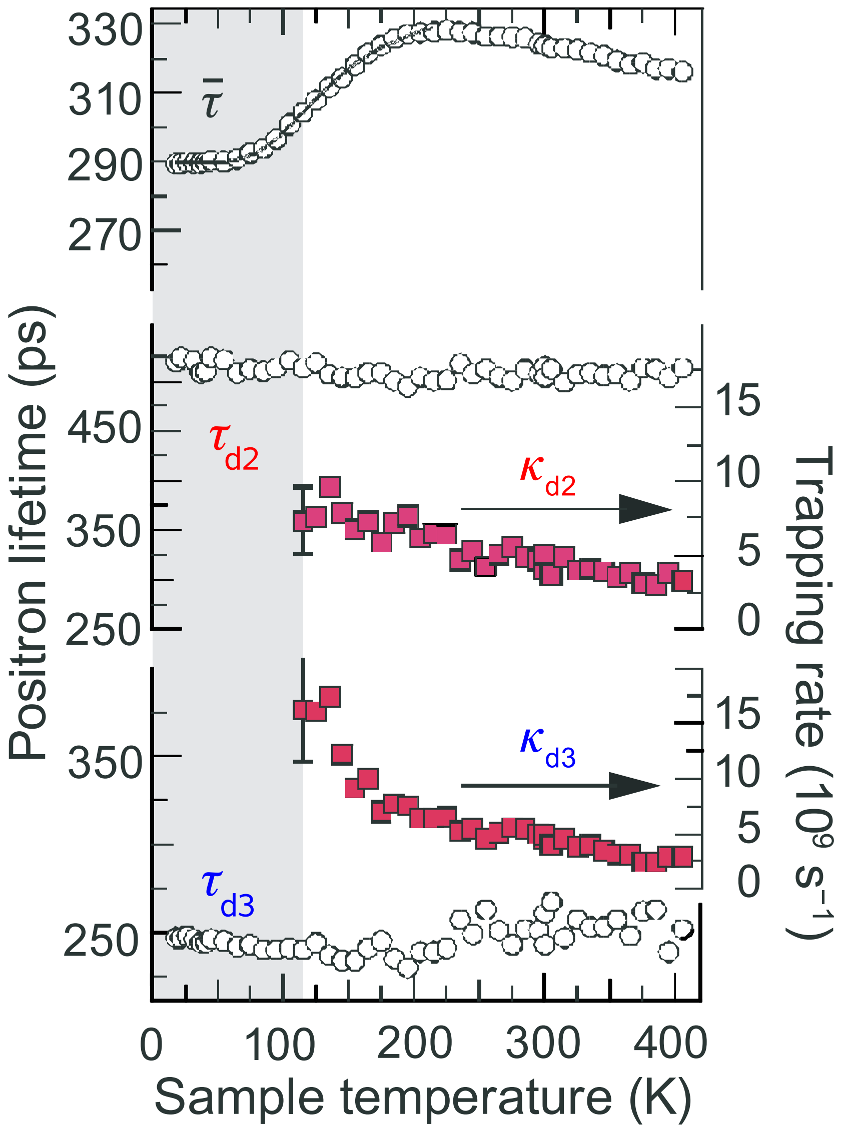
$$\rho_{\mathrm{v}} = \frac{l_{\mathrm{g}}\,\zeta\, c_{\mathrm{j}}}{l\, b^2\, m}\,\varepsilon$$

Point defect density as a function of deformation conditions (ii)



Total number of vacancies in the bulk (□), vacancies bound to dislocations (○), as well as number of Ga_{As} antisites (◇) in plastically deformed GaAs. Deformation temperature 773 K, strain 3 %, strain rate 7.5×10^{-5} s^{-1} (*above*), 3×10^{-4} s^{-1} (*below*).

Positron lifetimes and capture rates in deformed GaAs



Lifetime components:

- $\tau_2 = \tau_{d3} = (260 \pm 5)$ ps

  corresponds to a defect with the open volume of a monovacancy

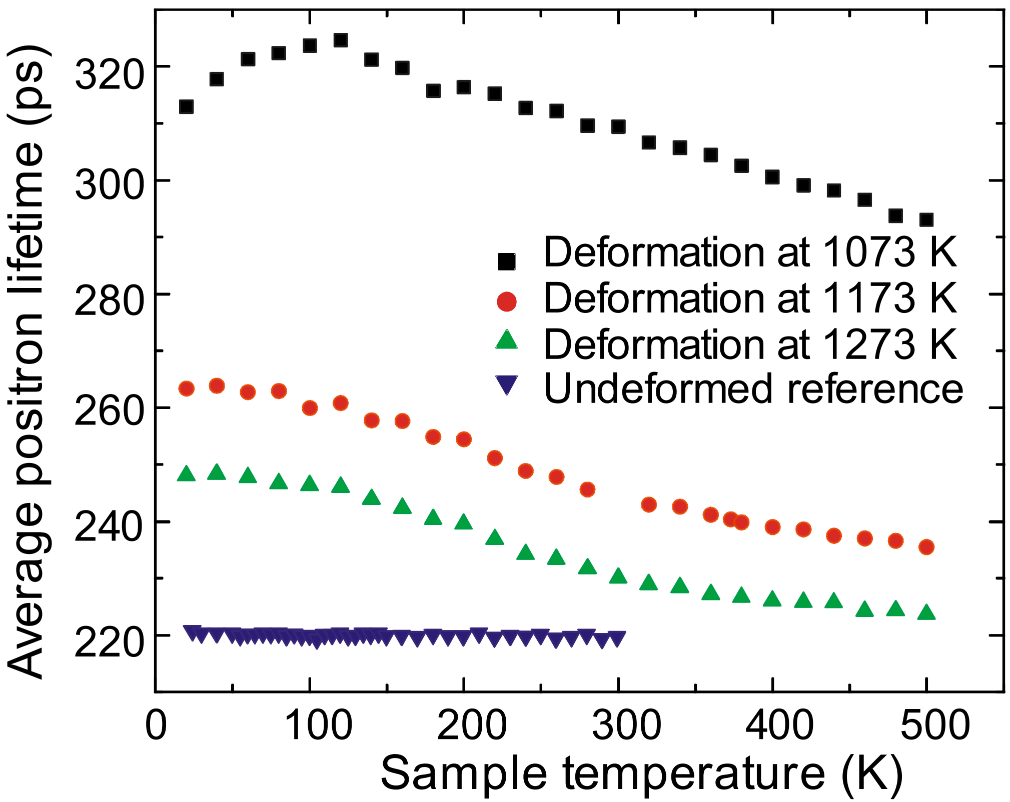
- $\tau_3 = \tau_{d2} = (477 \pm 20)$ ps

  corresponds to a defect with a large open volume (vacancy cluster)

- At low sample temperatures, another positron trap without open volume becomes active (*e. g.* antisite defects).

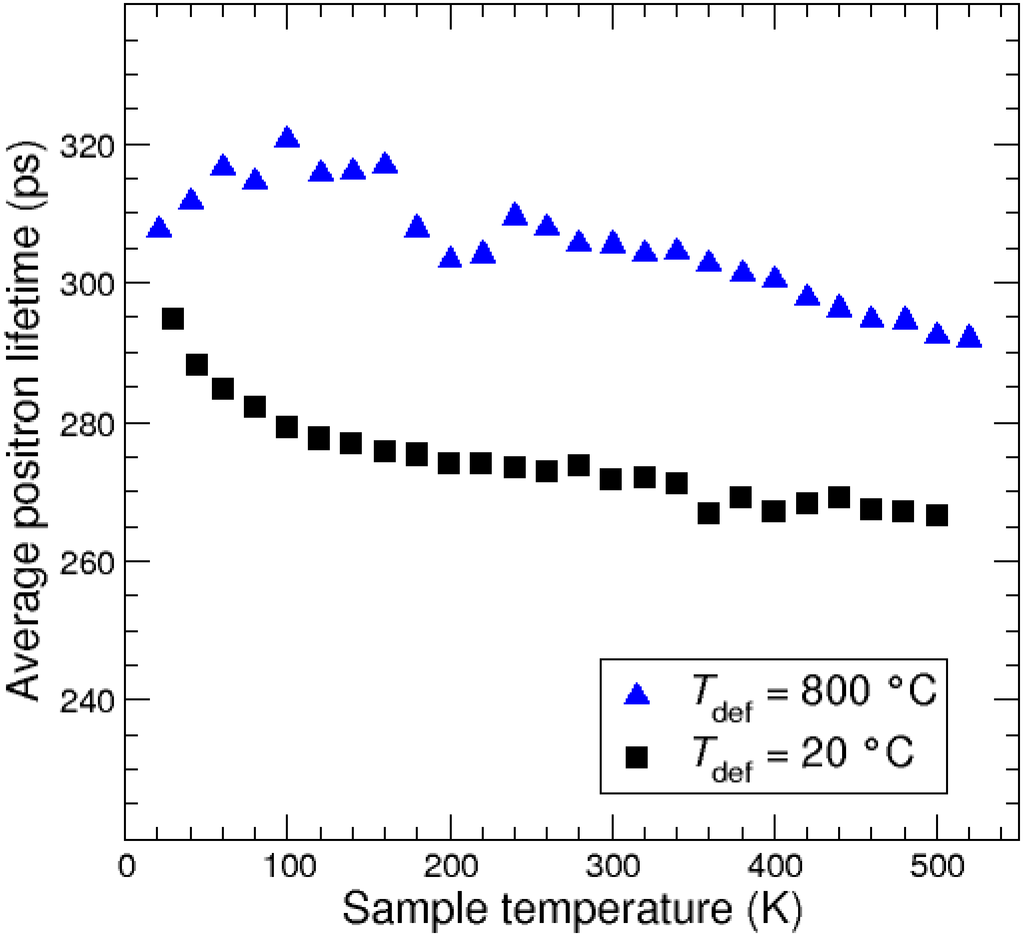
  $\tau_{d1} \approx \tau_b$

Plastic deformation of silicon



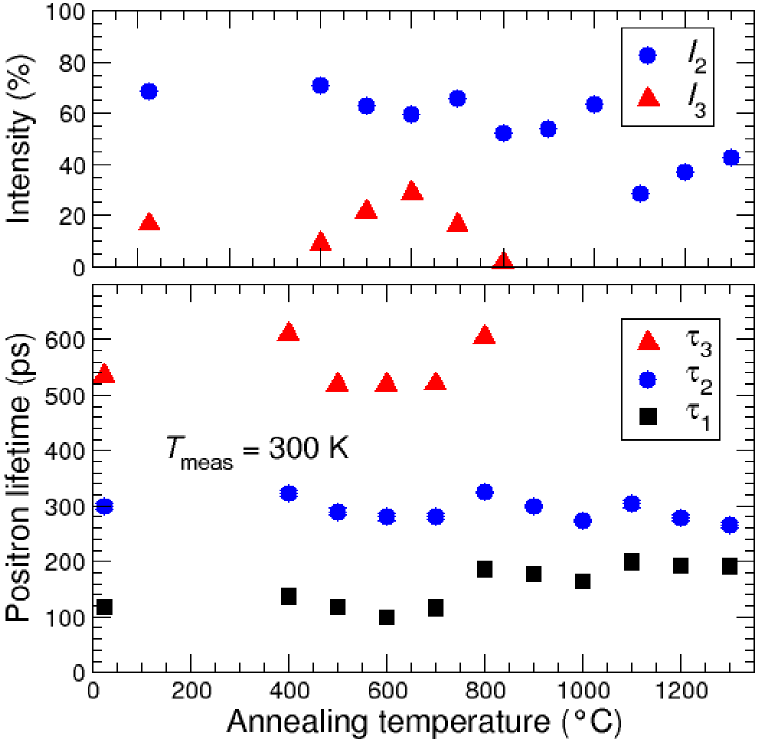
Average positron lifetime a a function of the sample temperature in lightly P-doped FZ Si deformed in [110] direction. 7 % deformation, 2.1×10^{-5} s^{-1} strain rate.

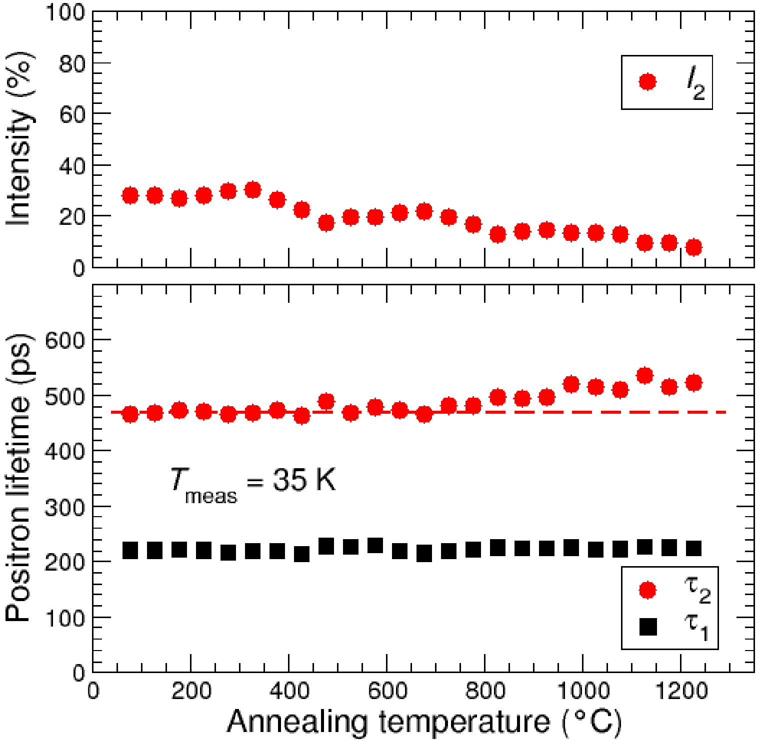
Comparison of high and low deformation temperatures



Positron lifetime as a function of the sample temperature in P-doped Si deformed at room temperature in comparison to high-temperature deformation

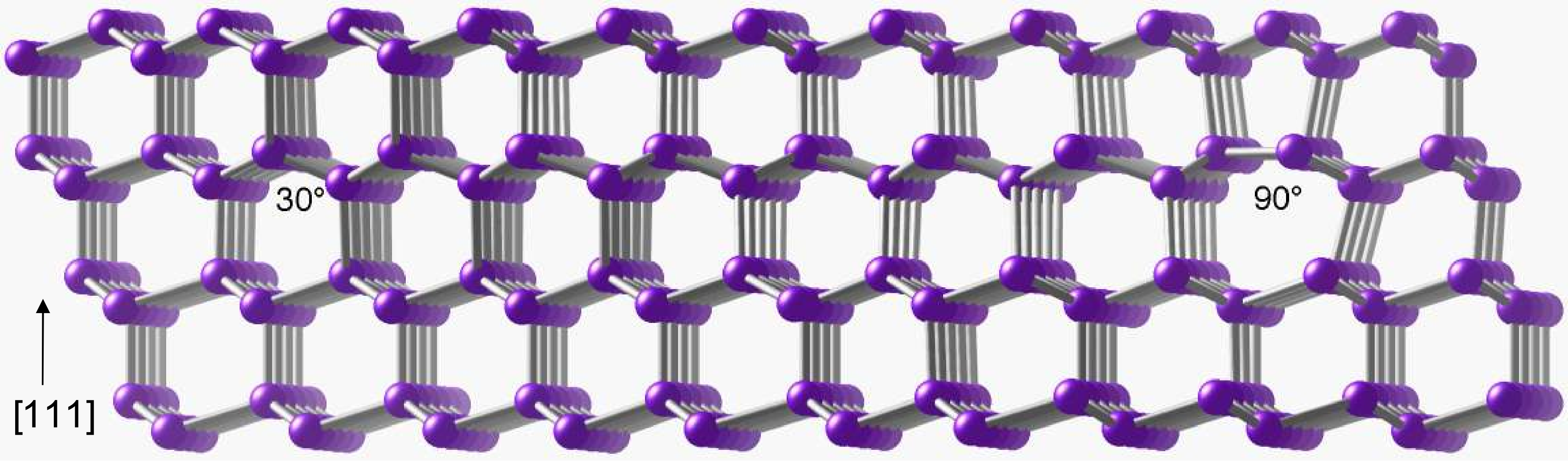
Thermal stability of deformation-induced defects





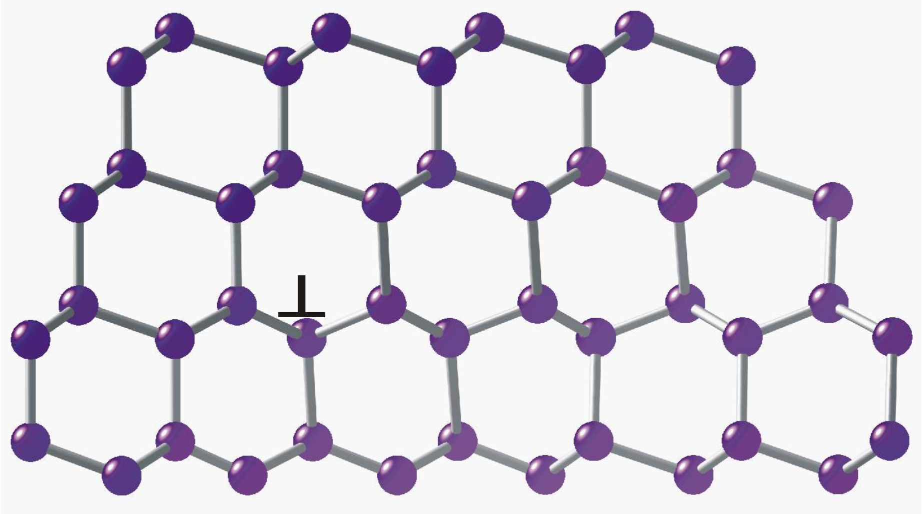
$T_{def} = 800$ °C	$T_{def} = 20$ °C	
$\tau_{d2} = 540$ ps	460 ps	(as deformed)
–	530 ps	(after annealing)
$\tau_{d3} = 280$ ps	–	(as deformed)
280 ps	–	(after annealing)

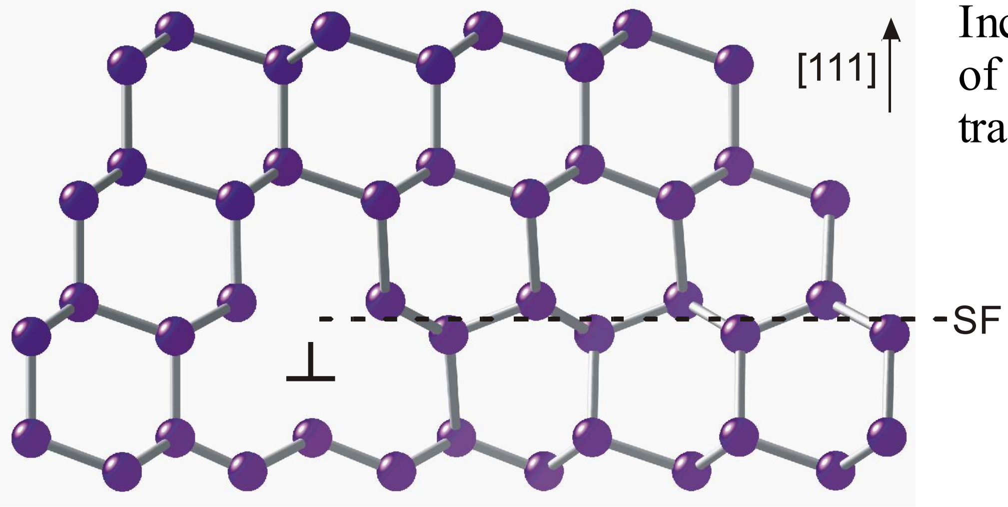
Dissociated dislocation in the diamond structure



Dissociation of a perfect 60° dislocation in the glide set in a 30° and a 90° partial dislocation. There is an intrinsic stacking fault between the two partials. The drawing is along the $(\bar{1}10)$ plane.

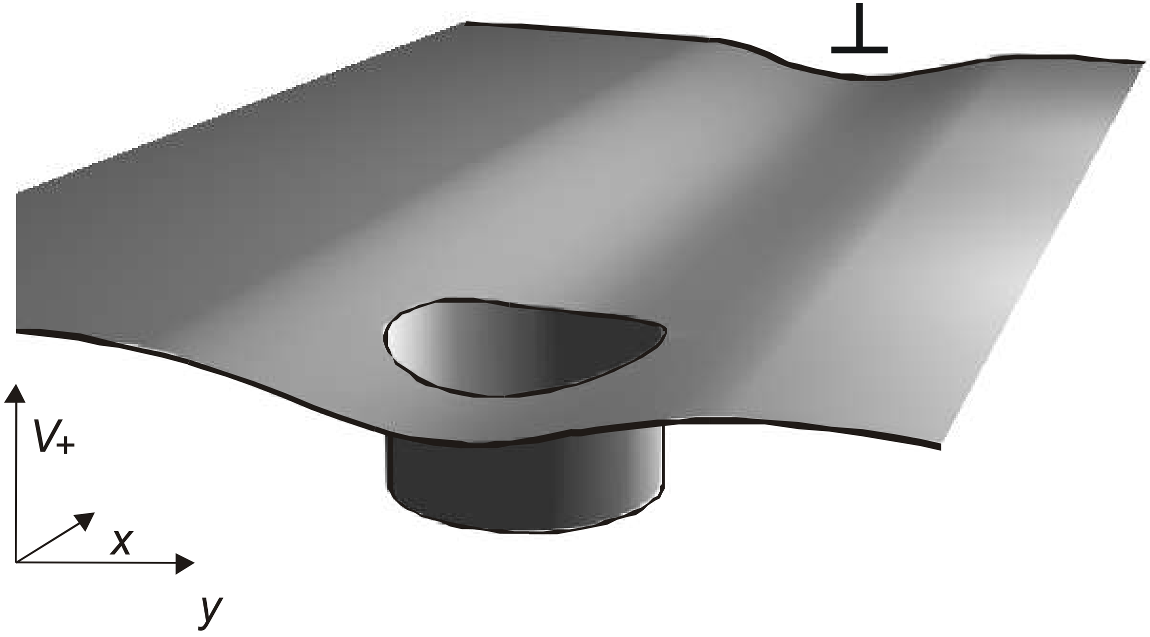
Vacancy incorporation in dislocations





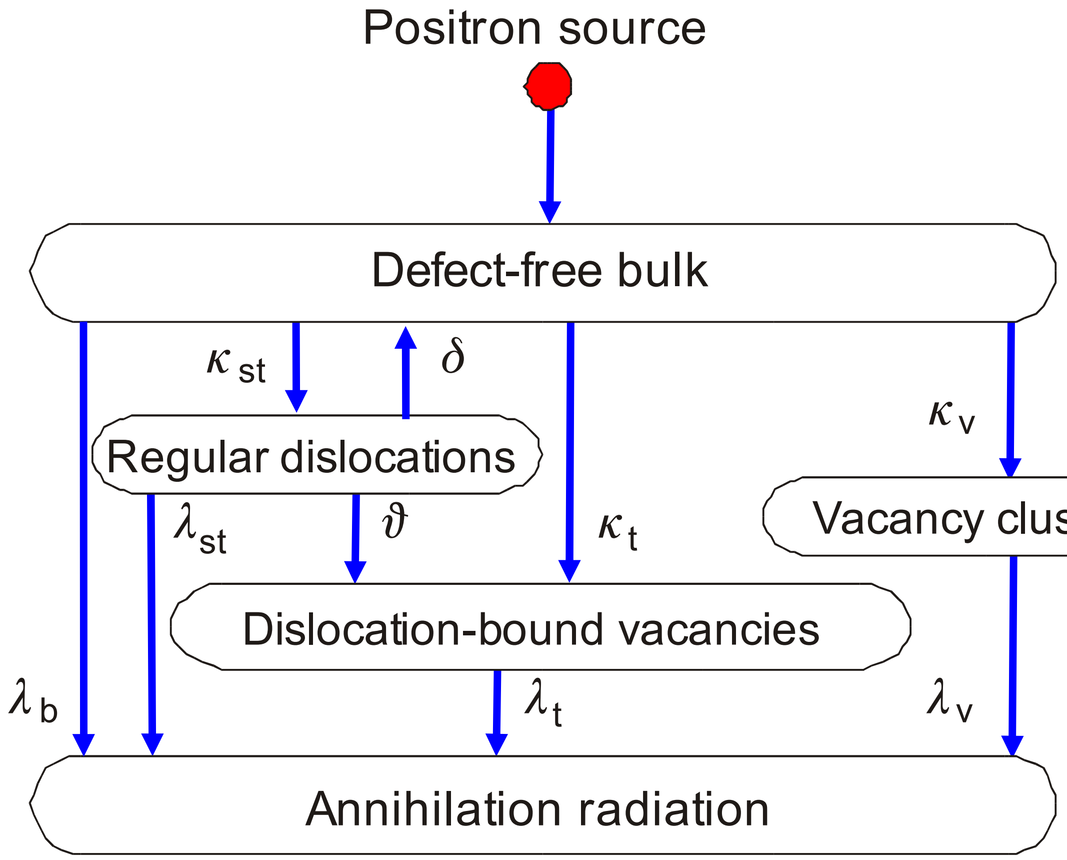
Incorporation of a vacancy in the core of a 30° partial dislocation as a local transition from glide to shuffle set.

Dislocations as positron traps



Positron potential $V_+(x,y)$ of a dislocation. The regular dislocation line is a shallow positron trap, while a bound vacancy acts as a deep trap.

Trapping model in deformed crystals



Positron source

Thermalization

Defect-free bulk

κ_{st}

δ

Trapping and detrapping

κ_{v}

Regular dislocations

Vacancy clusters

$(\tau_i = 1/\lambda_i)$

λ_{st}

ϑ

κ_{t}

Dislocation-bound vacancies

λ_{b}

λ_{t}

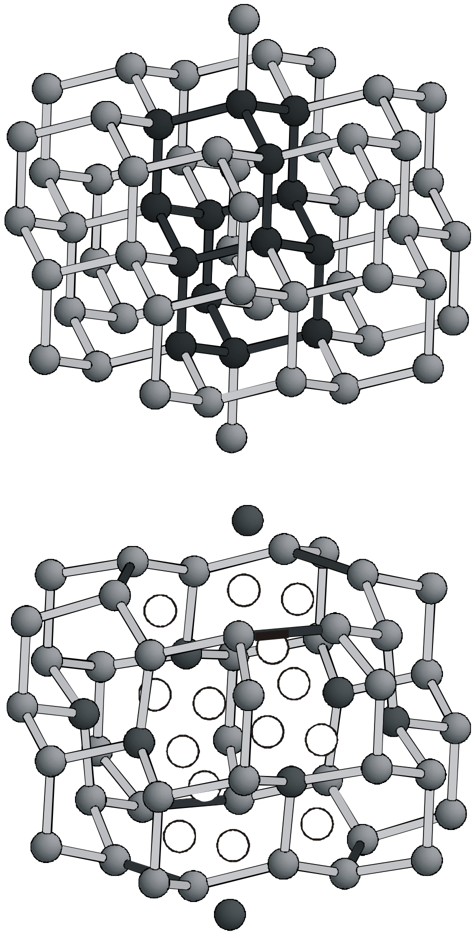
λ_{v}

Annihilation

Annihilation radiation

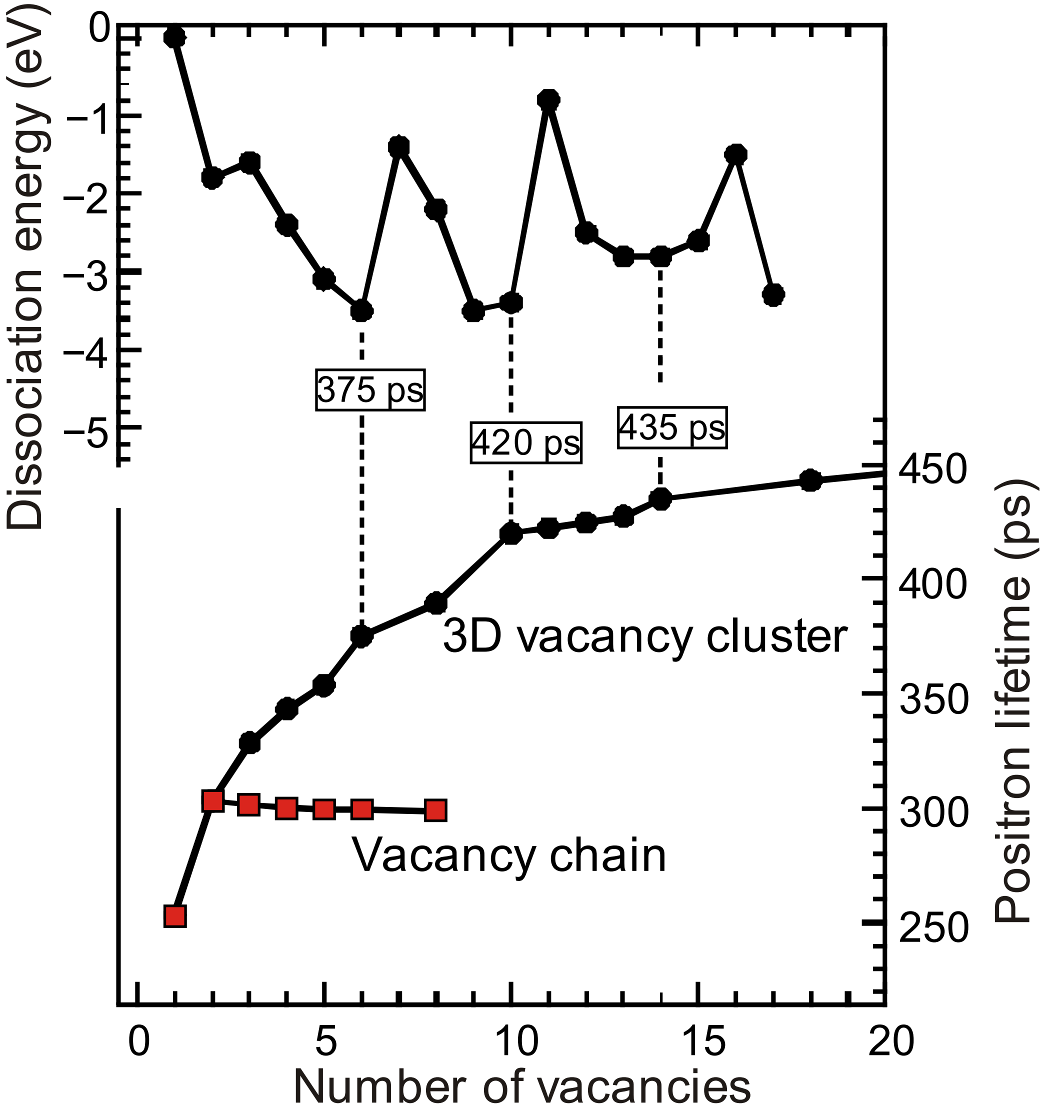
Calculation of vacancy clusters

- Construction of vacancy clusters and relaxation with a self-consistent charge-density-functional-based tight binding (SCC DFTB) method [Elstner *et al.* 1998]
- Method allows the modeling of large supercells (512 atoms), which are needed to avoid defect–defect interactions.
- Different vacancy aggregates were examined in respect of their stability.
- Construction scheme of closed structures with hexagonal rings of vacancies gives clusters of lowest total energy



Vacancy cluster in Si before and after relaxation

Calculation of vacancy clusters



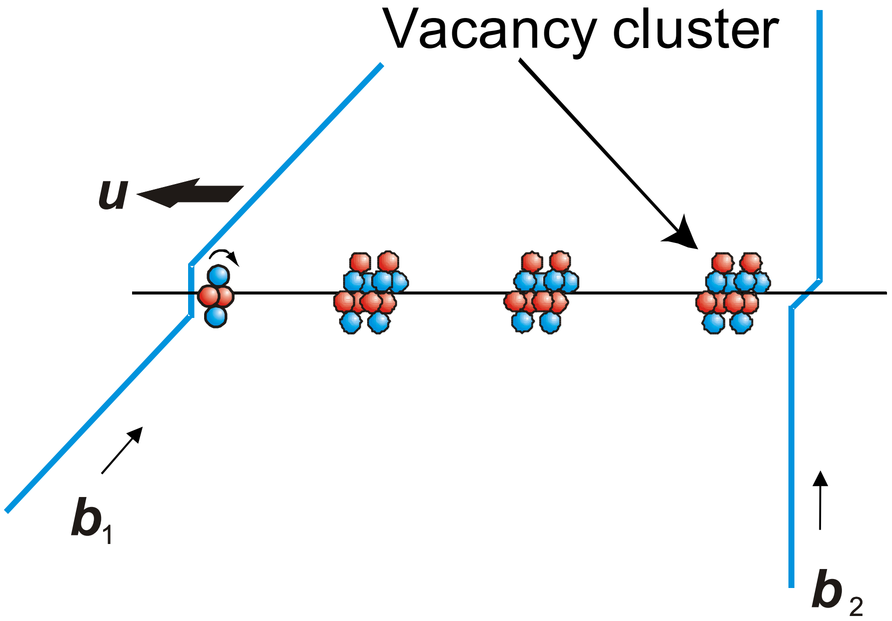
Energy gained by adding a monovacancy to an aggregate of $n - 1$ vacancies in Si (*upper part*) and the corresponding positron lifetime (*lower part*).

[Staab *et al*. 1999]

Results of calculations

- Especially stable structures ($n < 18$): V_{12} in GaAs
  V_6, V_{10}, V_{14} in Si
- Vacancy chains are not energetically favored structures
- The experimentally observed long-lived positron lifetime component may be attributed to V_{12} in GaAs and to V_{14} in Si.
- Magic numbers in silicon $n = 4i + 2$, $i = 1, 2, 3, \ldots$

Formation of vacancy clusters

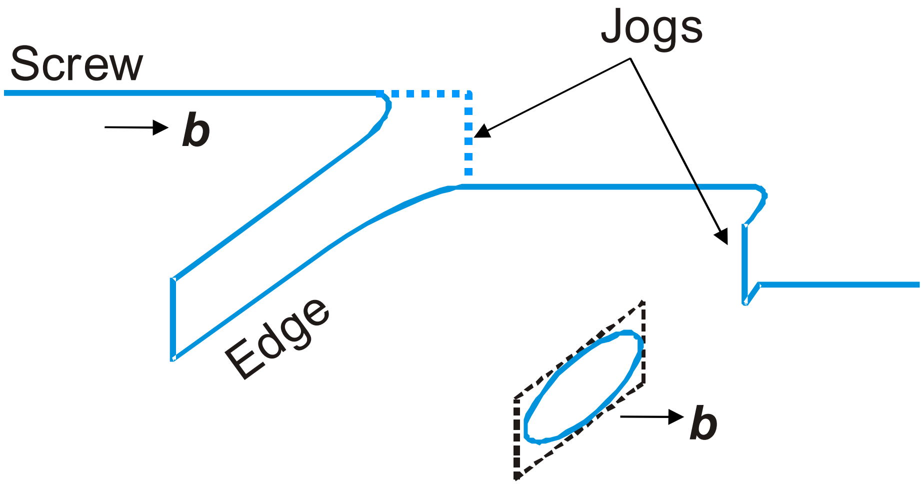


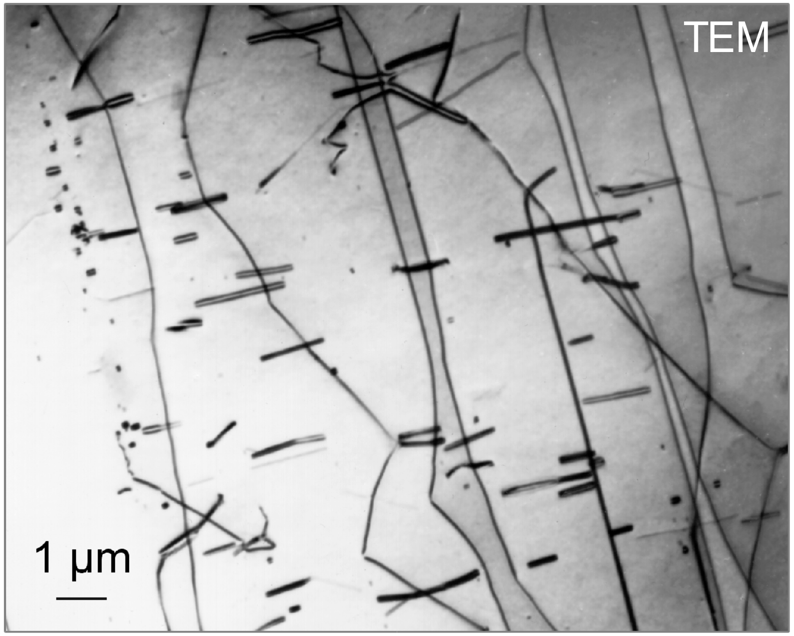
Number of point defects

$$C = \frac{1}{V} \frac{\xi_1 \cdot \boldsymbol{u} \times \xi_2}{|\xi_1 \cdot \boldsymbol{u} \times \xi_2|} \boldsymbol{b}_1 \cdot \boldsymbol{u} \times \boldsymbol{b}_2$$

Agglomeration of vacancies as a result of jog dragging at screw dislocations

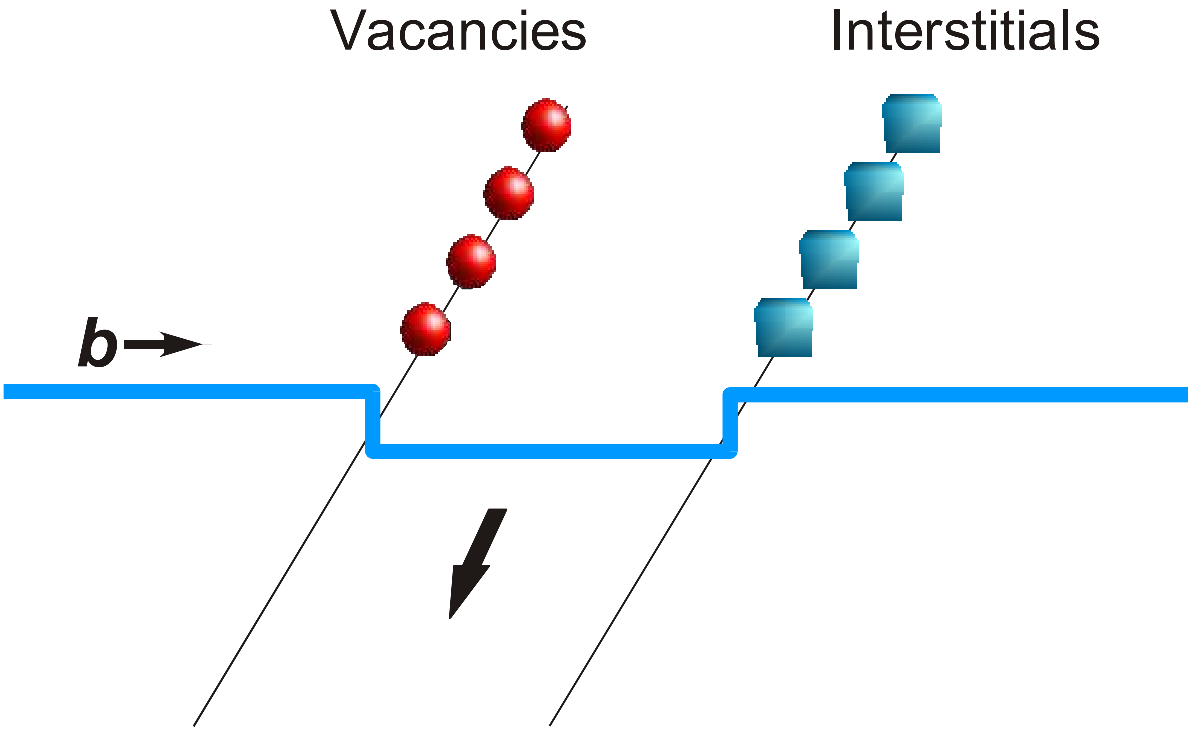
Superjogs





Formation of edge dipoles and prismatic dislocation loops

Vacancies *and* interstitials

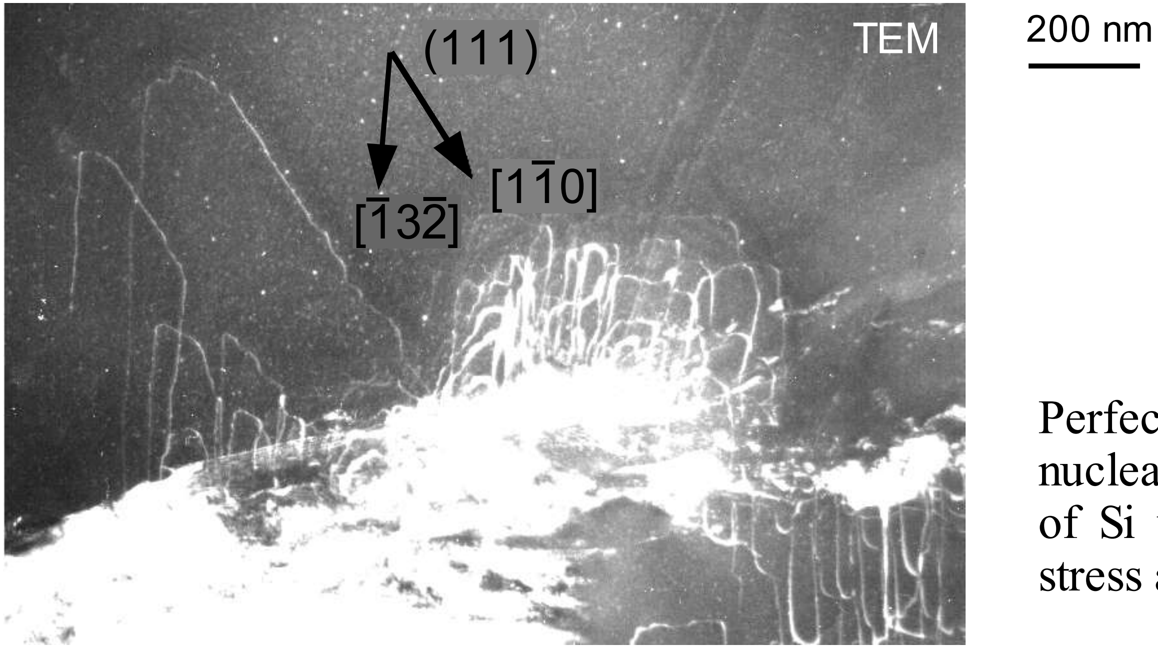


Secondary reactions lead to antisites:

$I_{Ga} + V_{As} \rightarrow Ga_{As}$ $\qquad$ $I_{As} + V_{Ga} \rightarrow As_{Ga}$

Room temperature deformation of Si

- No evidence of dislocations acting as shallow positron traps → low average dislocation density due to inhomogeneous deformation or due to other dislocation character ?
- Large thermally stable vacancy clusters → formation by a jog dragging or cross slip mechanism ?



Perfect shuffle set dislocations nucleated during plastic deformation of Si under conditions of very high stress and low temperatures

[Rabier *et al*. 2002]

Summary

☑ The formation of point defects during plastic deformation of semiconductors can be related to dislocation motion.

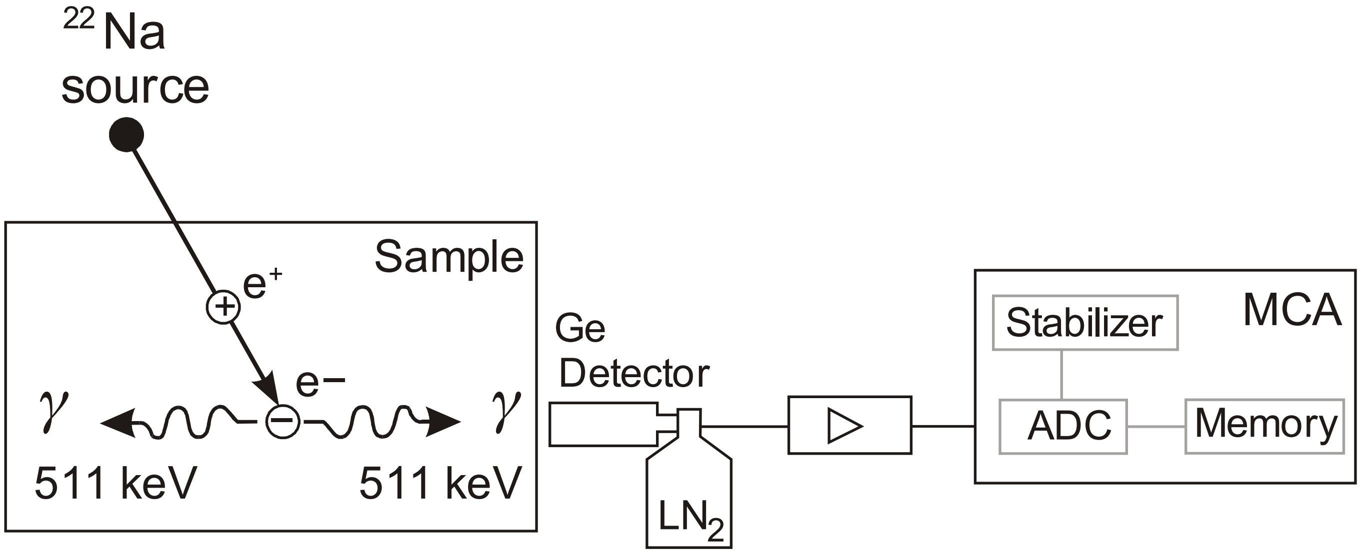
☑ The basic mechanism is the emission of vacancies and interstitials by screw dislocations containing jogs.

☑ Formation of long rows of vacancies is energetically unfavorable.

☑ Stable three-dimensional vacancy agglomerates are formed in a primary process by atomic re-arrangement directly at the climbing jog.

☑ Dislocations are combined positron traps with the regular dislocation line representing a shallow positron trap and bound vacancies as deep traps.

Doppler-broadening spectroscopy



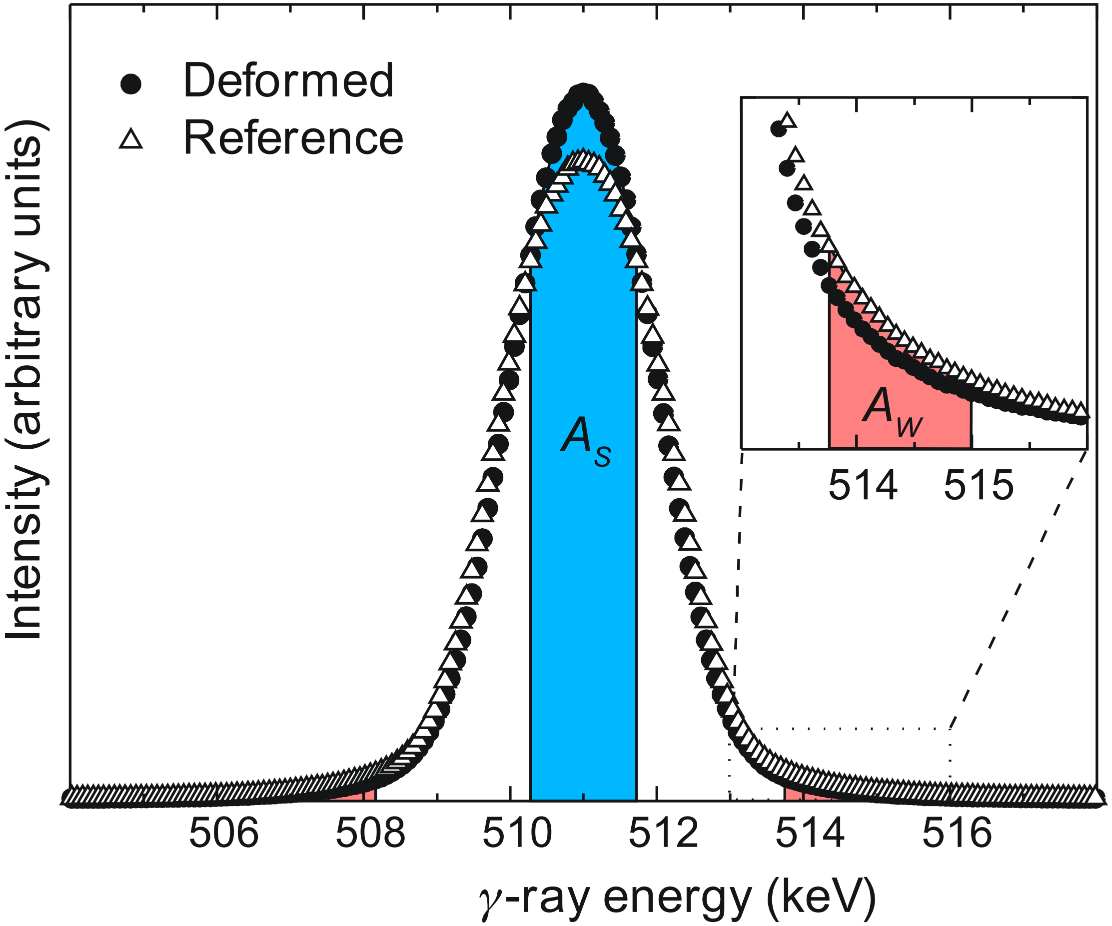
- Momentum conservation during annihilation

  → Doppler shift of the annihilation energy: $\Delta E = p_z c/2$

- Doppler spectrum consists of 10^6 events

  → Doppler-broadening of the annihilation line

Line-shape parameters



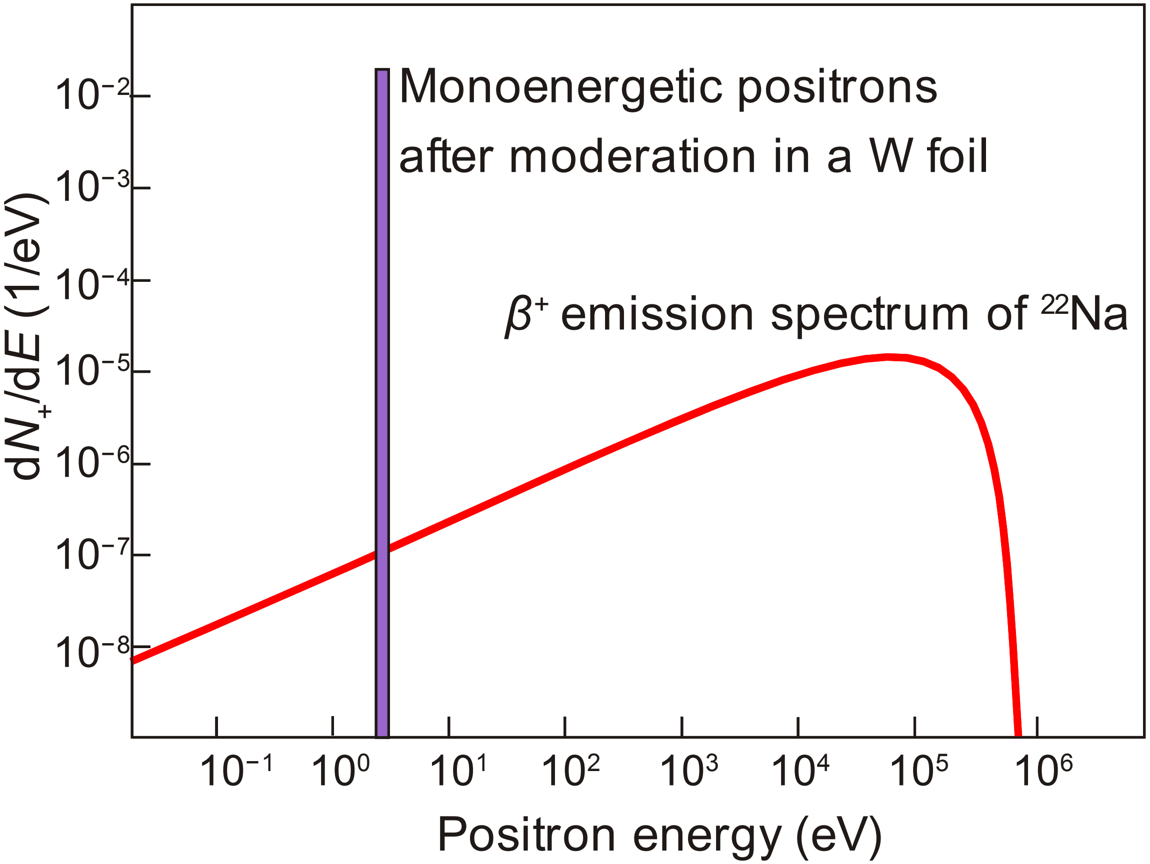
Open-volume defects

- *S* parameter ↗
- *W* parameter ↘

Different sensitivity

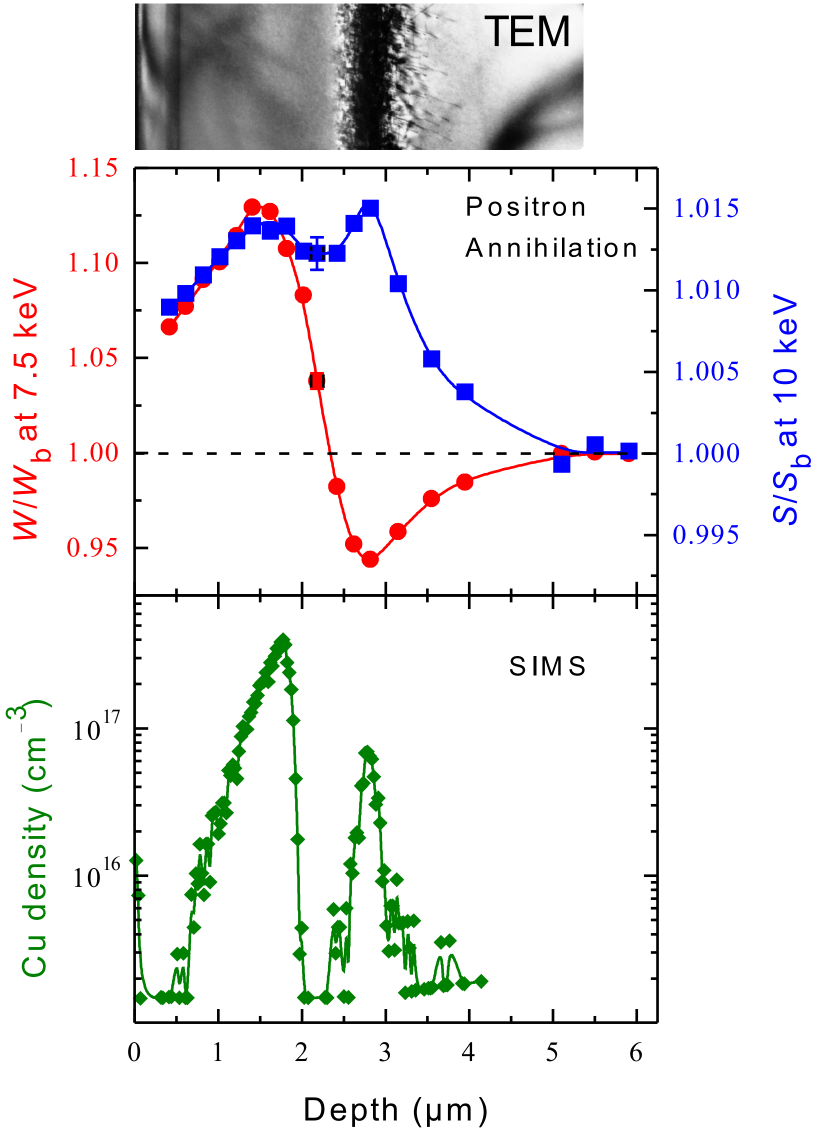
- *S* parameter – valence electron annihilation → open volume
- *W* parameter – core electron annihilation → chemical environment

Monoenergetic positrons



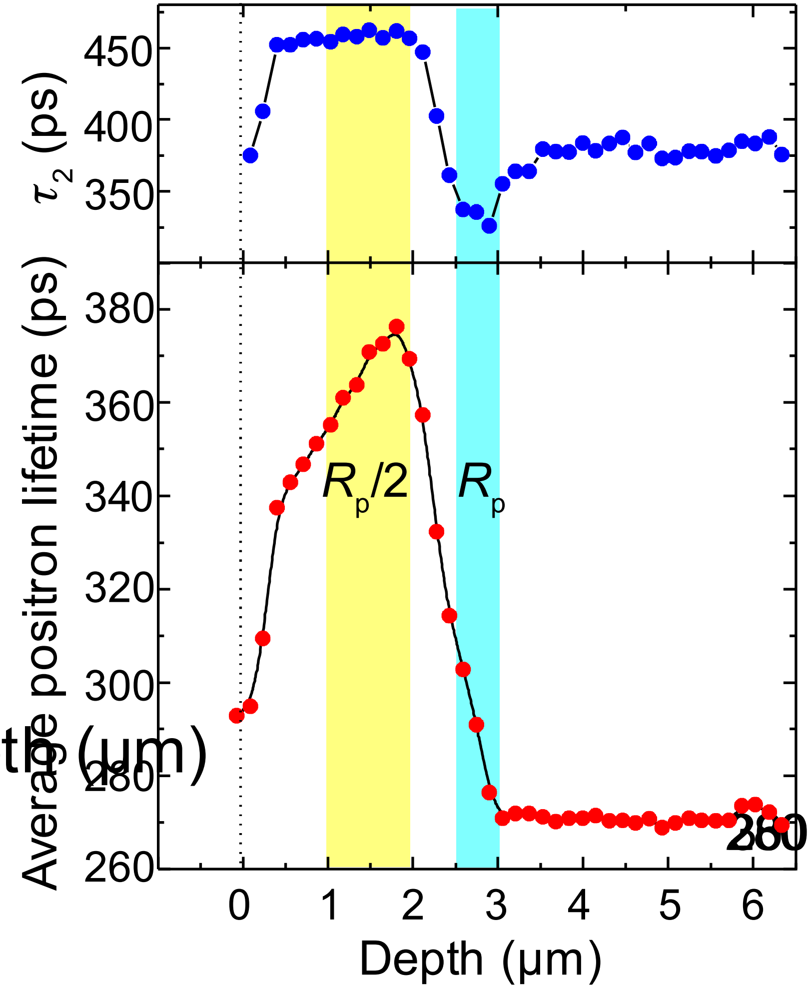
The broad emission positron emission spectrum of a radioactive source (mean e^+ penetration depth in silicon of 50 µm) can be moderated in a tungsten foil.

Gettering centers in self-implanted Si



- After high-energy (3.5 MeV) self-implantation of Si (5×10^{15} cm^{-2}) and RTA annealing (900 °C, 30 s) two gettering zones appear at R_p and $R_p/2$
  (R_p projected range of Si^+)
- Visible by secondary ion mass spectrometry profiling after intentional Cu contamination

Positron lifetime microscopy

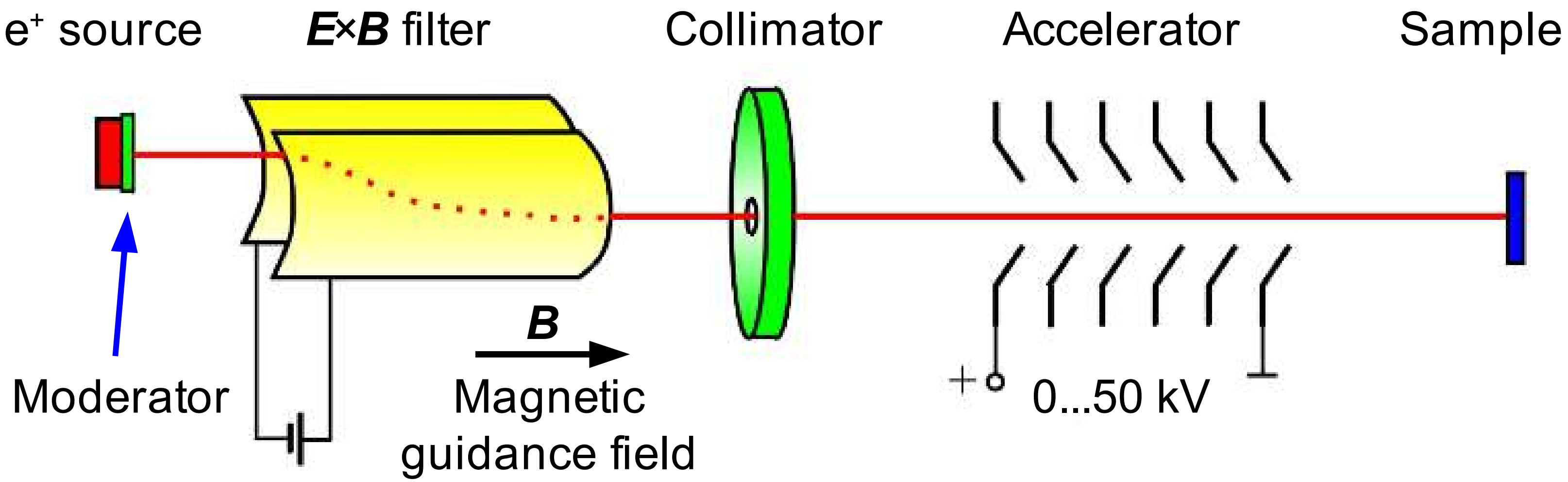


- At $R_p/2$, $\tau_d = 450$ ps (vacancy clusters, V_{14})
- At R_p, $\tau_d = 320$ ps (divacancy-type defect, related to dislocation loops)

Defect profile using the Munich positron lifetime microscope

[Krause-Rehberg *et al.* 2001]

Variable-energy positron beam



- Penetration depth in the sample: 0...5 µm
- Spot diameter: 5 mm
- Time per single Doppler broadening measurement: 20 min
- Time per depth scan: 8 h
- No lifetime measurements possible without bunching

Defect profiling