Forschergruppenkolloquium
Institut für Geowissenschaften, Christian-Albrechts-Universität Kiel

Investigation of dislocations and vacancy clusters by means of positron annihilation

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Overview

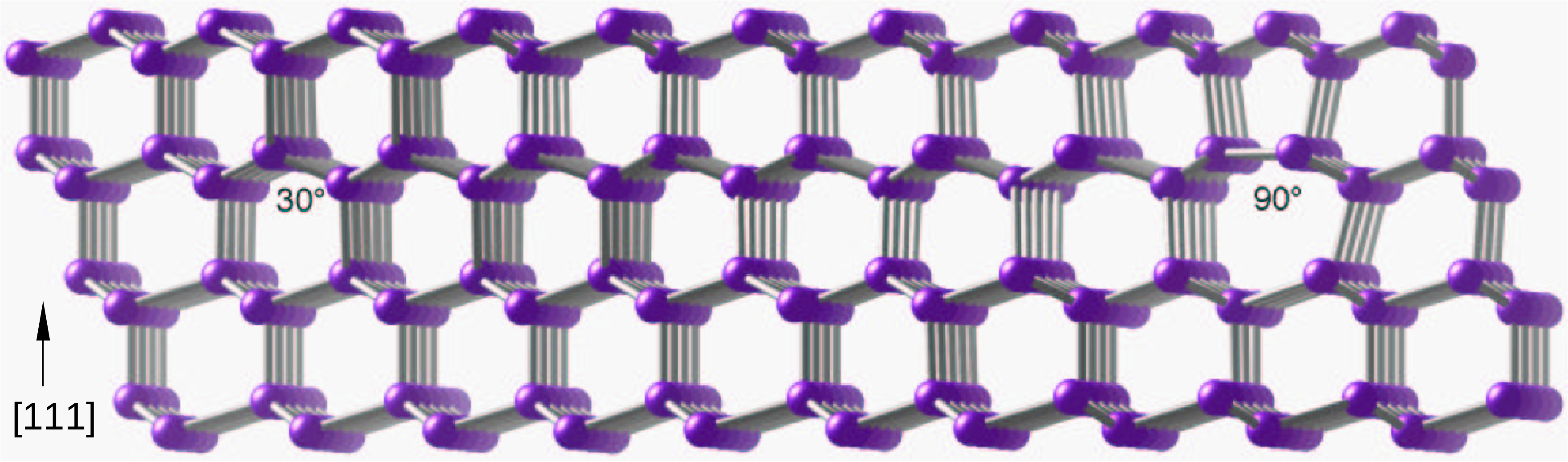
- Dislocations in semiconductors – core structure
- Dislocation dynamics – plastic deformation
- Formation of point defects during plastic deformation
- What we can learn from positron annihilation about defect structures?
- Calculations of vacancy clusters
- Modell of point defect generation

Core structure of dislocations

60° dislocation in the diamond structure, $\boldsymbol{b} = \frac{a}{2}\langle 110\rangle$.
[Shockley 1953]

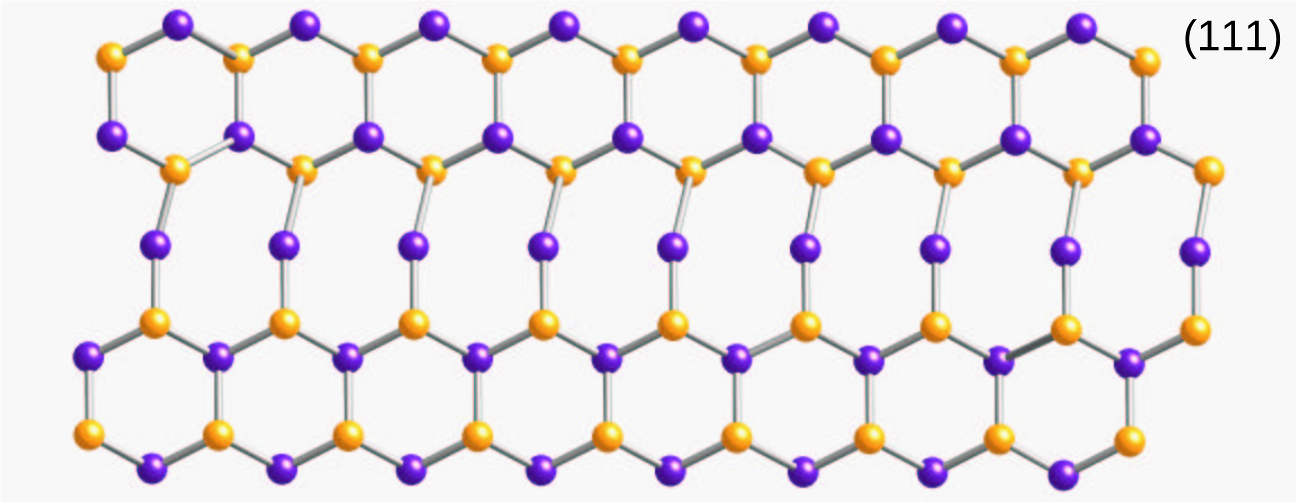
Not like this *!*

Dissociation

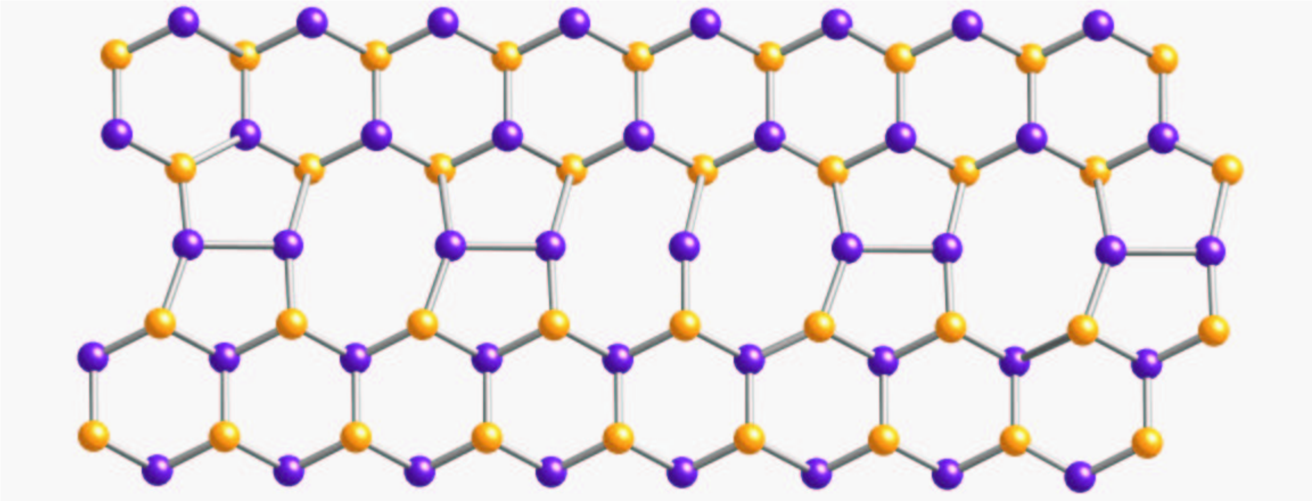


Dissociation of a perfect 60° dislocation in the glide set in a 30° and a 90° partial dislocation. There is an intrinsic stacking fault between the two partials. The drawing is along the $(1\bar{1}0)$ plane.

Reconstruction

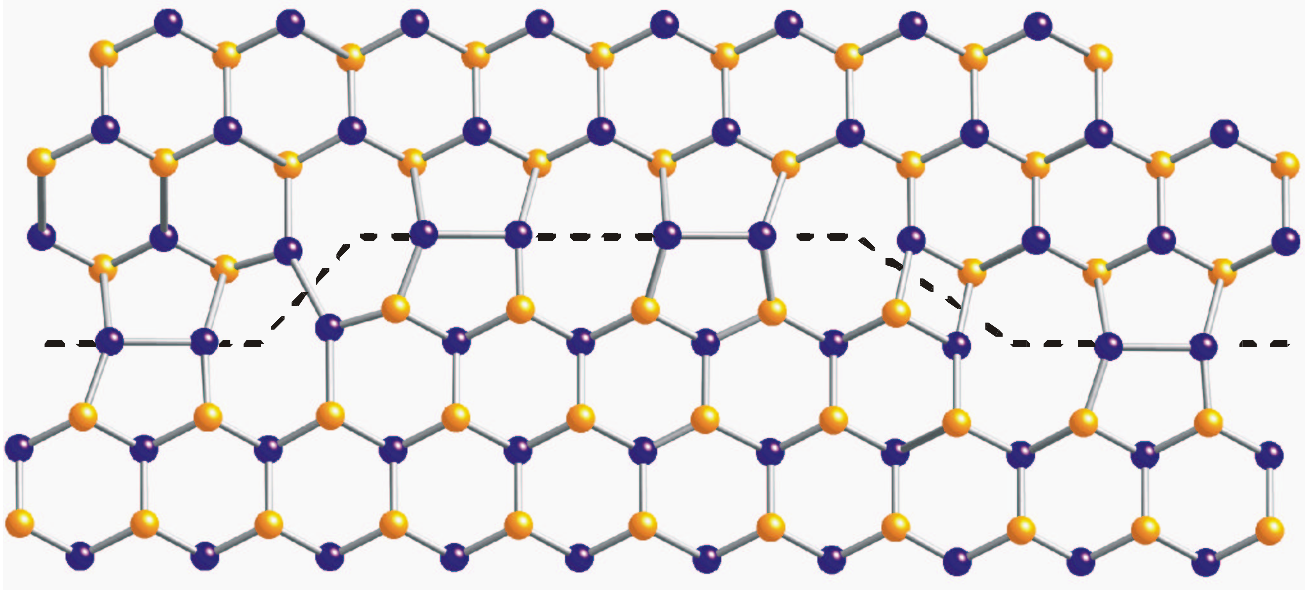


Unreconstructed
30° partial dislocation



Reconstructed
30° partial dislocation

Dislocation defects



Kink pair on a 30° partial dislocation

Analysis of the stress–strain curve

- ***Dislocation velocity***

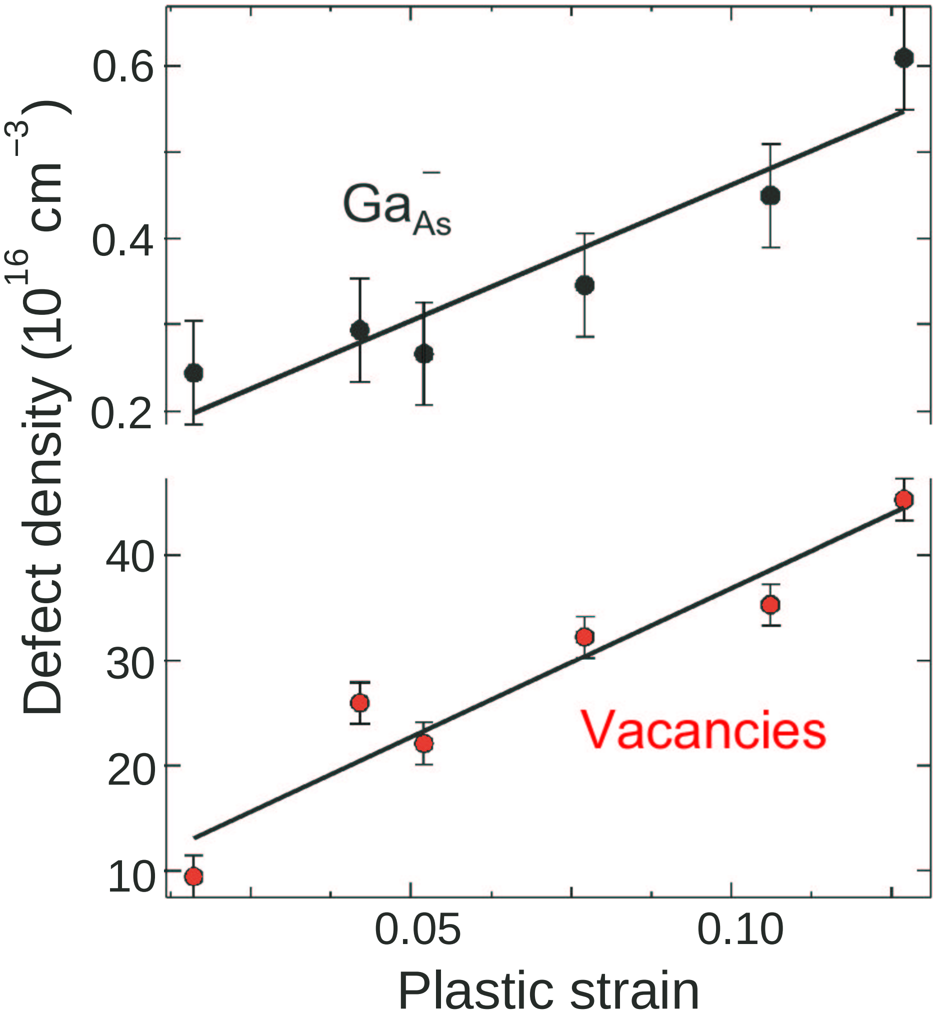
$$v = B\,\tau_{\mathrm{eff}}^{m}\exp\left(-\frac{U}{k_B T}\right)$$

- ***Lower yield stress***

$$\tau_{\mathrm{ly}} = C\,\dot{\varepsilon}^{1/(2+m)}\exp\left[\frac{U}{(2+m)\,k_{\mathrm{B}}\,T}\right]$$

	$2 + m$	U/eV	Q_{d}/eV	Q_{d}/U
Si	2.3	2.30	3.5	1.52
InSb	3.1	0.96	1.5	1.56
InP	2.9	1.43	2.3	1.61
GaAs	3.6	1.35	2.0	1.48
GaSb	3.0	1.20	1.7	1.42

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

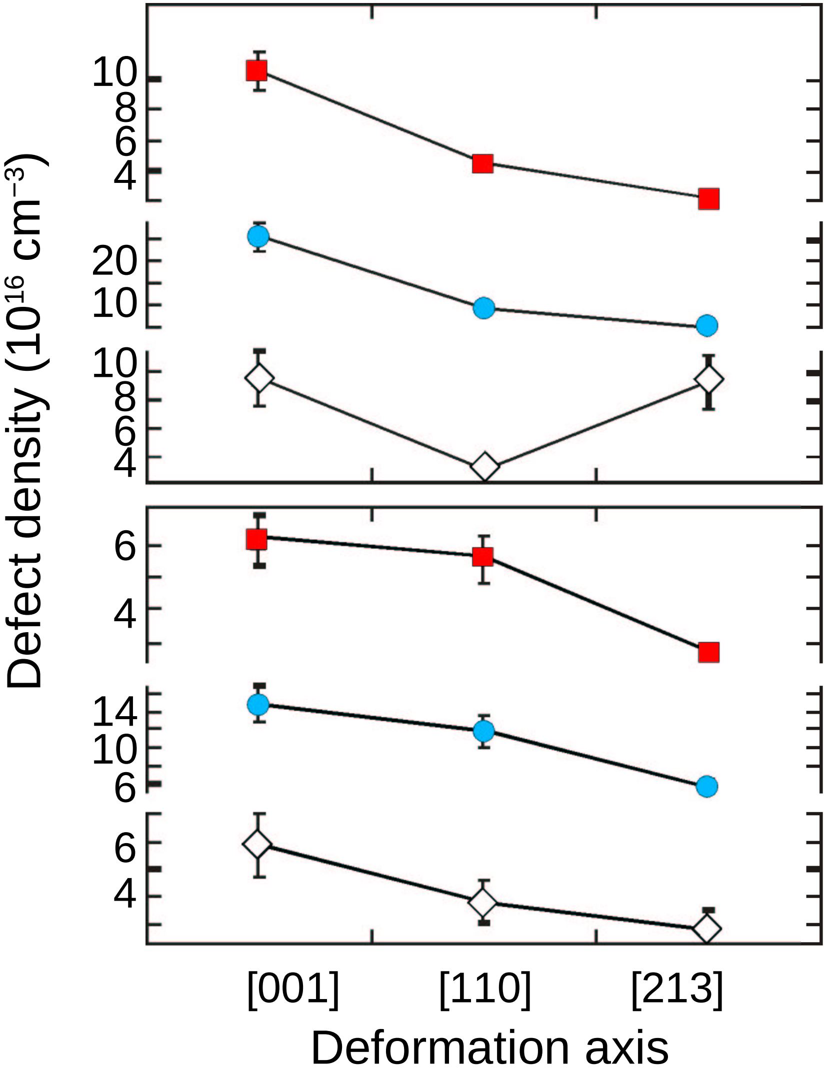


Density of vacancies and antisite defects as a function of the strain. Result of measurements by positron annihilation in plastically deformed GaAs. Uniaxial compression in [110] direction at 773 K, strain rate 1×10^{-3} s^{-1}.

Relation between excess vacancy density and strain

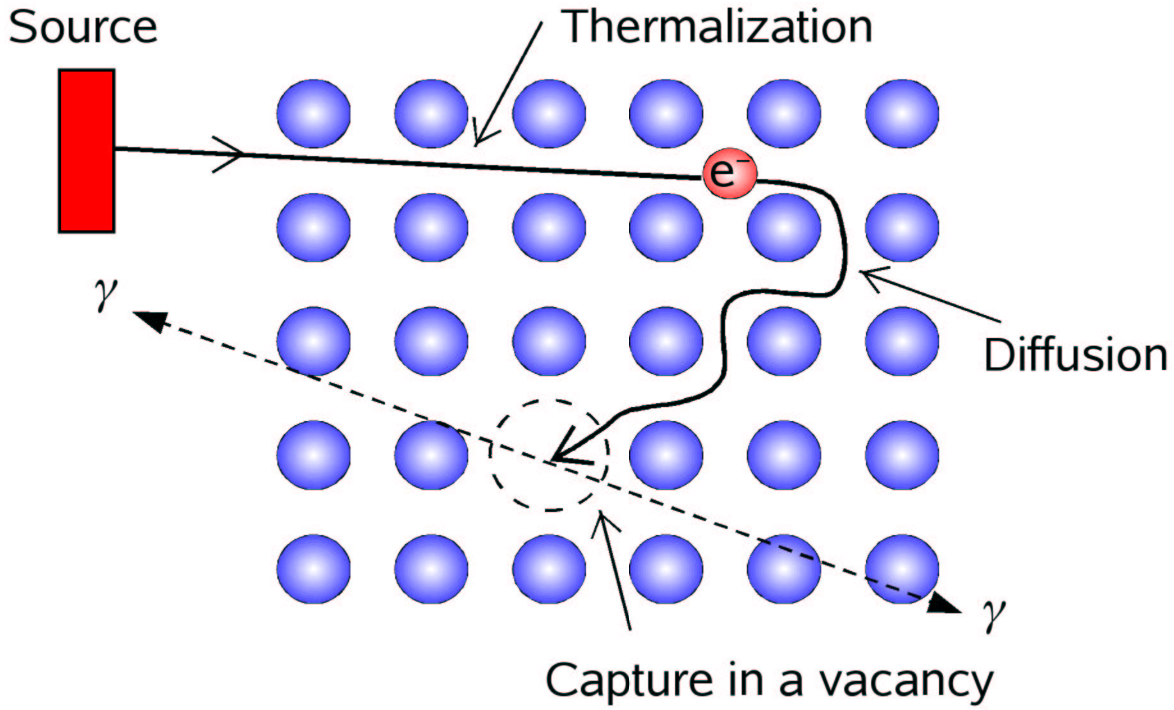
$$\rho_v = \frac{l_g \zeta c_j}{l\, b^2 m} \varepsilon$$

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



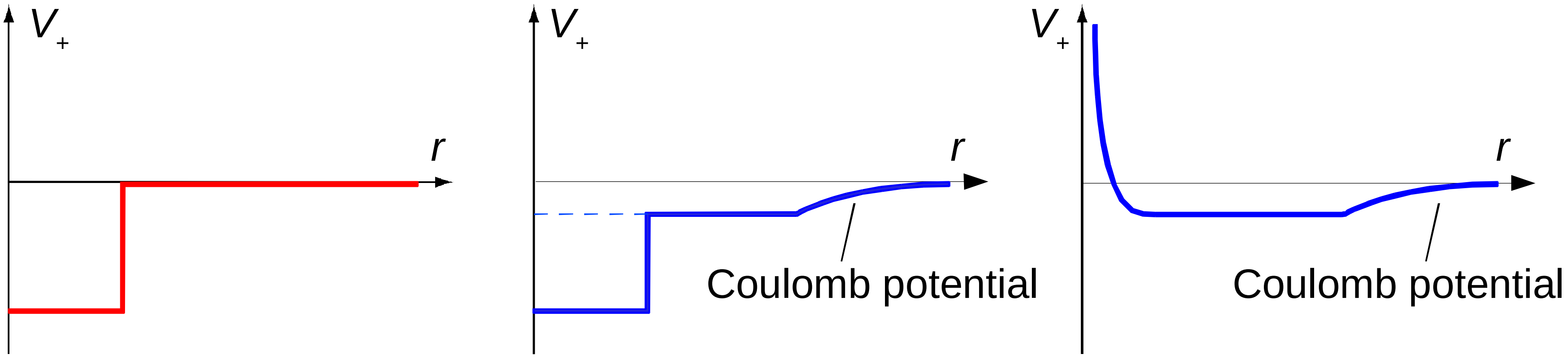
Total number of vacancies in the bulk (□), vacancies bound at dislocations (○), as well as number of Ga_{As} antisites (◇) in plastically deformed GaAs. Deformation temperature 773 K, strain 3 %, strain rate 7.5×10^{-5} s^{-1} (*above*), 3×10^{-4} s^{-1} (*below*).

Positron annihilation



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

Positron capture in defects

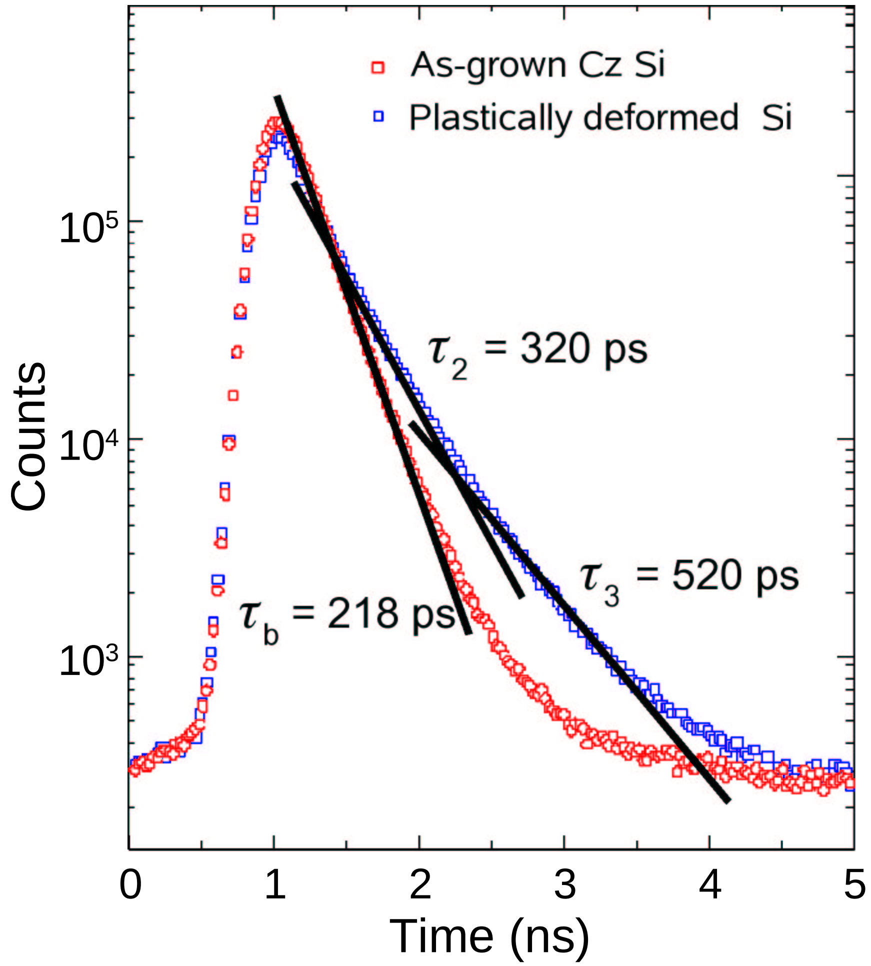


$\lambda \propto$ open volume

$\lambda \approx \lambda_b$

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).

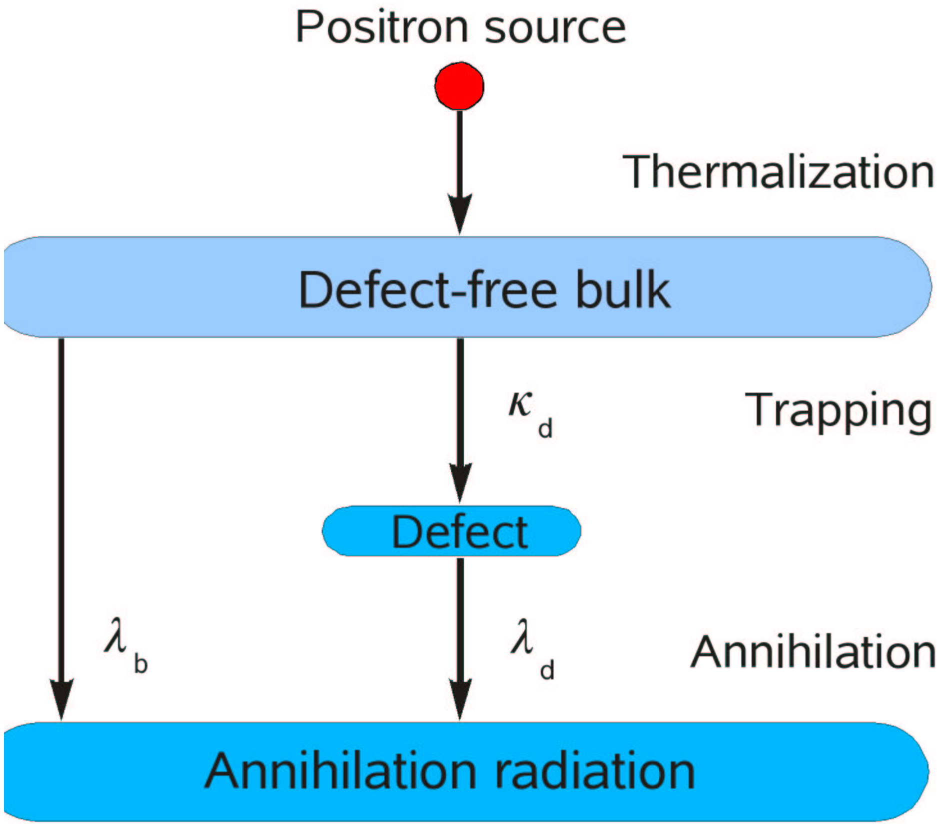
Positron lifetime spectrum



Decomposition of experimental positron lifetime spectra:

- Undeformed Czochralski Si:
  one component, τ_b = 218 ps
- Plastically deformed Si:
  (3 %, 1050 K)
  three components
  τ_1 = 120 ps (not shown),
  τ_2 = 320 ps, τ_3 = 520 ps

Trapping model



Positron source

Thermalization

Defect-free bulk

κ_d

Trapping

Defect

λ_b

λ_d

Annihilation

Annihilation radiation

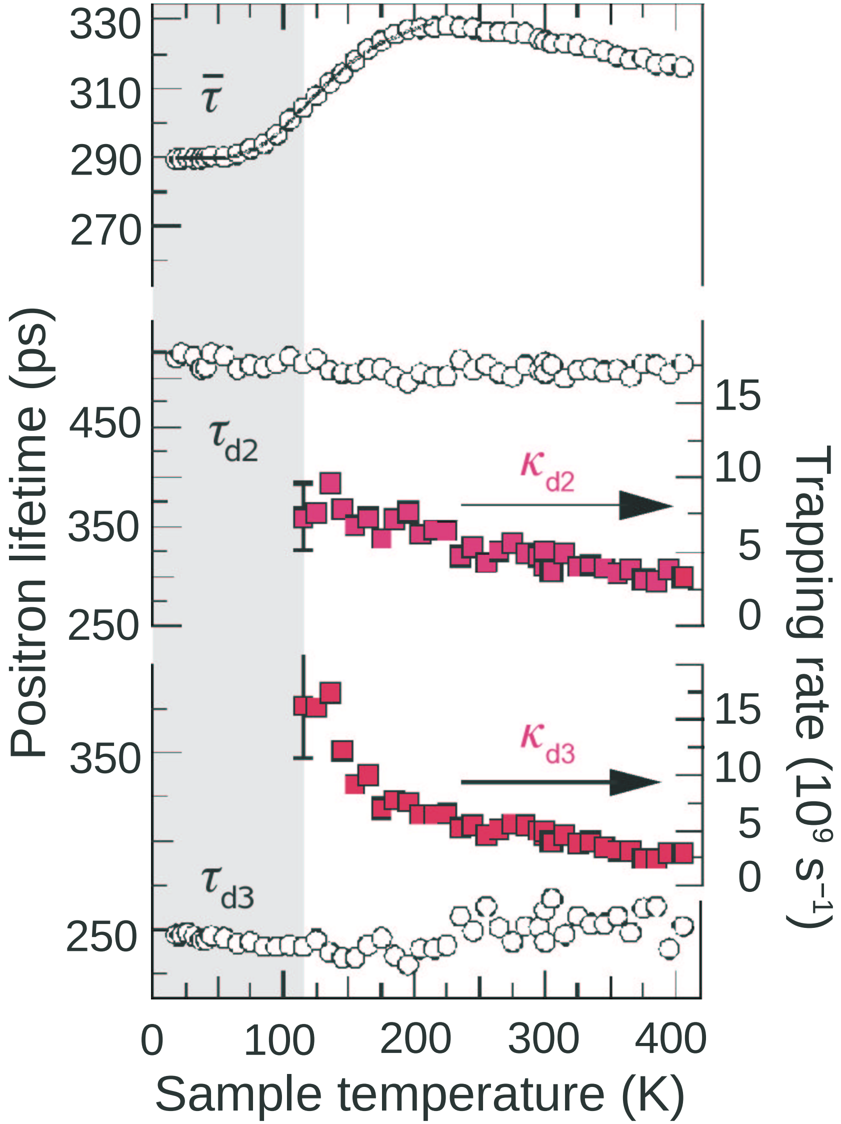
- Quantitative analysis of positron trapping by a set of rate equations
- Solution (lifetime spectrum):

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

Trapping rate: $\kappa_\mathrm{d} = \mu C_\mathrm{d}$

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

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

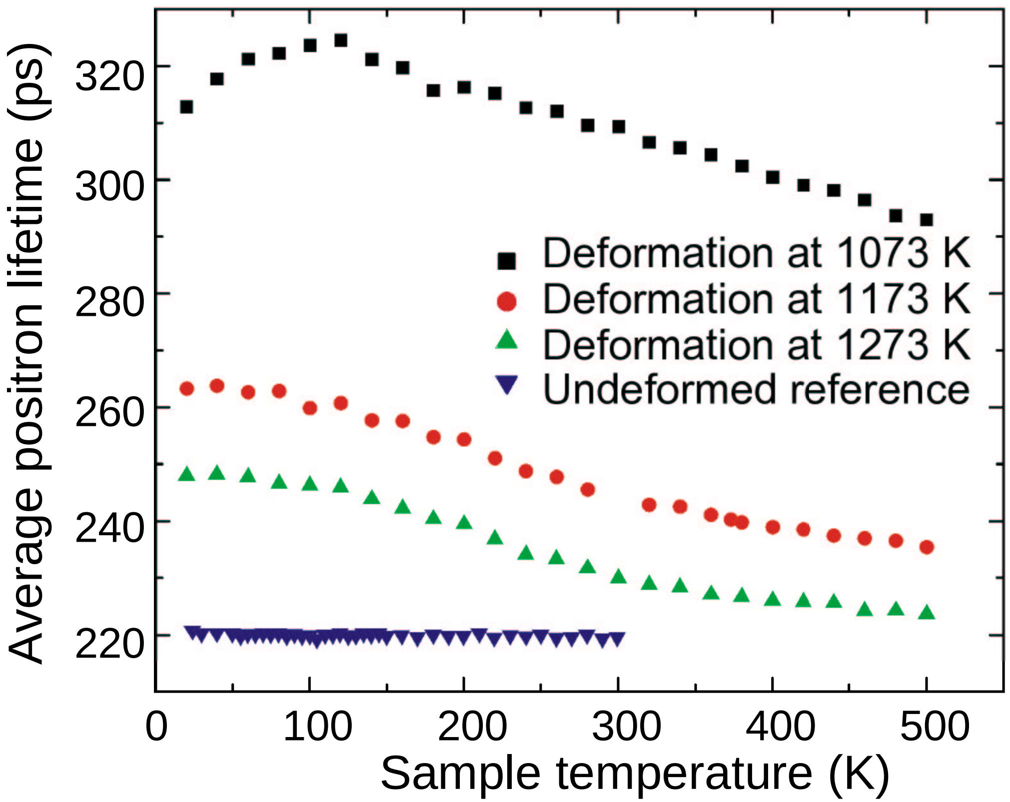
- $\tau_3 = \tau_{d2} = (477 \pm 20)$ ps

  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).

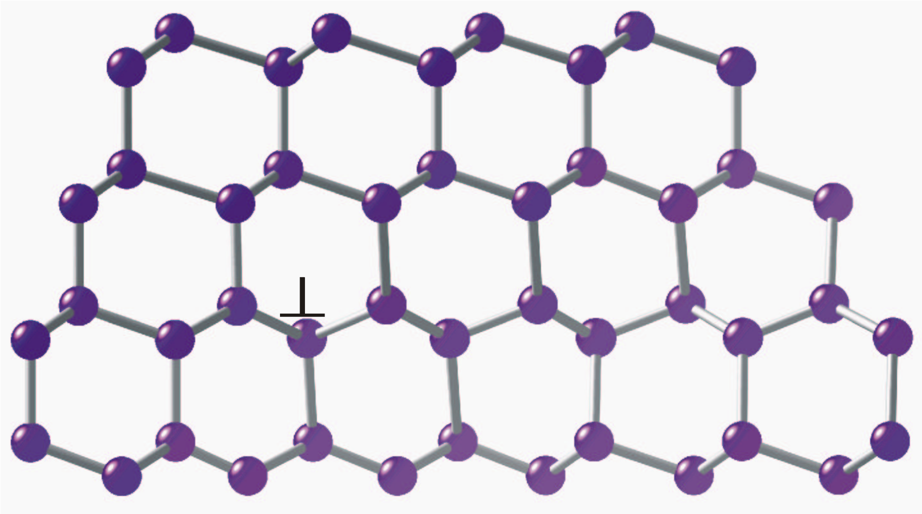
  $\tau_{d1} \approx \tau_b$

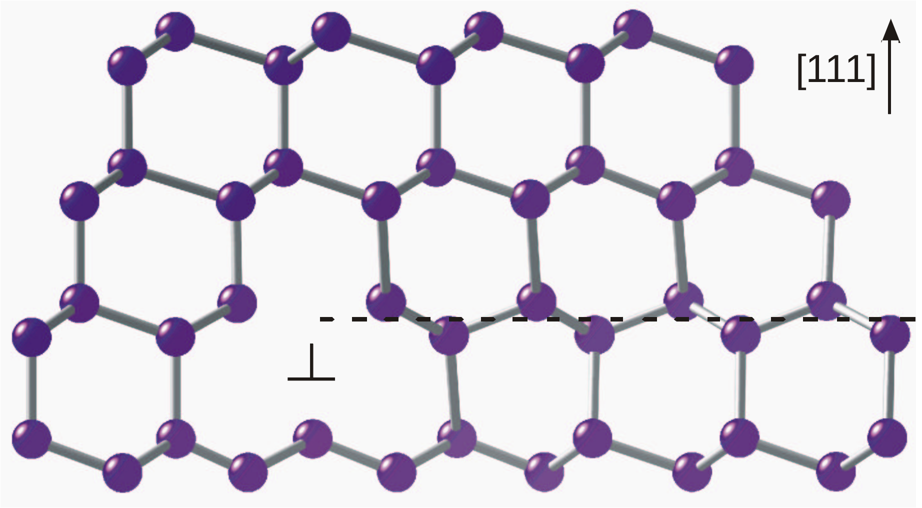
Plastic deformation of silicon



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.

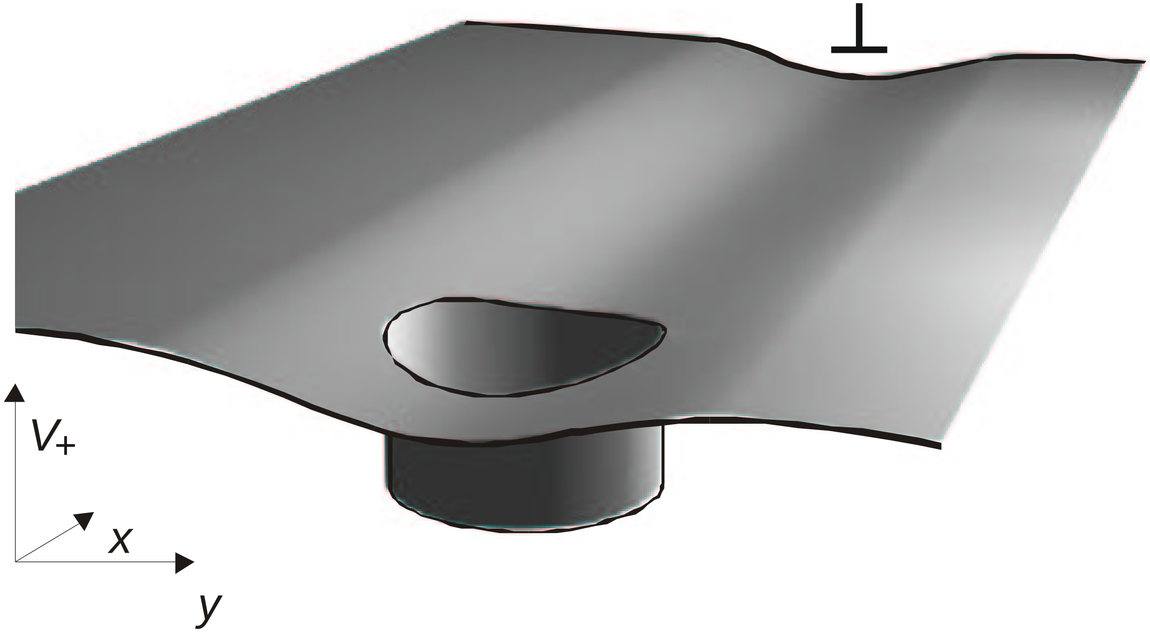
Vacancy incorporation in dislocations





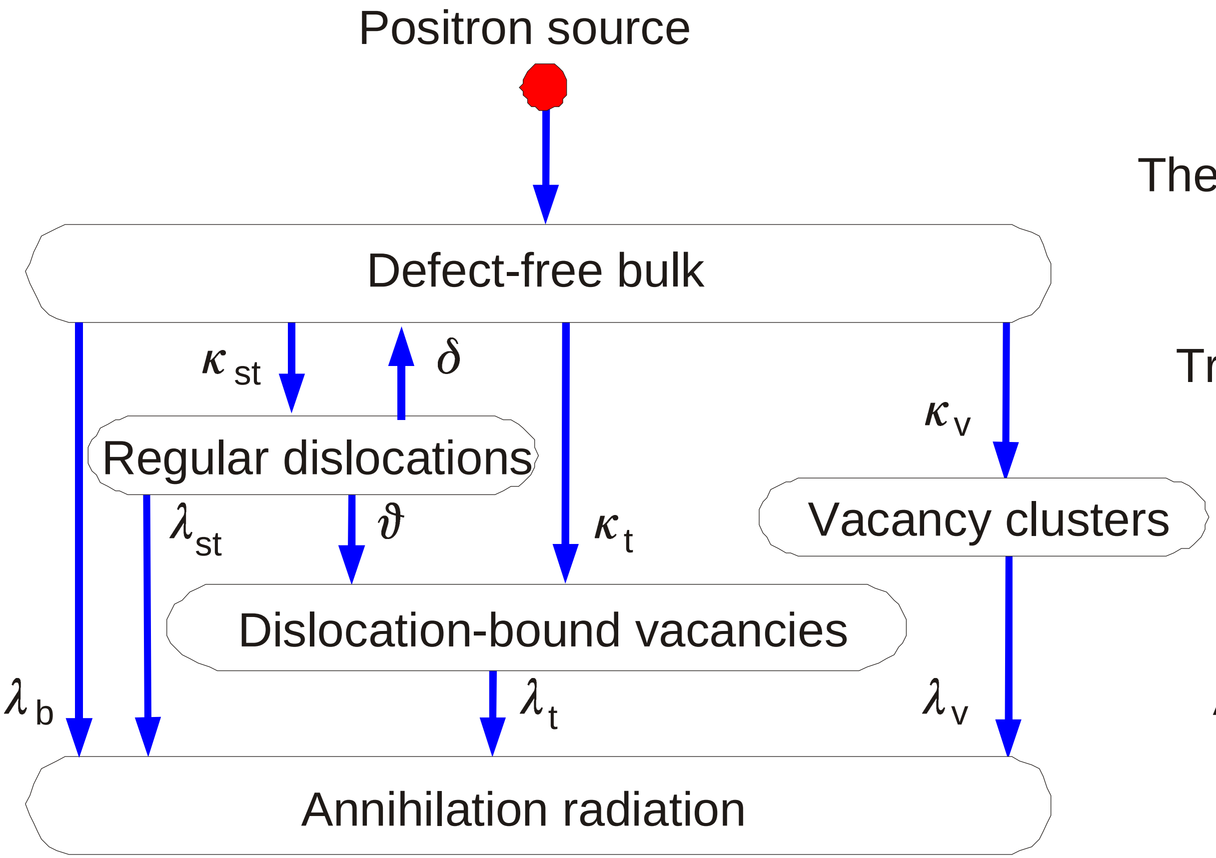
Incorporation of a vacancy in the core of a 30° partial dislocation as a local transition from glide to shuffle set.

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

Defect-free bulk

κ_{st} δ

Regular dislocations

κ_{v}

Vacancy clusters

λ_{st} ϑ κ_{t}

Dislocation-bound vacancies

λ_{b} λ_{t} λ_{v}

Annihilation radiation

Thermalization

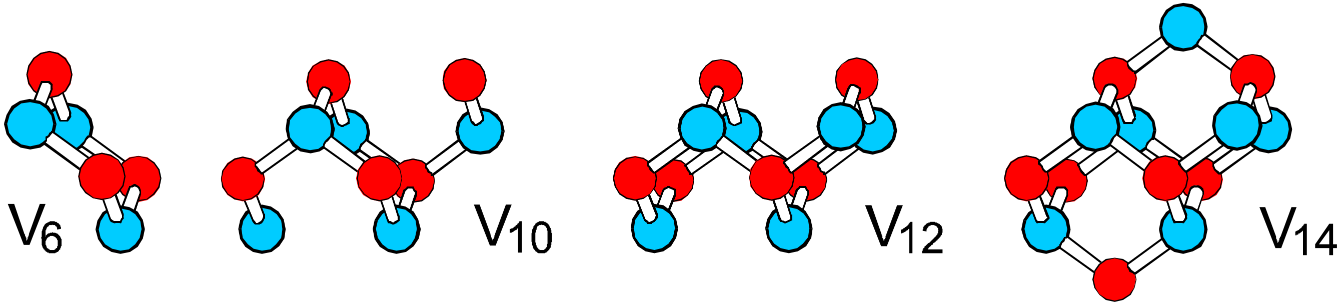
Trapping and
detrapping

Annihilation

$(\tau_i = 1/\lambda_i)$

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

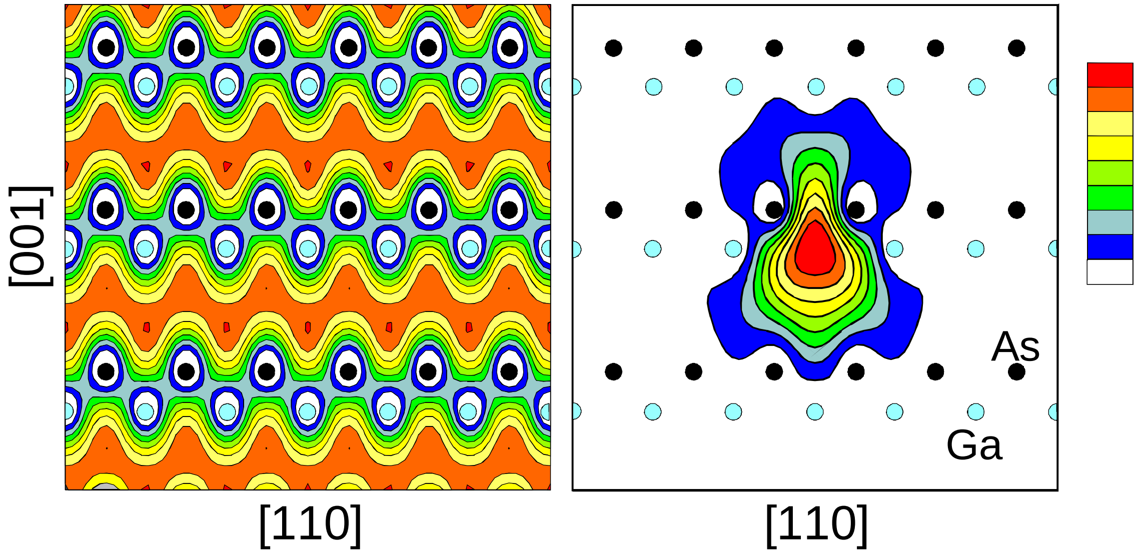


Structure of some unrelaxed V_n clusters in GaAs

Calculation of the positron lifetime

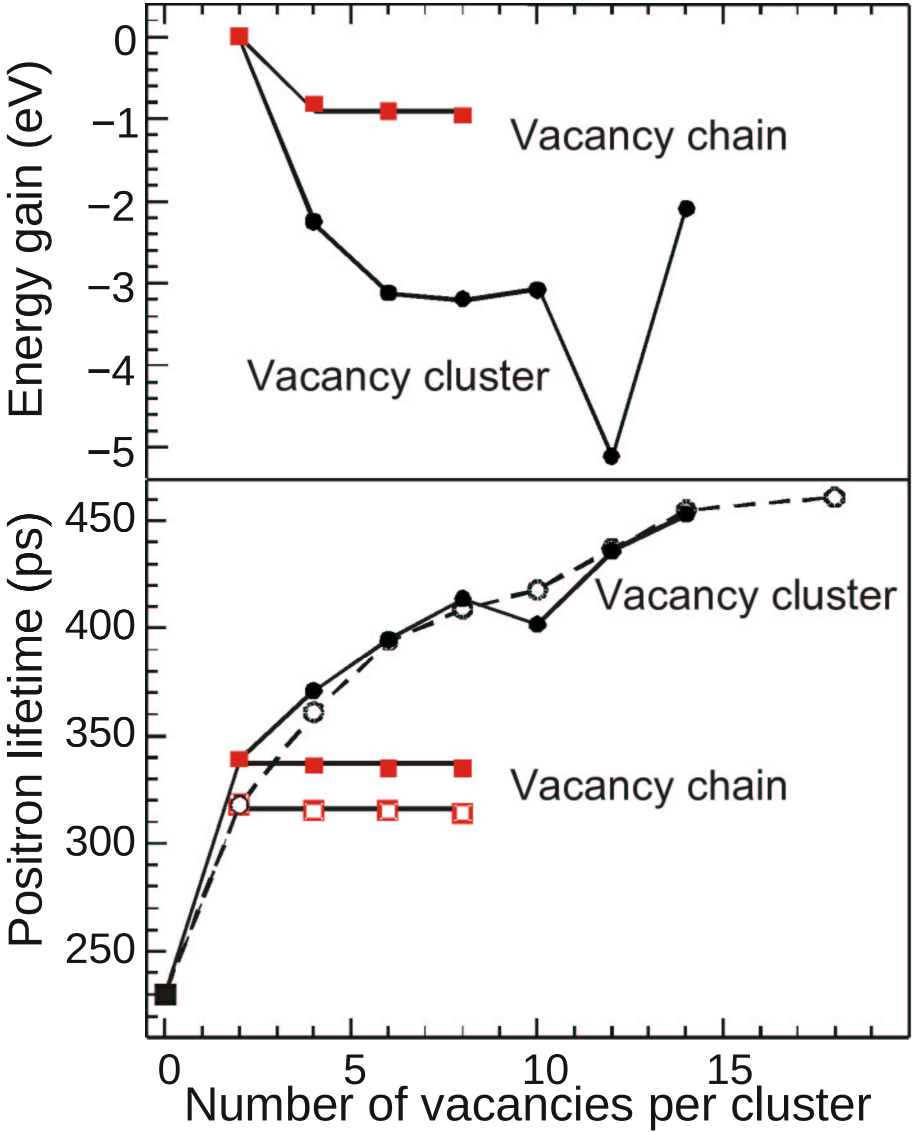
Calculation of positron lifetimes for various vacancy cluster configurations using the superimposed-atom model of Puska *et al*. (1989)

Annihilation rate $$\lambda \propto \int \Gamma n^{-} |\Psi^{+}(\boldsymbol{r})|^{2} \, \mathrm{d}\boldsymbol{r}$$



Positron wave function in bulk GaAs (*left*) and in a gallium vacancy (*right*)

Stability of vacancy clusters and cluster-related positron lifetimes

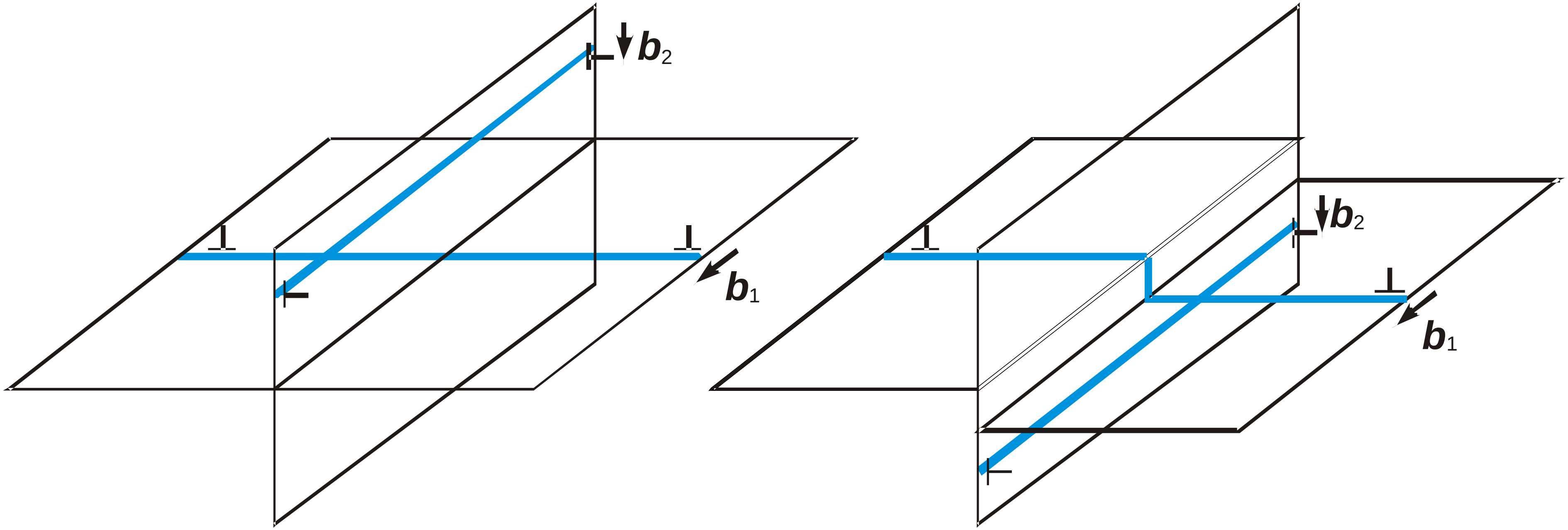


Energy gained by adding a divacancy to an aggregate of *n* – 2 vacancies in GaAs (*upper part*) and positron lifetimes in vacancy aggregates (*lower part*). *Open/closed symbols*: configuration before/after relaxation.

Results of calculations

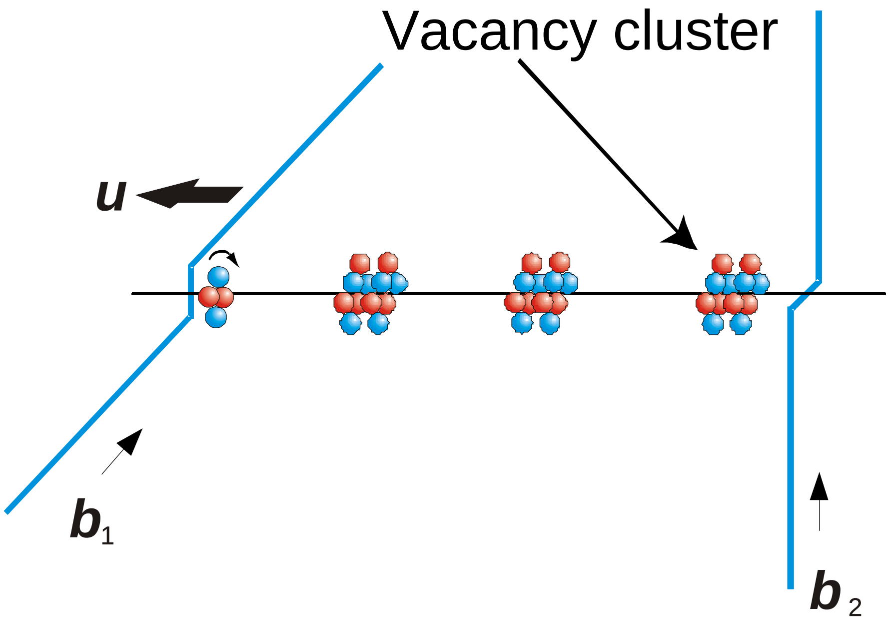
- Especially stable structures ($n < 18$): V_{12} in GaAs
  V_6, V_{10}, V_{14} in Si
- Vacancy chains are not energetically favored structures
- The experimentally observed long-lived positron lifetime component may be attributed to V_{12} in GaAs and to V_{14} in Si.
- Magic numbers in silicon $n =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

Cutting of dislocations



Cutting of edge dislocations

Formation of vacancy clusters

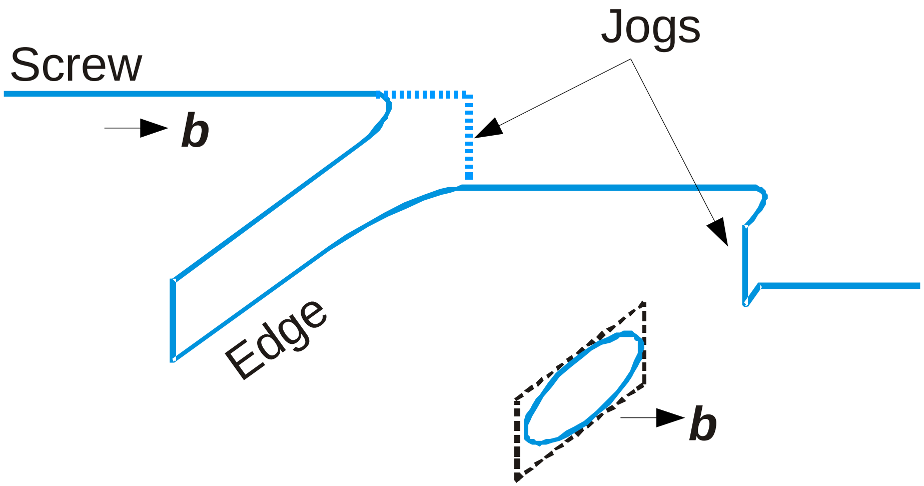


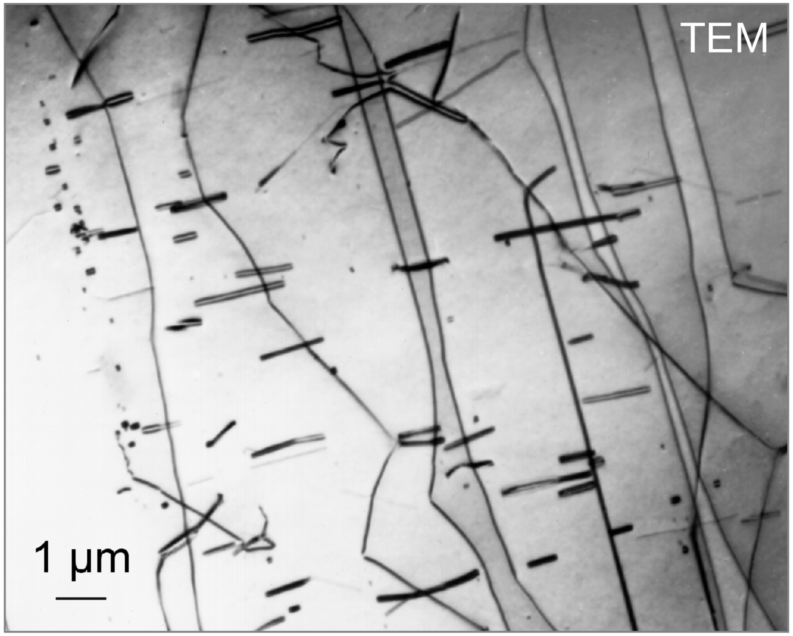
Number of point defects

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

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

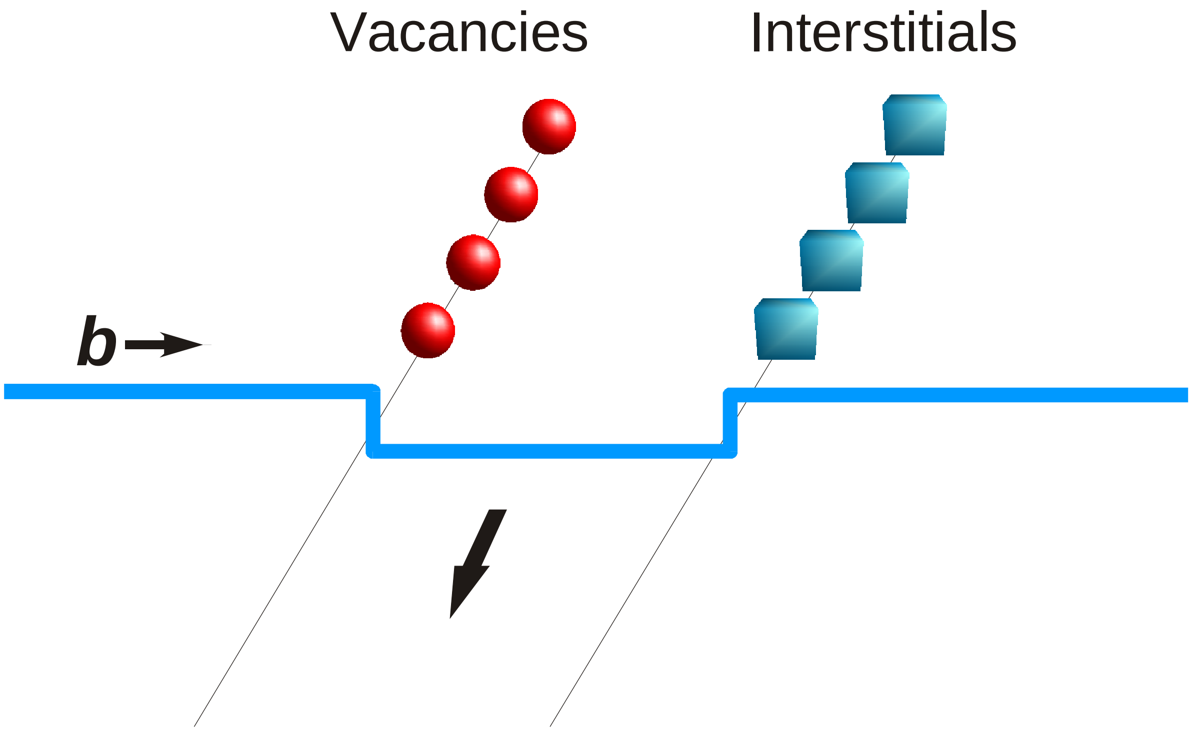
Superjogs





Formation of edge dipoles and prismatic dislocation loops

Vacancies *and* interstitials



Secondary reactions lead to antisites:

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

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.