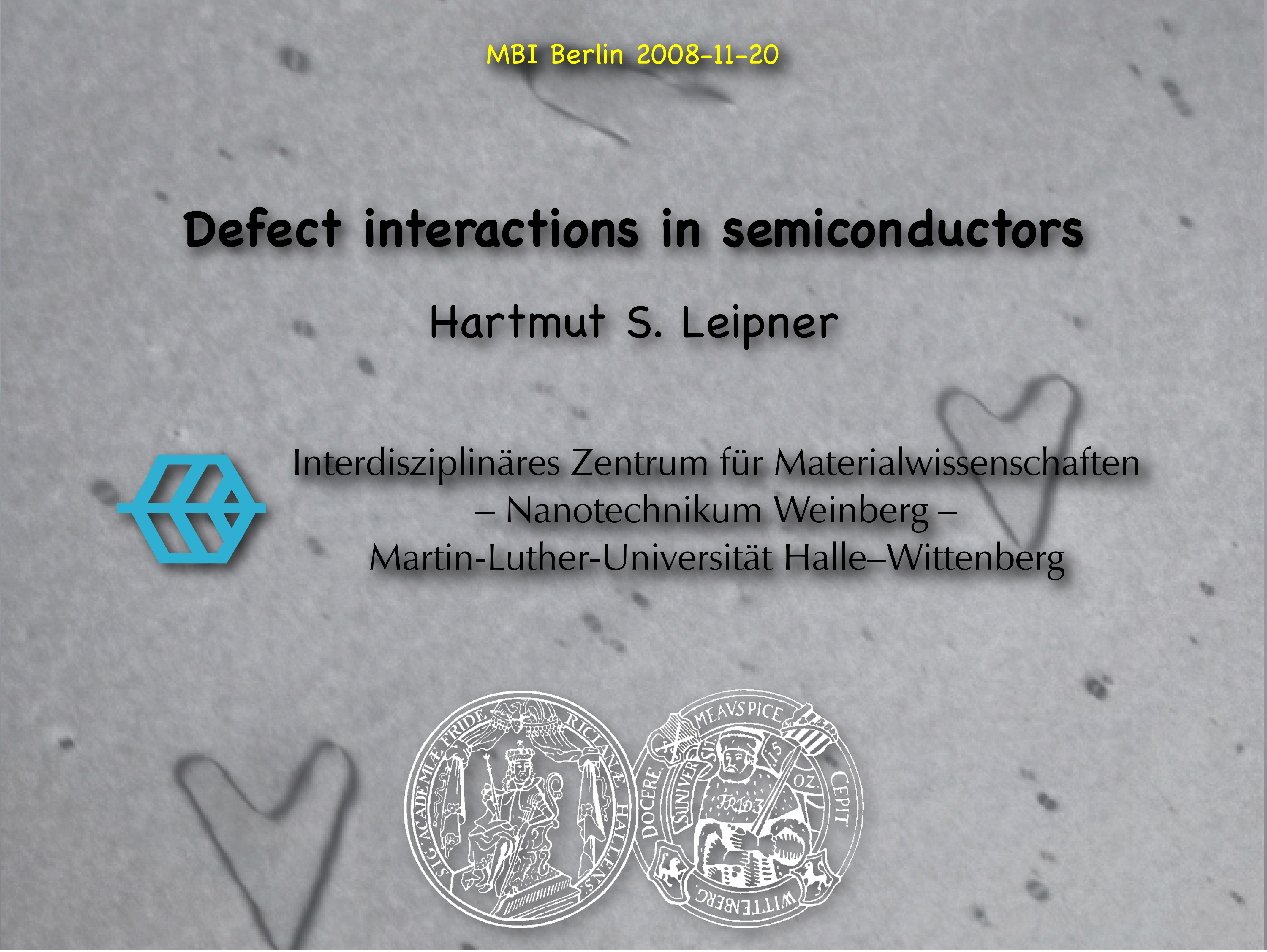

MBI Berlin 2008-11-20

Defect interactions in semiconductors

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Interdisziplinäres Zentrum für Materialwissenschaften
– Nanotechnikum Weinberg –
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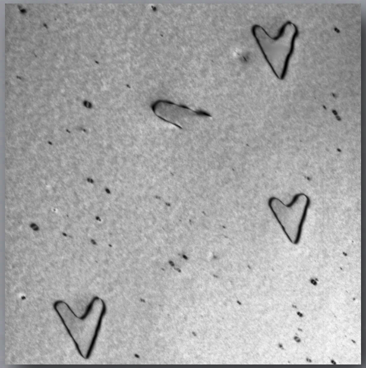
Nanotechnikum Weinberg

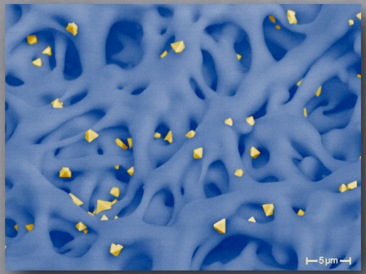
In operation since 2007, 1800 m^2 labs, 210 m^2 cleanroom class 100

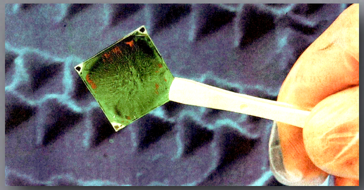

Central labs (IZM@MLU): Nanostructuring/-analytics, electron microscopy, lithography, positron annihilation, deposition

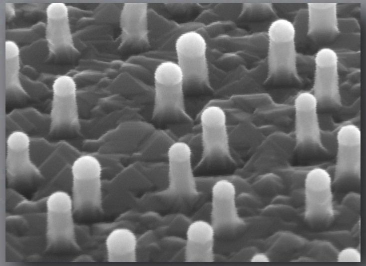
Reseach disposal areas (*Bio–Nano-Zentrum*) for physics, chemistry, material science, bioscience

Topics



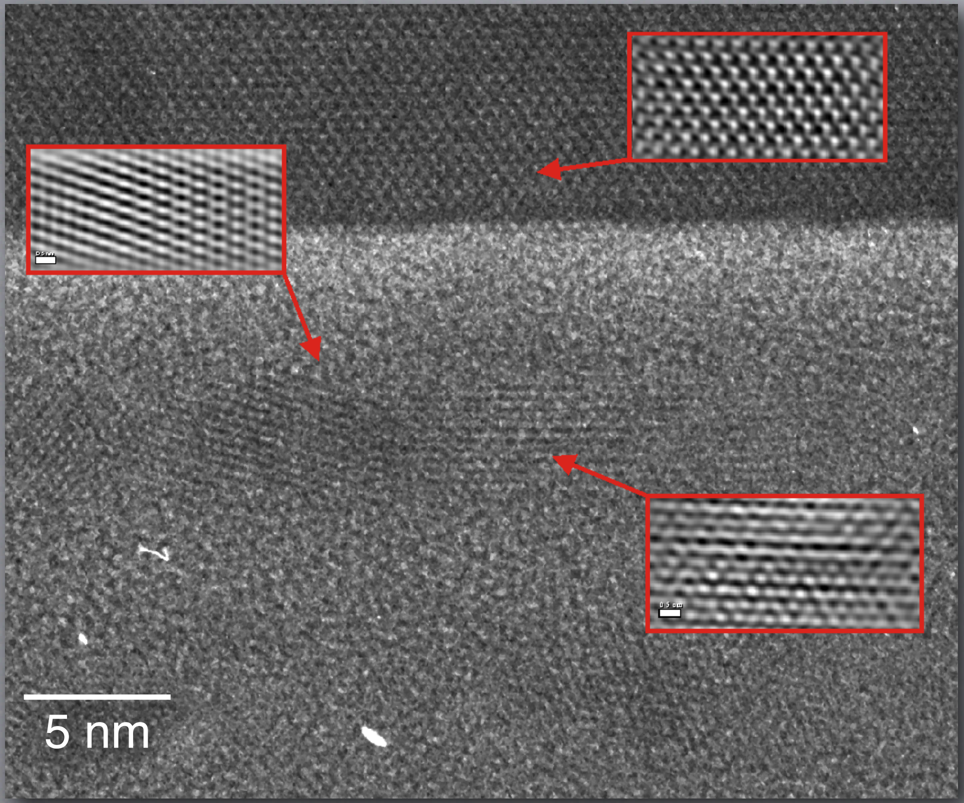


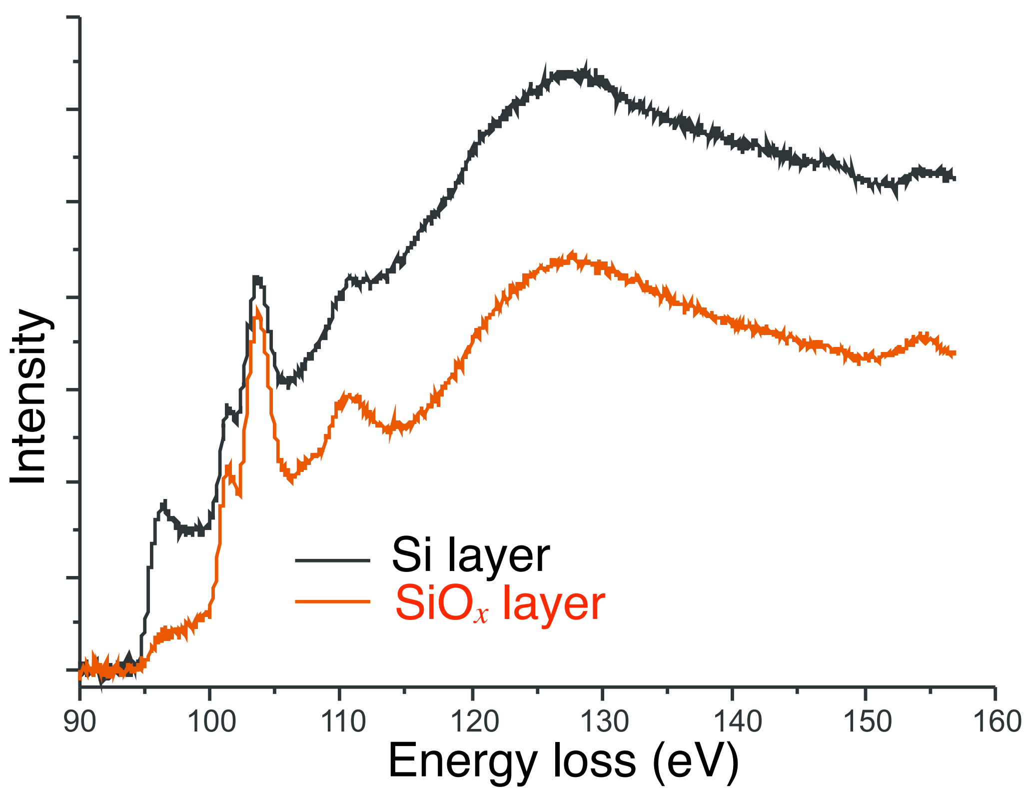




- Nanostructuring/-analysis
  (patterning, characterization of thermoelectric and photovoltaic materials, defect investigations in semiconductors)
- Nanolithography
  (nanosphere lithography, nanoimprint, EBL)
- Positron annihilation
  (crystal defects, porosimetry, EPOS project)
- High resolution materials characterization
  (FESEM, STEM, EFTEM, AFM, Raman microscopy, cathodoluminescence microscopy)

Analytics on Si for 3rd generation photovoltaics



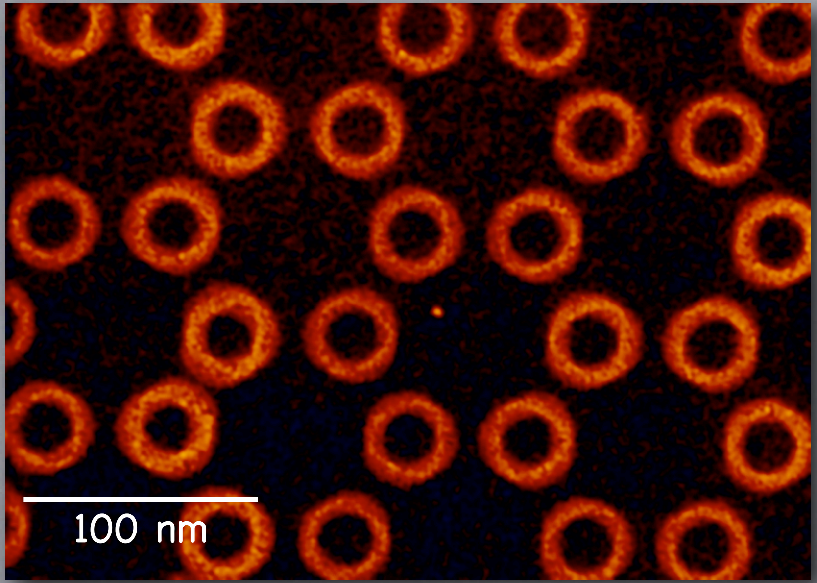


Superlattice with 2 nm Si/3 nm SiO$_x$
after RTA (1100 °C, 30 s)

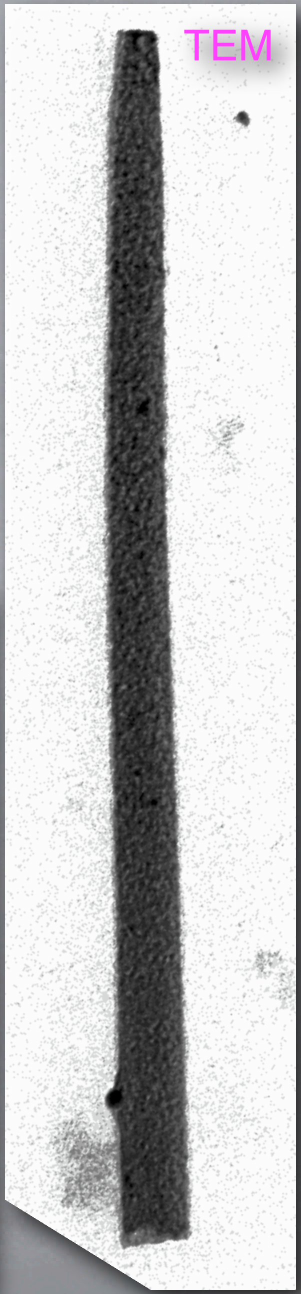
EELS in different layers

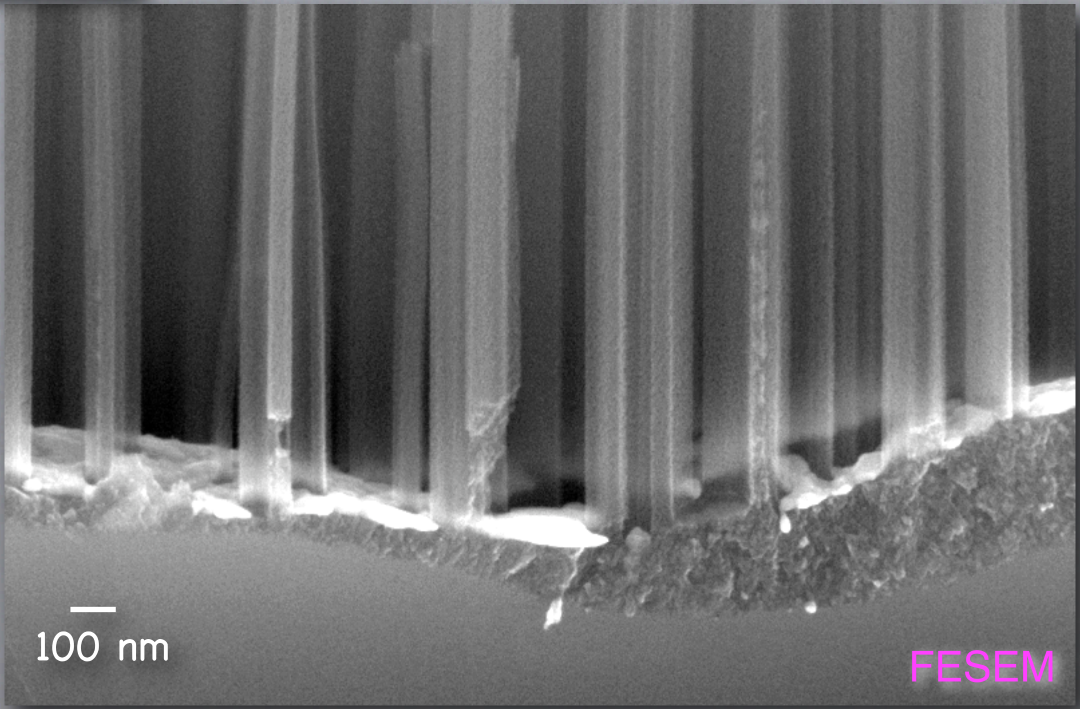
[Schade et al. 2008]

Nanosphere lithography



Development of a “nano pinhole camera“

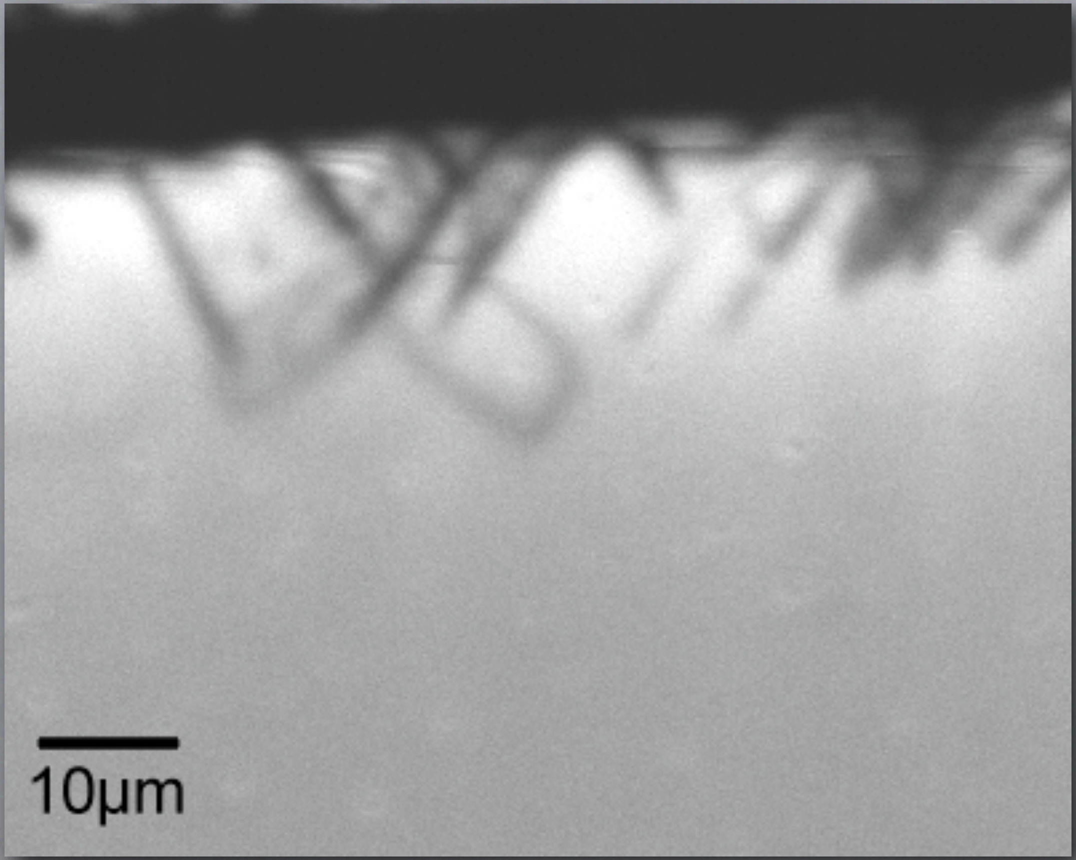




Silicon nanowires
by catalytic etching
[Geyer et al. 2008]

Defects at IZM@MLU

- Defects in semiconductors
(interaction of point defects with dislocations, dislocation dynamics – TEM, SEM, positron annihilation)

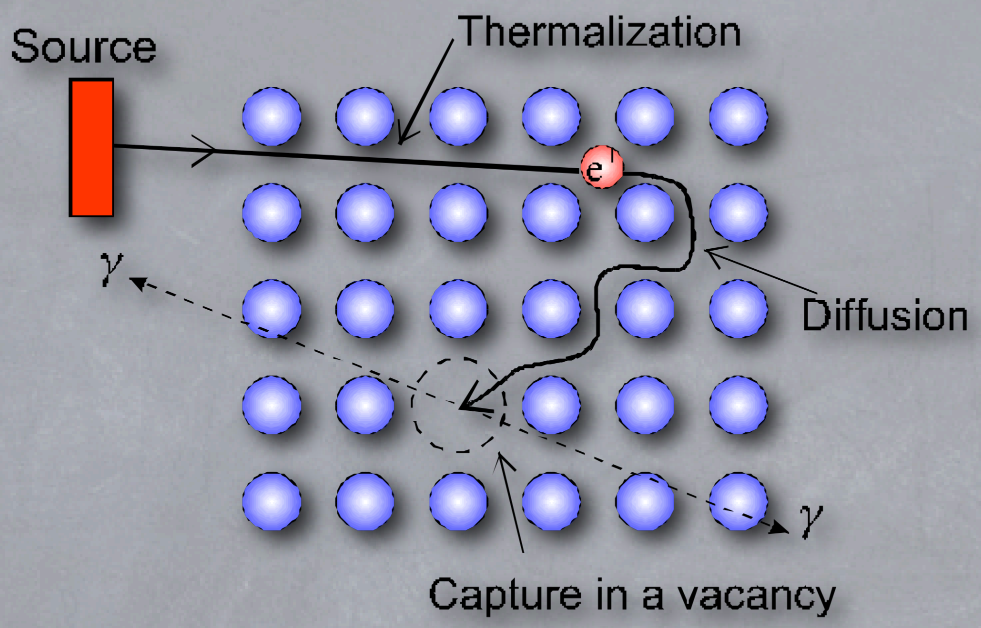


Gliding dislocations in GaAs, cathodoluminescence microscopy [Schreiber et al.]

Defect interaction: Key issues

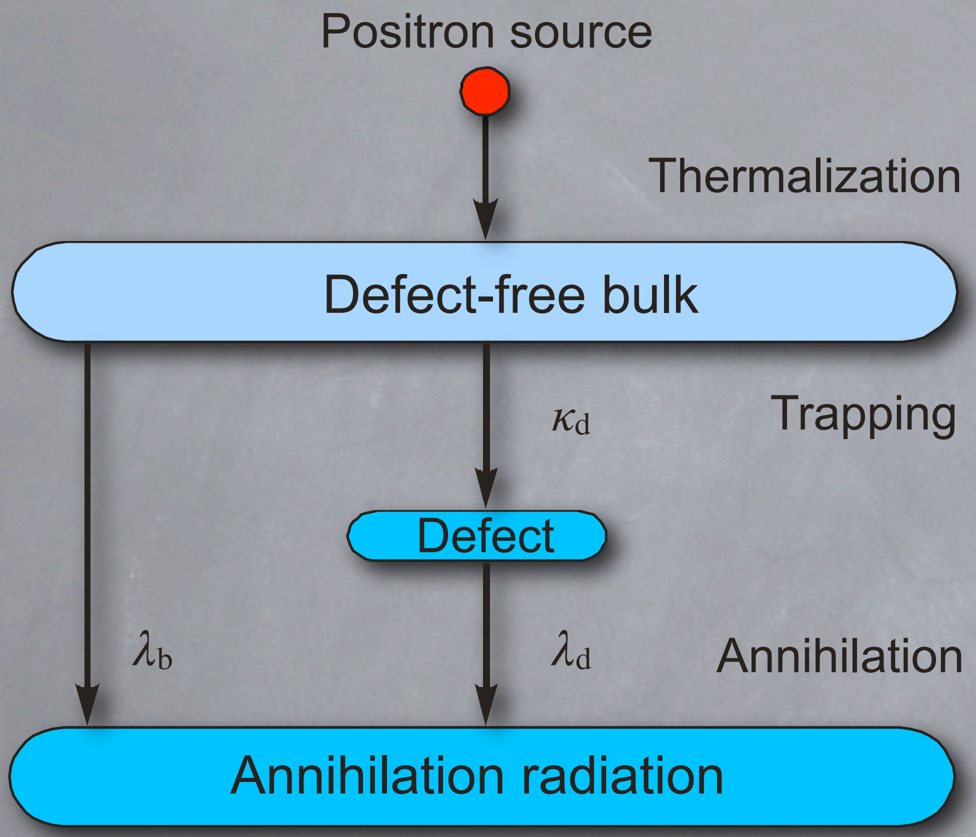
- Dislocations and point defects are not independent from each other.
  - The motion of dislocations leads to the generation of intrinsic defects.
  - The existing point defect population is altered by the presence of dislocations.
- Formation of intrinsic defects during plastic deformation of elemental and compound semiconductors

Positron annihilation



- Positrons may be captured during diffusion in lattice defects.
- Annihilation rate (reciprocal lifetime) depends on the local electron concentration at the annihilation site.
- Positron lifetime: kind of defect, trapping rate: defect density

Trapping model



Positron source

Thermalization

Defect-free bulk

κ_d

Trapping

Defect

λ_b

λ_d

Annihilation

Annihilation radiation

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

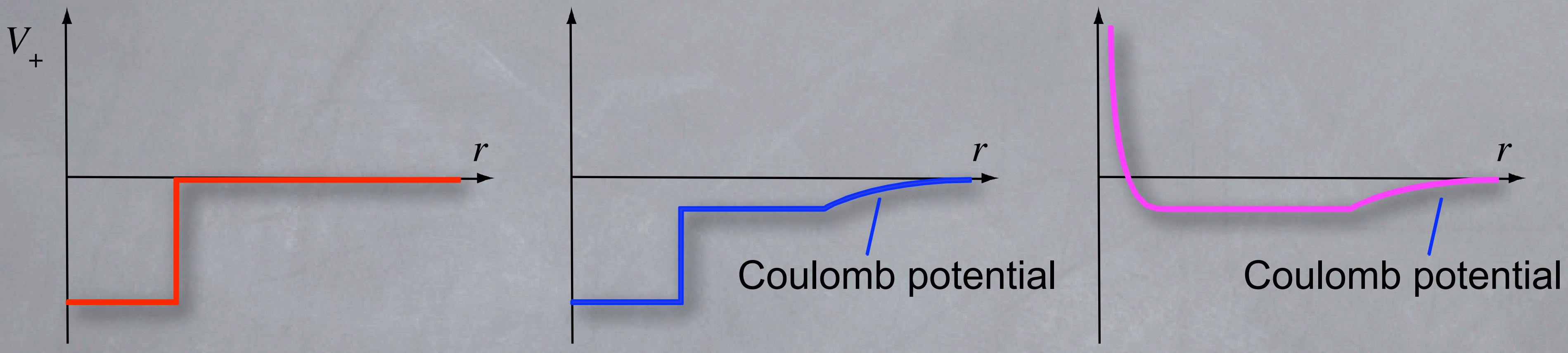
- Quantitative analysis of positron trapping by a set of rate equations
- Solution (lifetime spectrum):

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

- Intensity I_i relates to the trapping rate:

$$\kappa_d = \mu \rho_d$$

Positron capture in defects

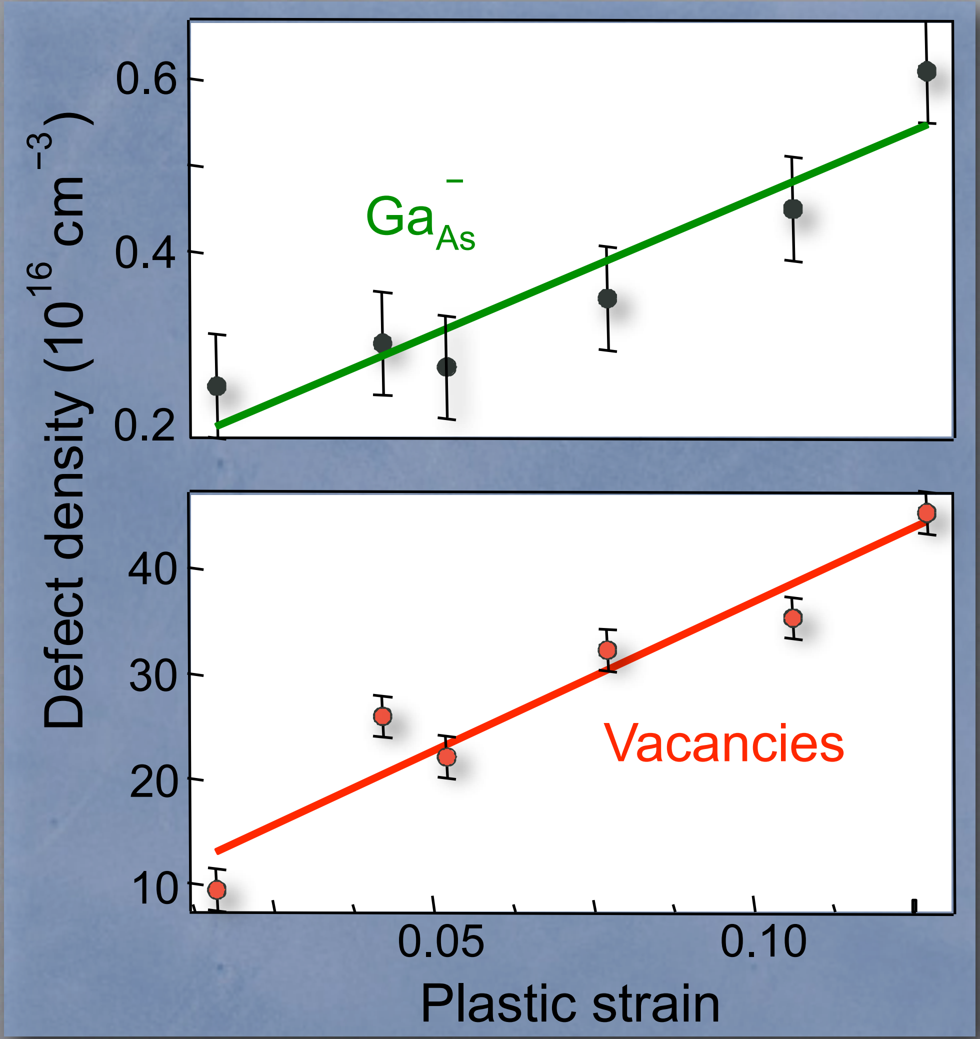


$\tau \propto$ open volume

$\tau \approx \tau_b$

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. The trapping rate $\kappa = \kappa(T)$ is constant for neutral defects and a function of temperature T for charged defects.

Point defect densities after plastic deformation

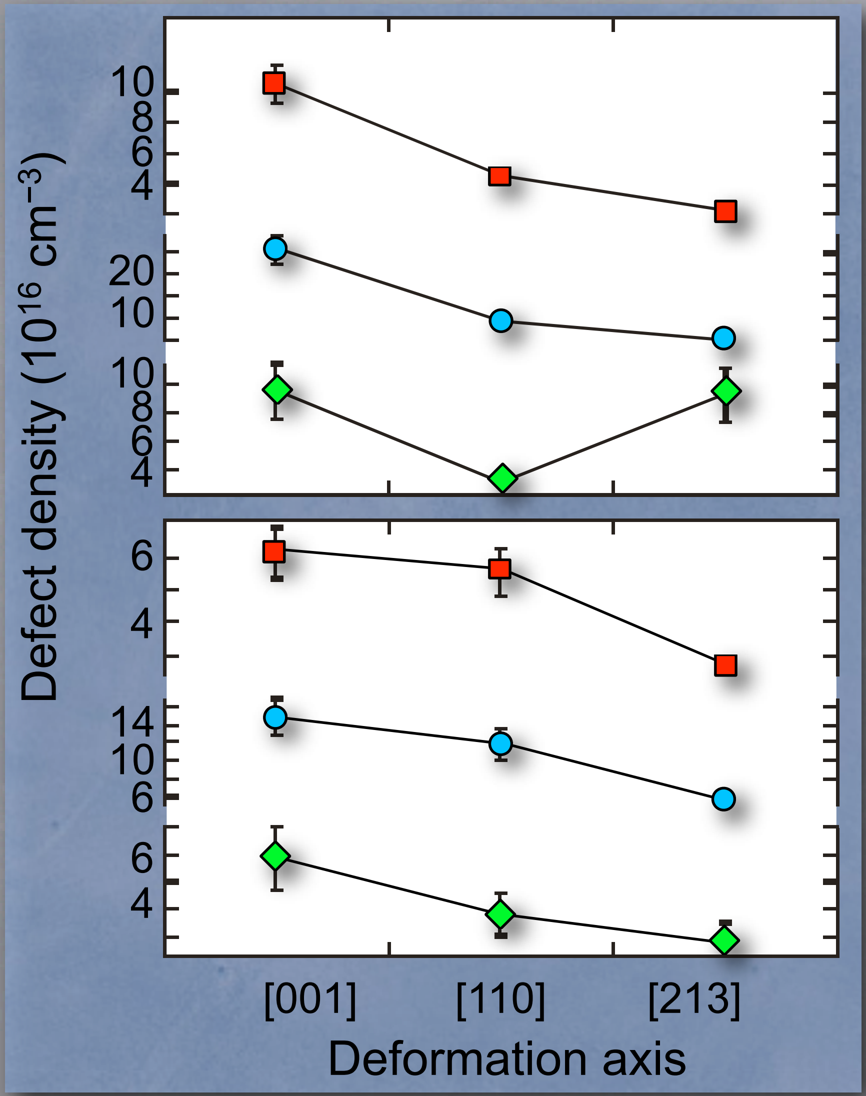


Total density of vacancies and antisite defects as a function of the strain. Result of measurements by positron annihilation in plastically deformed GaAs. Uniaxial compression in [110] direction at 773 K, strain rate 1×10^{-3} s^{-1}.

Relation between density of excess vacancies and strain

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

Deformation conditions



Total number of vacancies in the bulk 🟥, vacancies bound to dislocations 🔵, as well as number of GaAs antisites ◆ in plastically deformed GaAs.

Deformation temperature $773\ \mathrm{K}$, strain $3\ \%$, strain rate $7.5\times10^{-5}\ \mathrm{s}^{-1}$ (above), $3\times10^{-4}\ \mathrm{s}^{-1}$ (below).

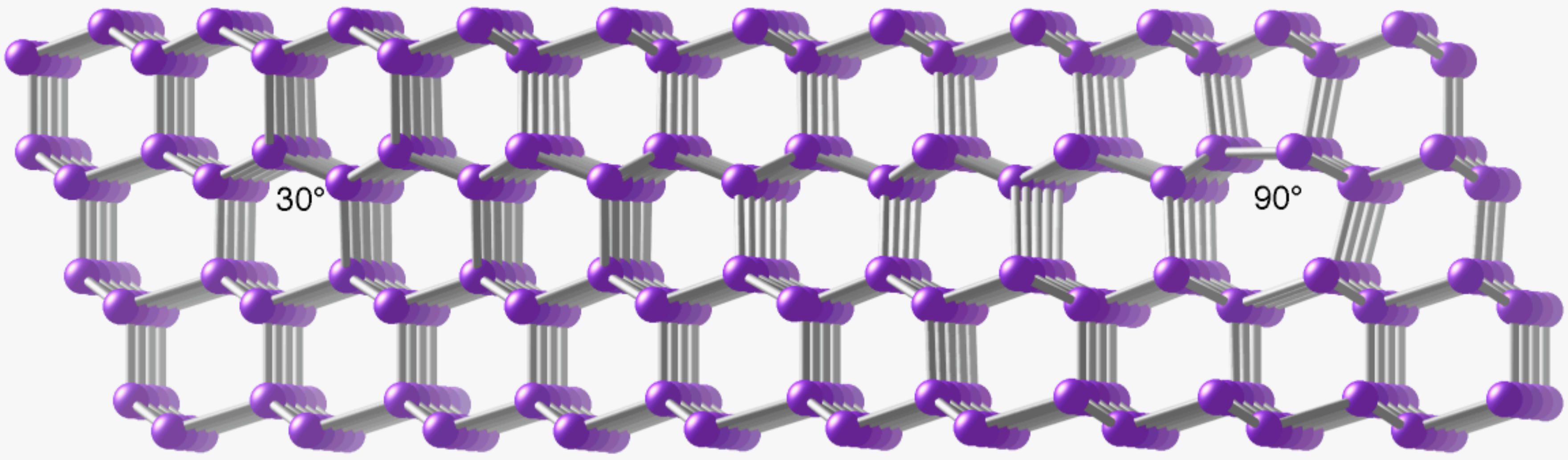
→ Defect densities higher for multislip orientation

Positron lifetimes in GaAs

Lifetime components:

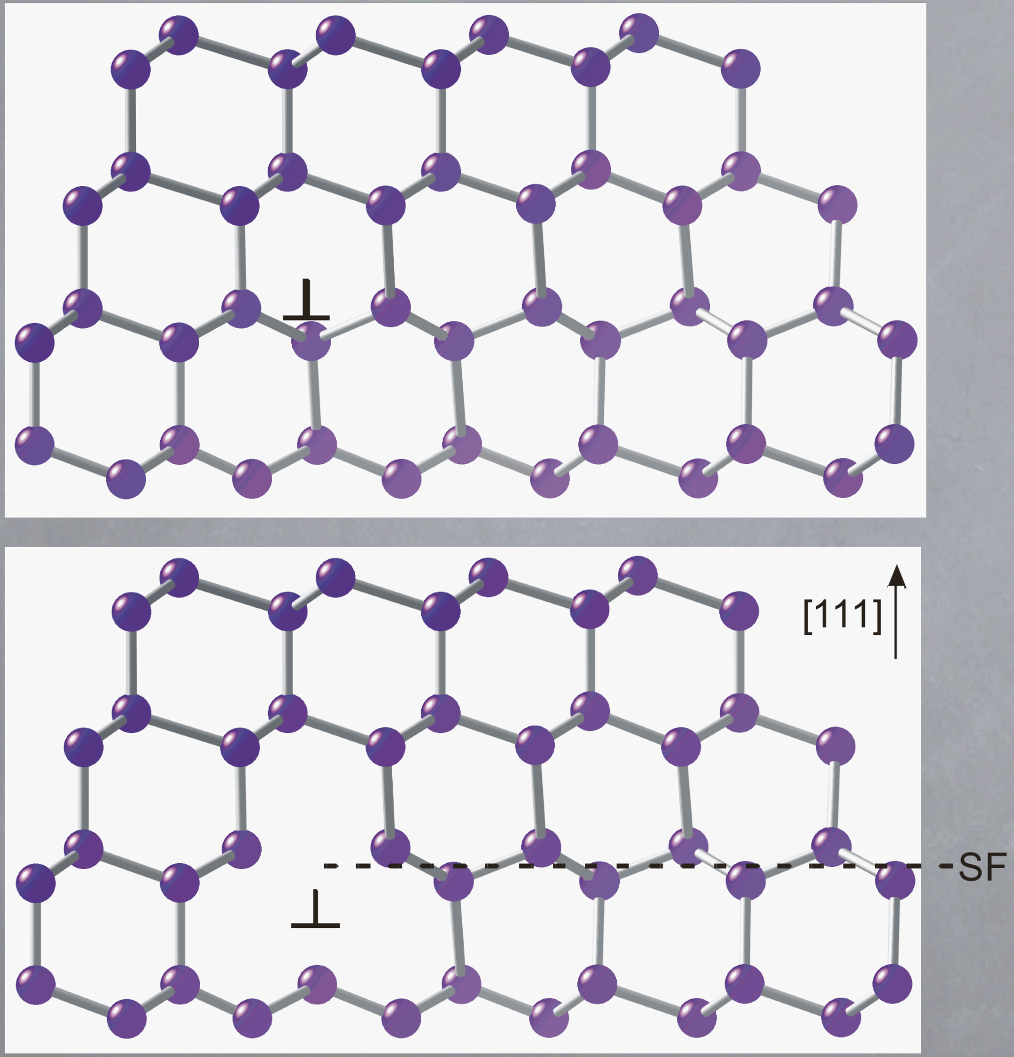
- $\tau_2 = \tau_{d3} = (260 \pm 5)$ ps
  corresponds to a defect with the open volume of a monovacancy
- $\tau_3 = \tau_{d2} = (477 \pm 20)$ ps
  corresponds to a defect with a large open volume
  (vacancy cluster)
- At low sample temperatures, another positron trap without open volume becomes active (antisite defects).
  $\tau_{d1} \approx \tau_b$

Dissociated dislocation



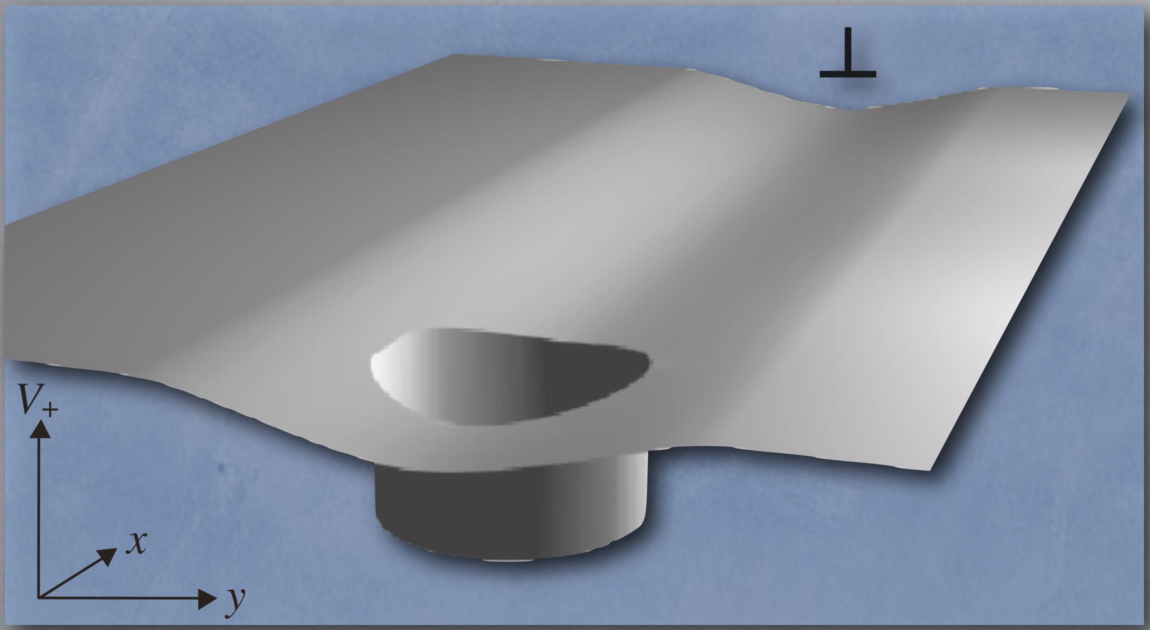
Dissociation of a perfect 60° dislocation in the glide set in a 30° and a 90° partial dislocation. There is an intrinsic stacking fault between the two partials. The drawing is along the (110) plane.

Vacancy incorporation



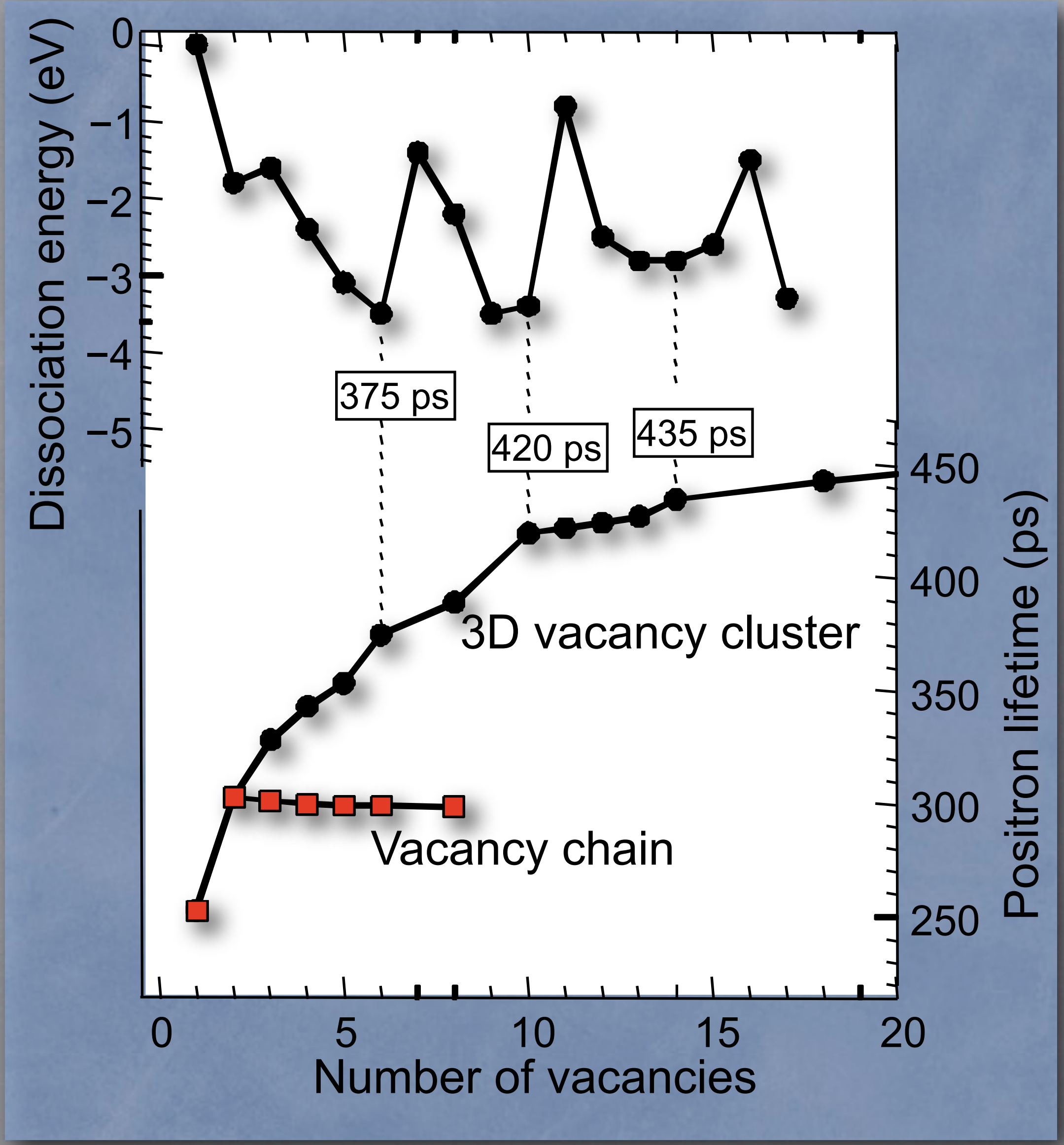
Incorporation of a vacancy in the core of a 30° partial dislocation as a local transition from glide to shuffle set.

Dislocation as a positron trap



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.

Calculation of vacancy clusters



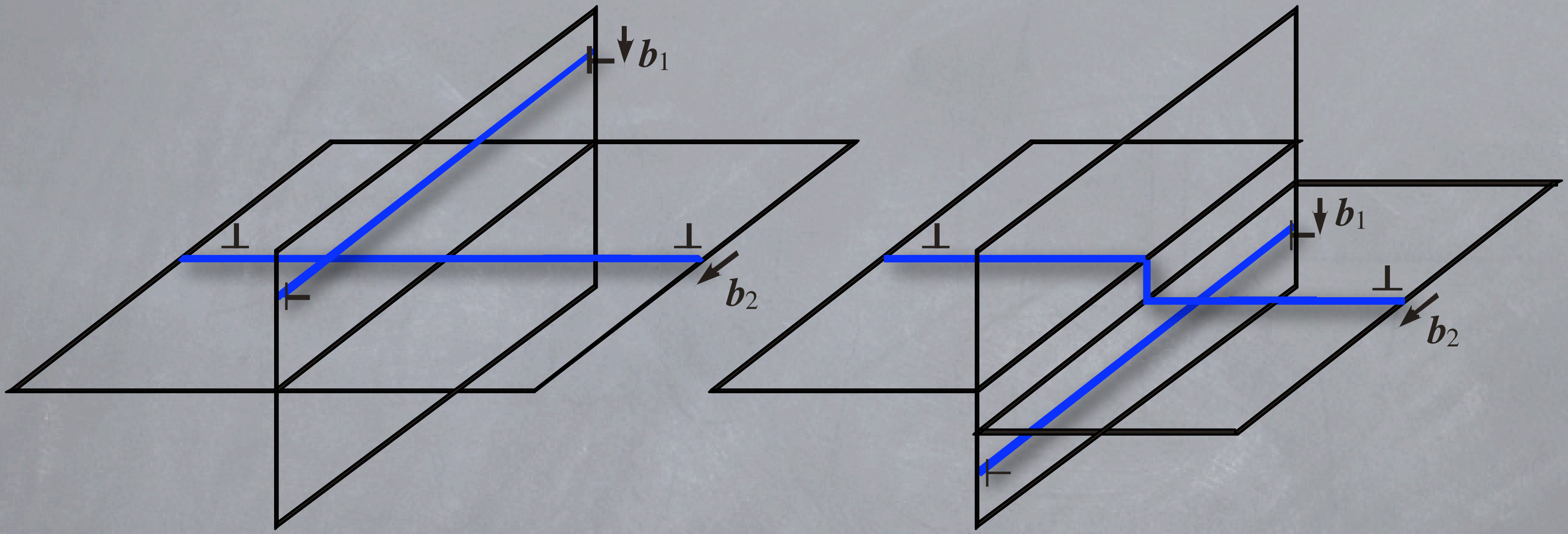
Energy gained by adding a monovacancy to an aggregate of $n-1$ vacancies in Si (upper part) and the corresponding positron lifetime (lower part).

[Staab et al. 1999]

Magic numbers

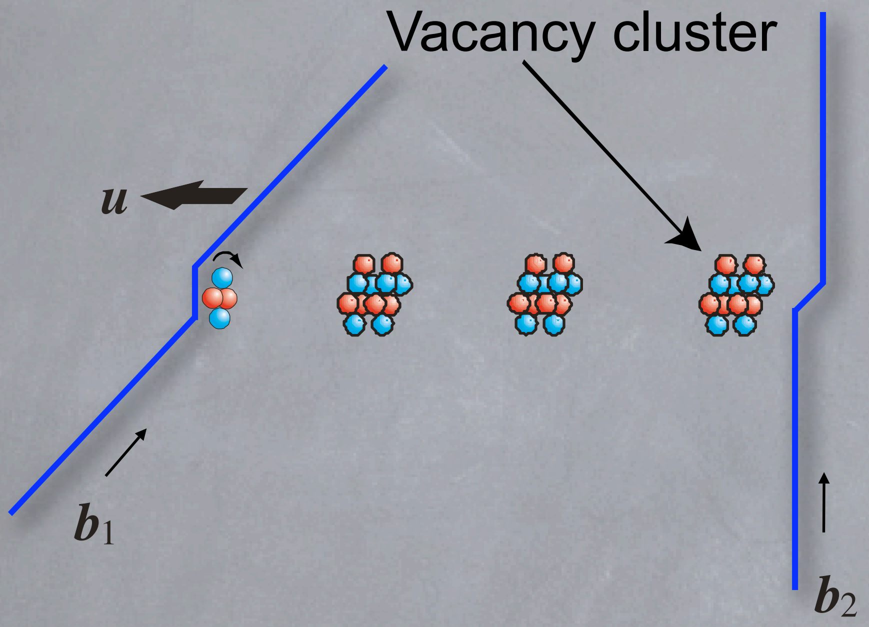
- Especially stable structures ($n < 18$): V_{12} in GaAs
  V_6, V_{10}, V_{14} in Si
- Vacancy chains are not energetically favored structures
- The experimentally observed long-lived positron lifetime component may be attributed to V_{12} in GaAs and to V_{14} or V_{18} in Si.
- Magic numbers in silicon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

Cutting of dislocations



Cutting of edge dislocations

Formation of vacancy clusters

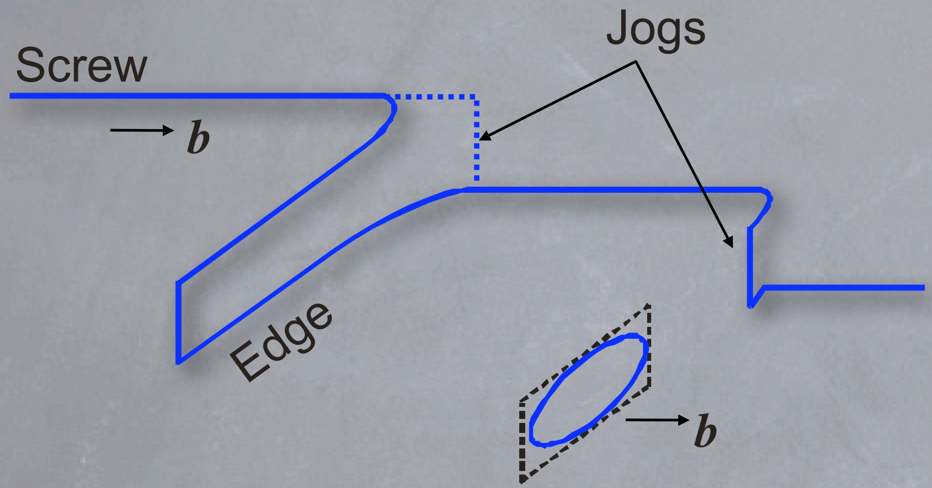


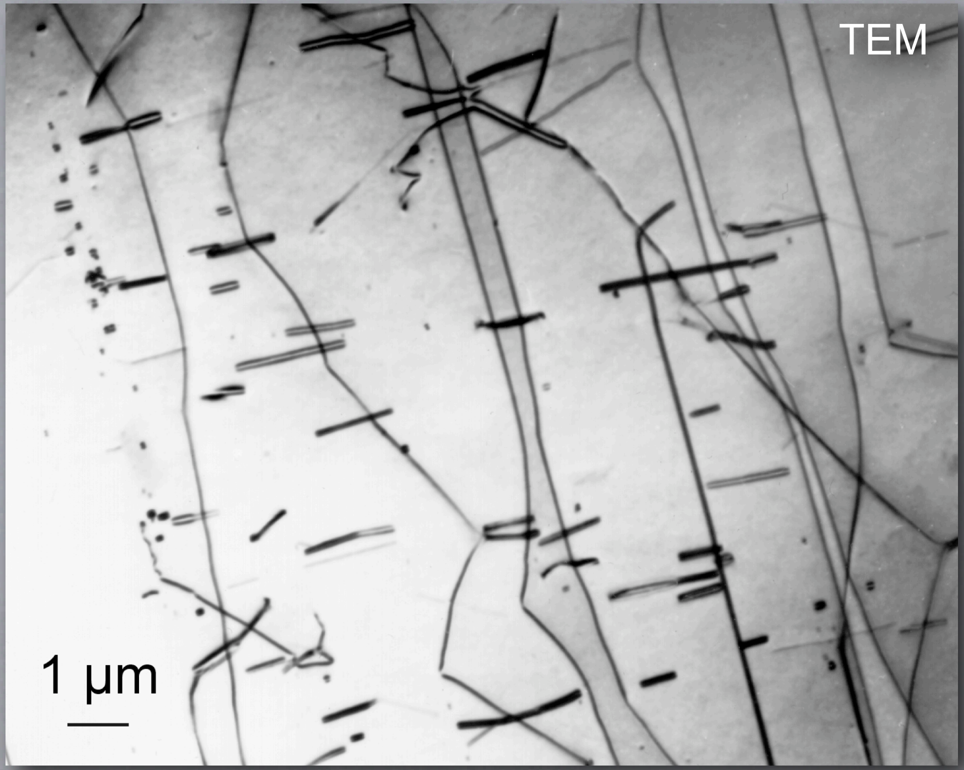
Number of vacancies

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

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

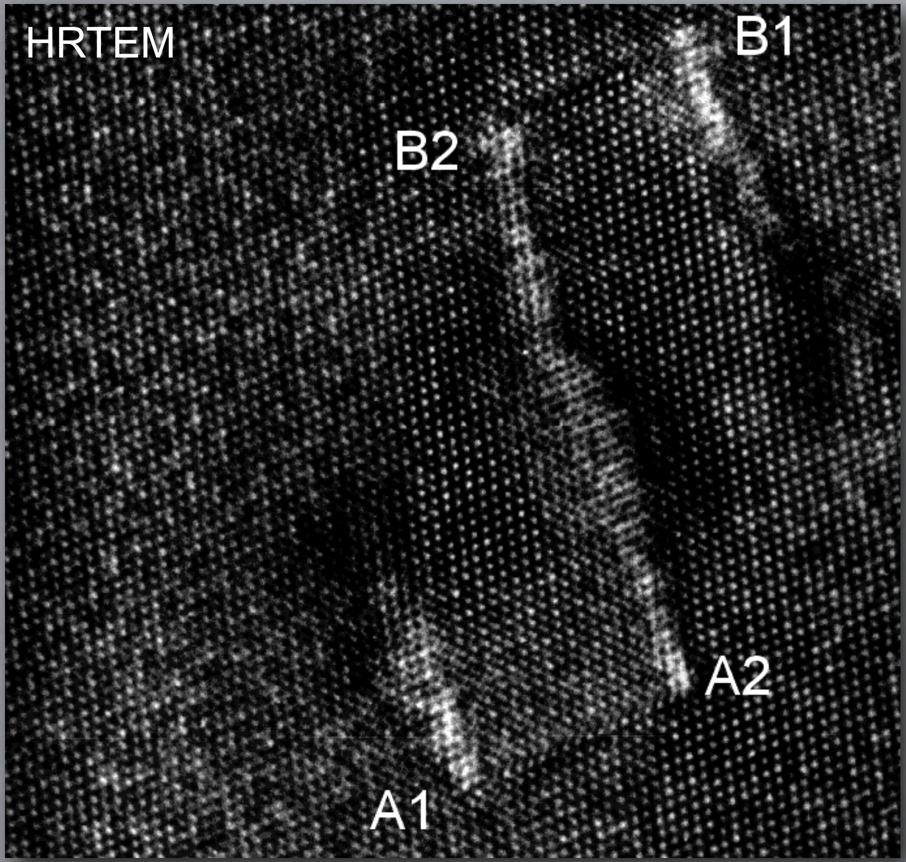
Superjogs

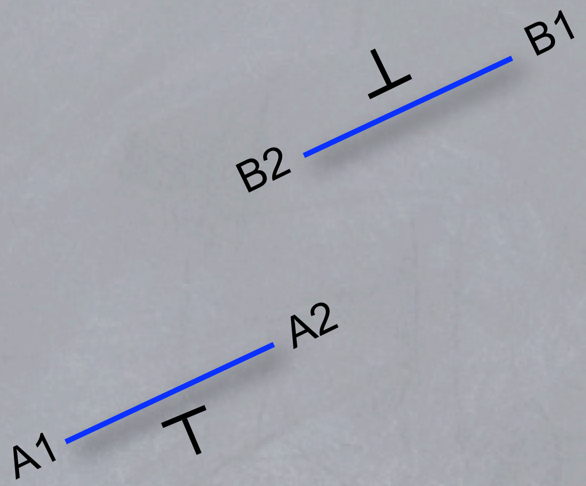




Formation of edge dipoles and prismatic dislocation loops

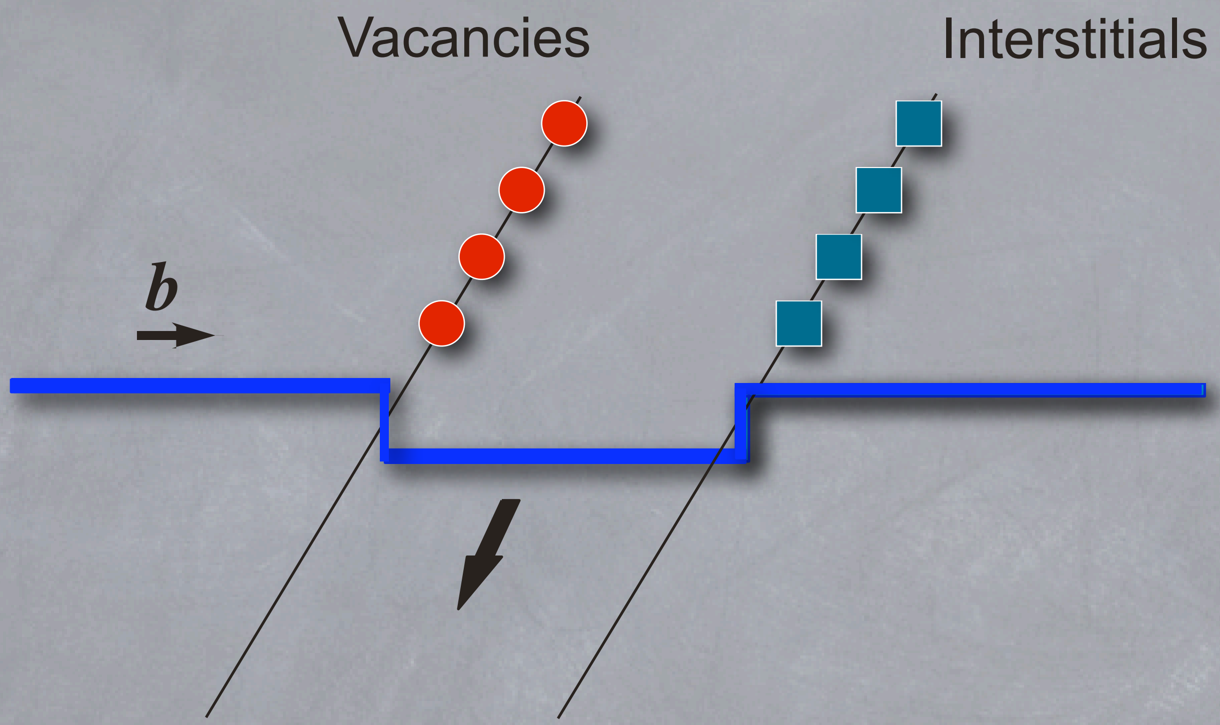
Dipole structure





Dislocation dipole in deformed Si. A1–A2 and B1–B2 are the two dissociated edge dislocations with their Shockley partial dislocations. The dissociation width amounts to 6 nm. HRTEM image of a (110) foil.

Vacancies *and* intersititals



Secondary reactions lead to the formation of antisites:

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

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.

☑ The 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.

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感谢您的关注

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