Workshop on Dislocations in multi-crystalline silicon
Freiberg, 2012-03-27/28

Interaction of point defects with dislocations

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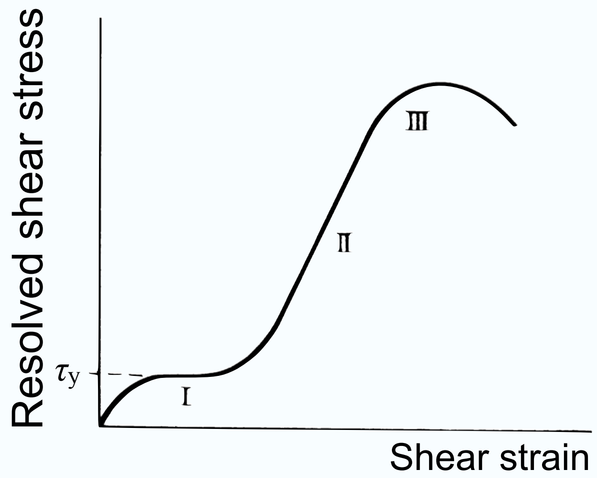
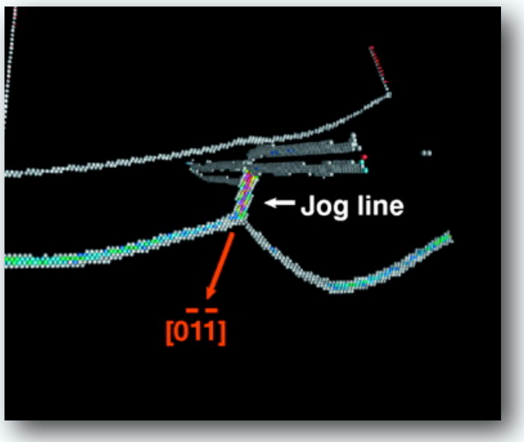
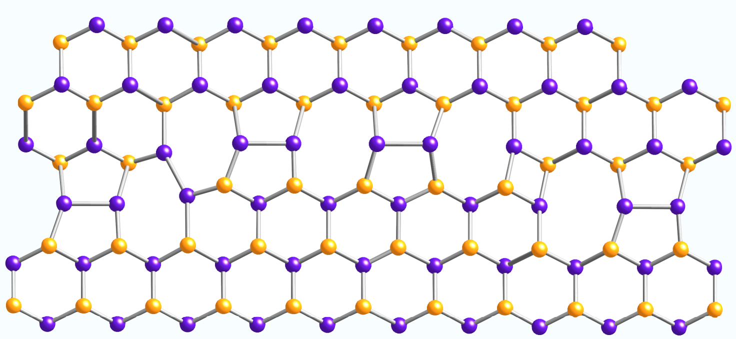
Dislocation models



Continuum mechanics/dislocation dynamics

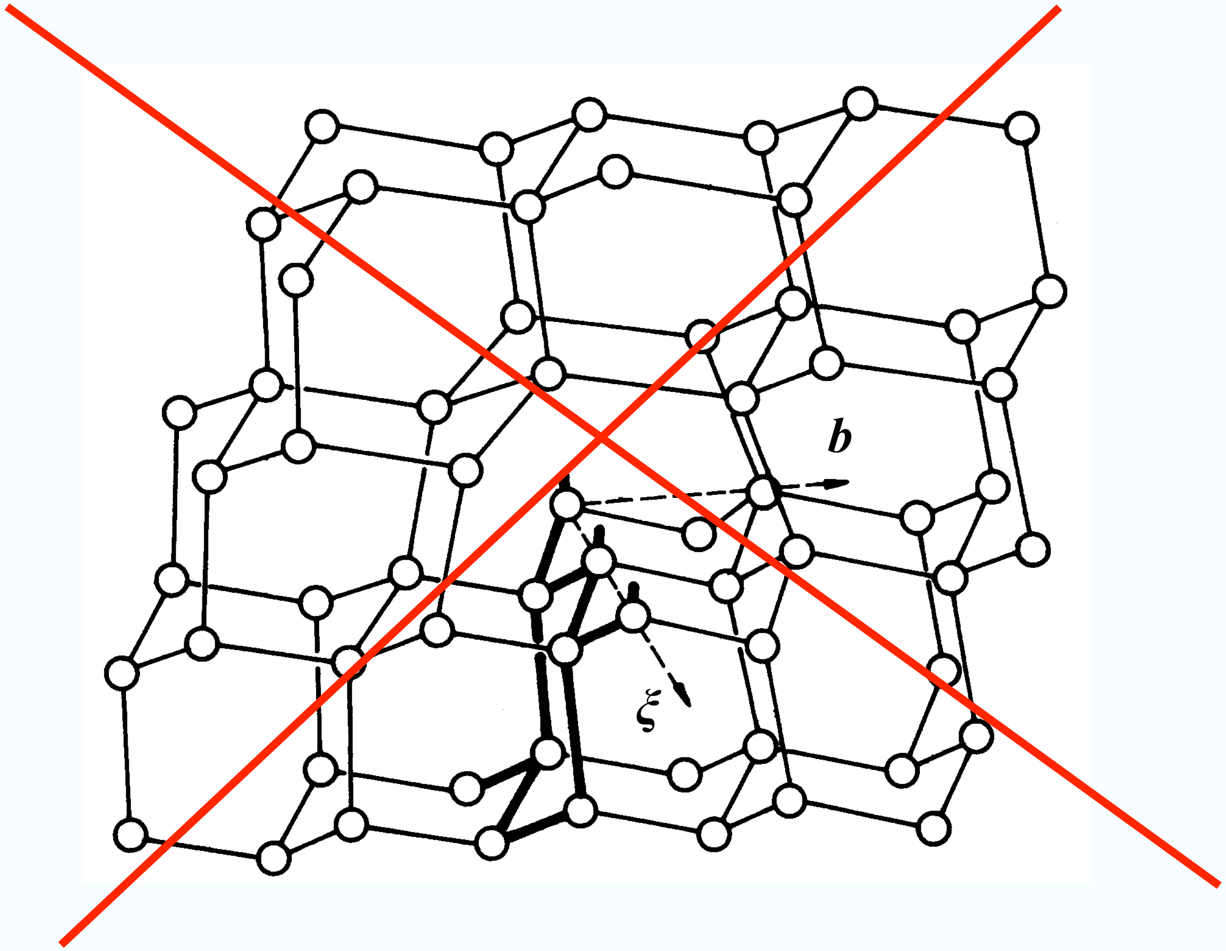


Molecular dynamics



Atomistic/quantum mechanics

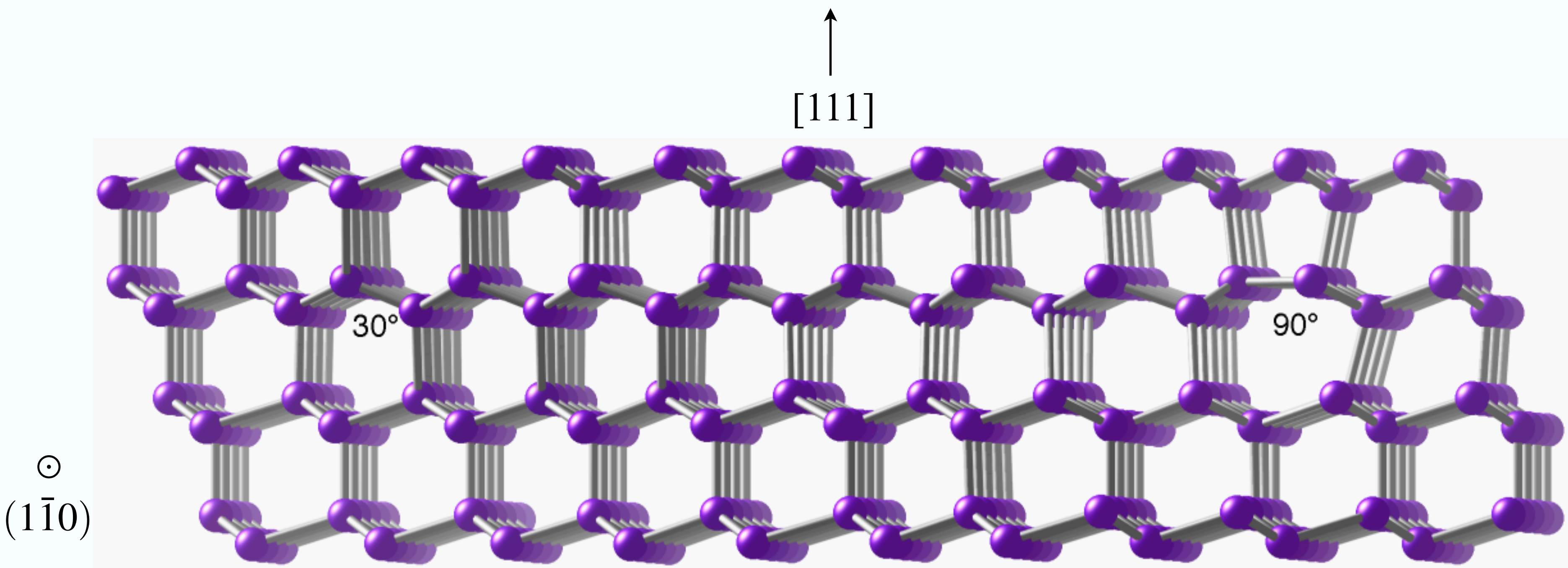
“Ptolemaic” model of dislocations



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

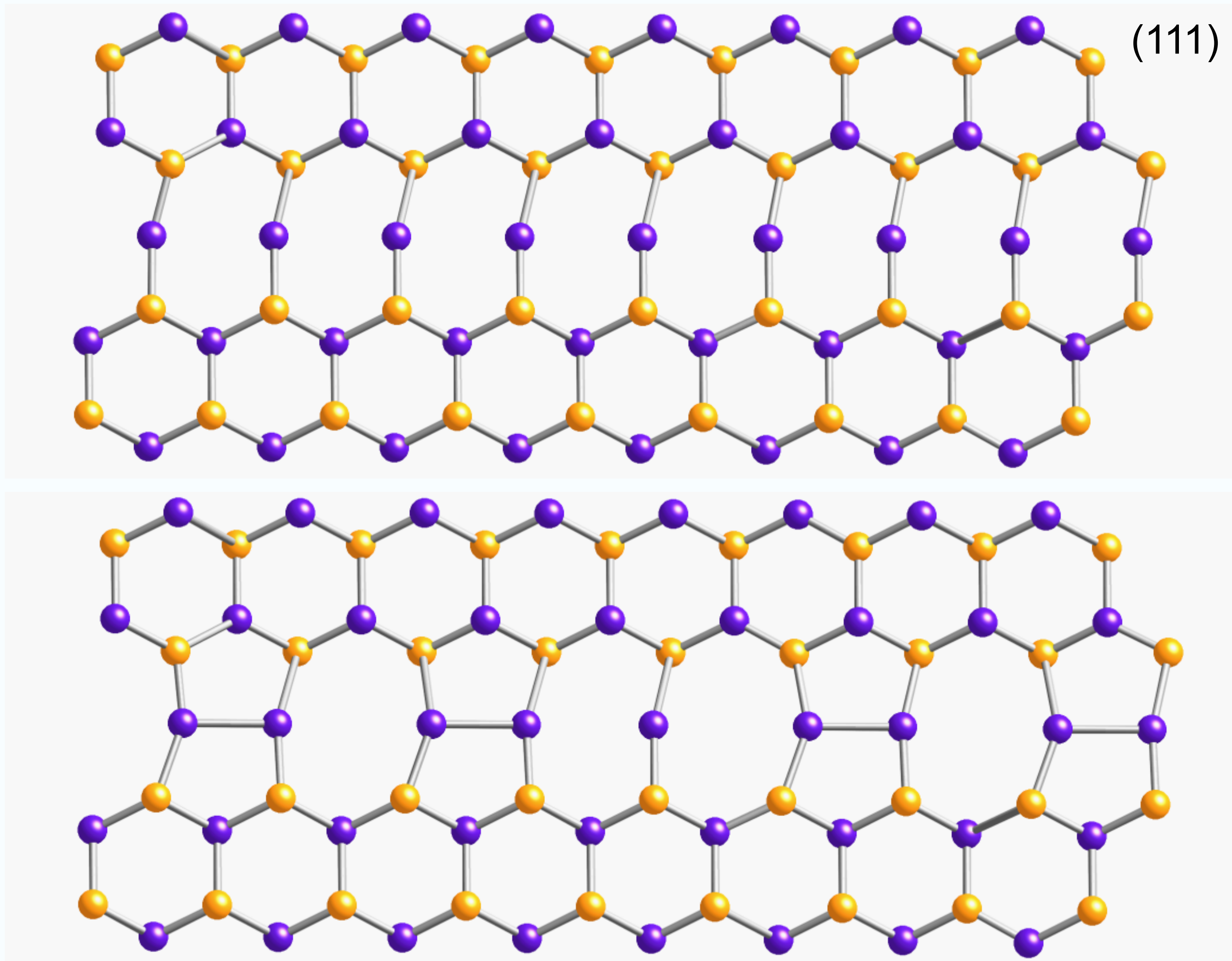
[Shockley 1953]

Dissociation



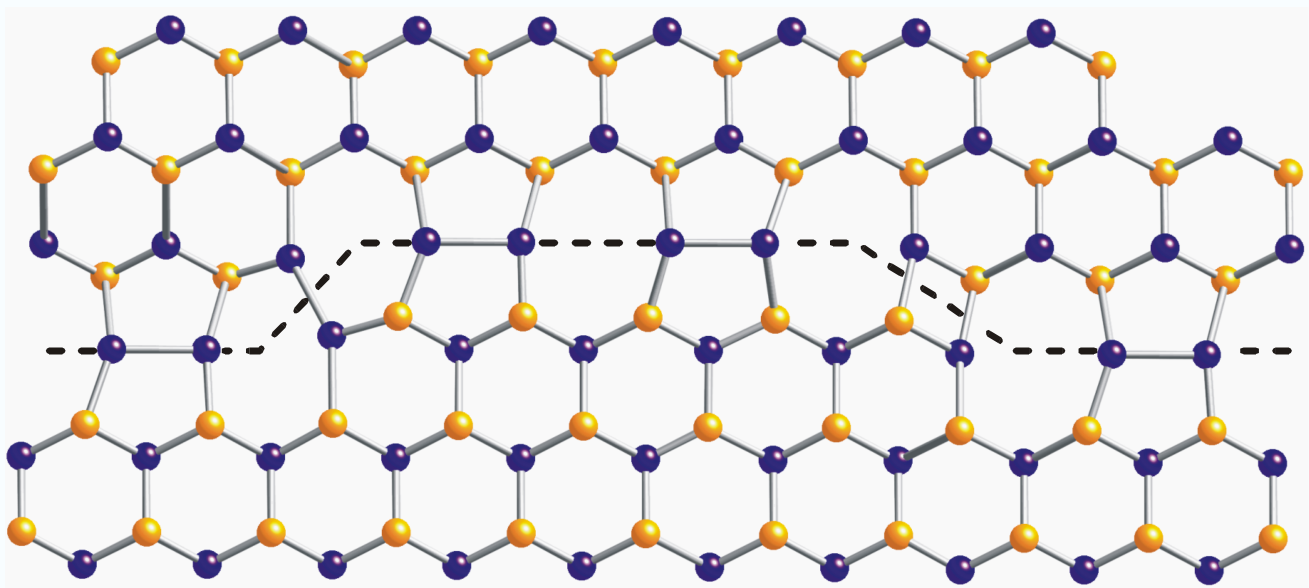
Dissociation of a perfect 60° dislocation in the diamond structure into a 30° and a 90° partial. The Shockley partial dislocations, $\boldsymbol{b} = \frac{\boldsymbol{a}}{6}\langle 211 \rangle$, are separated by a stacking fault.

Reconstruction



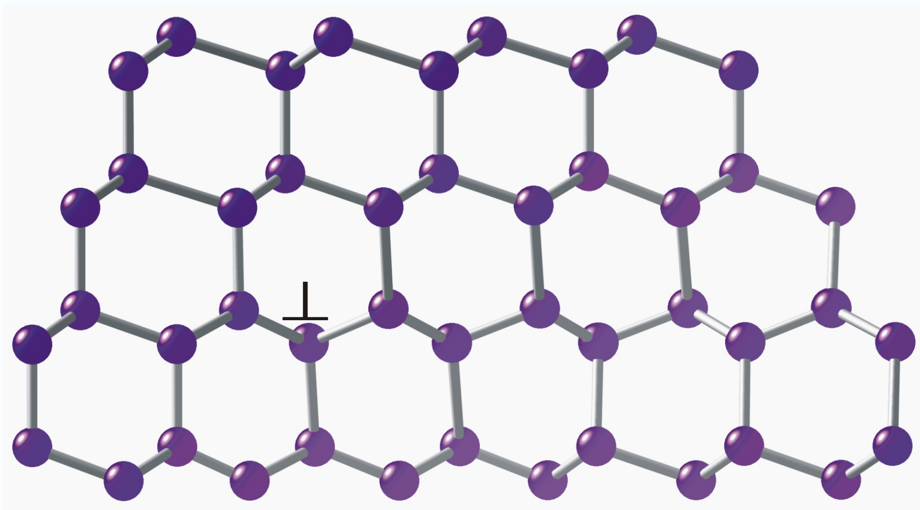
Unreconstructed and reconstructed 30° partial

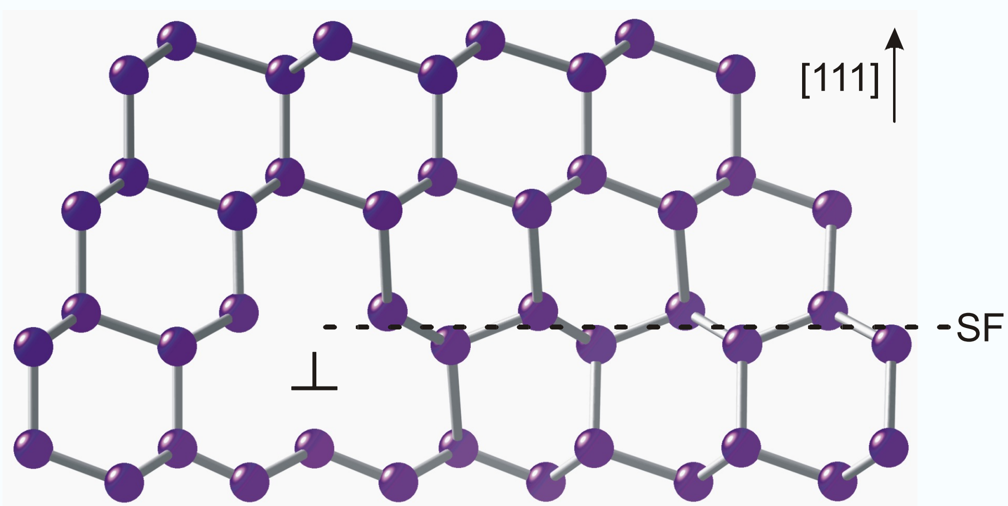
Dislocation defects



Left and right kink on the 30° partial

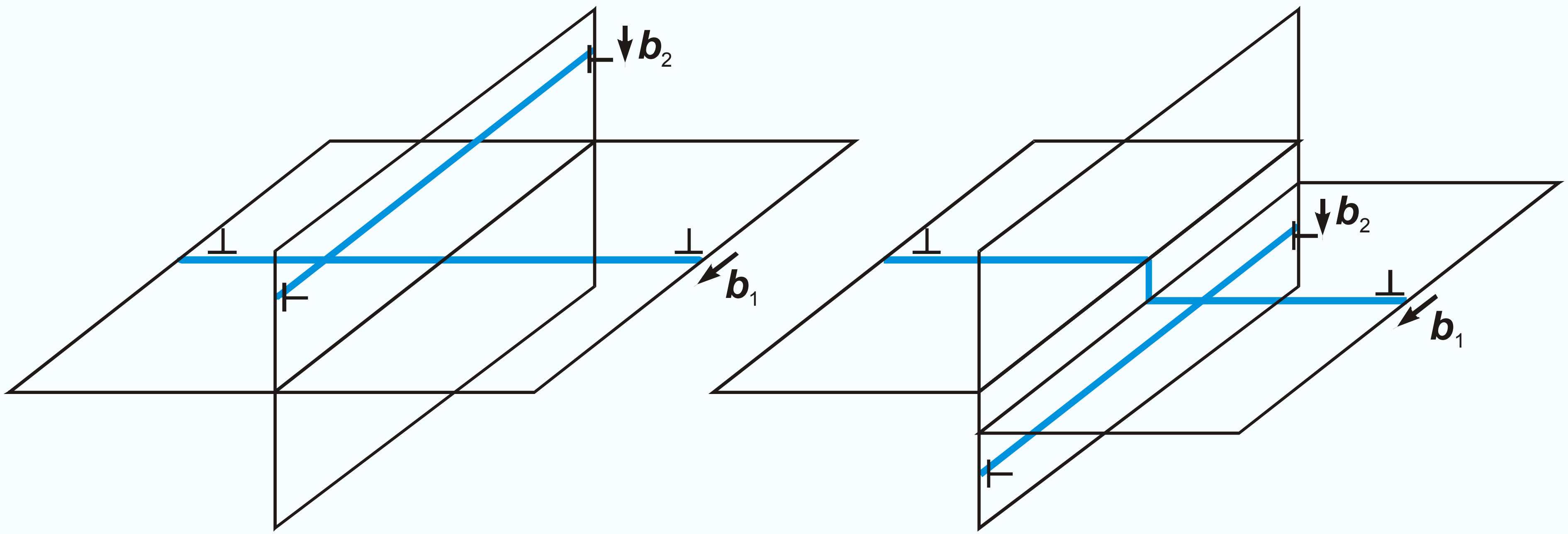
Incorporation of vacancies in the core





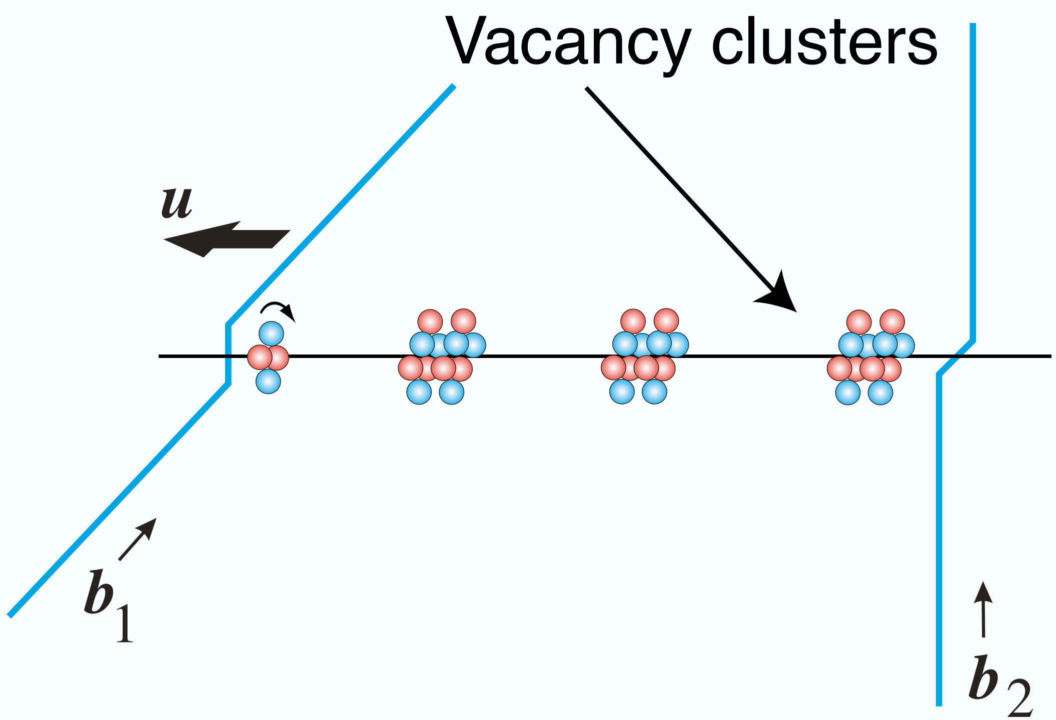
Vacancy in the core of a 30° partial as a local transition from the glide to the shuffle set

Cutting of dislocations



Cutting of edge dislocations

Formation of vacancy trails



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

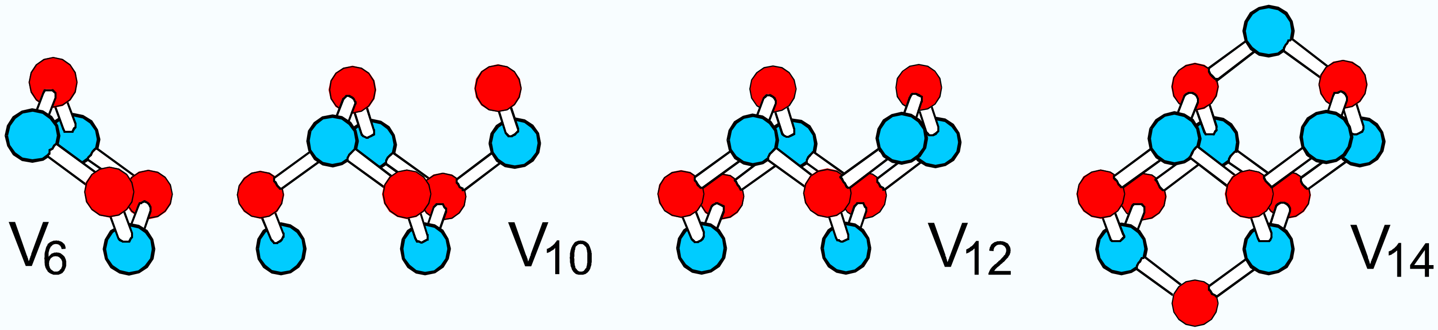
Number of point defects

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

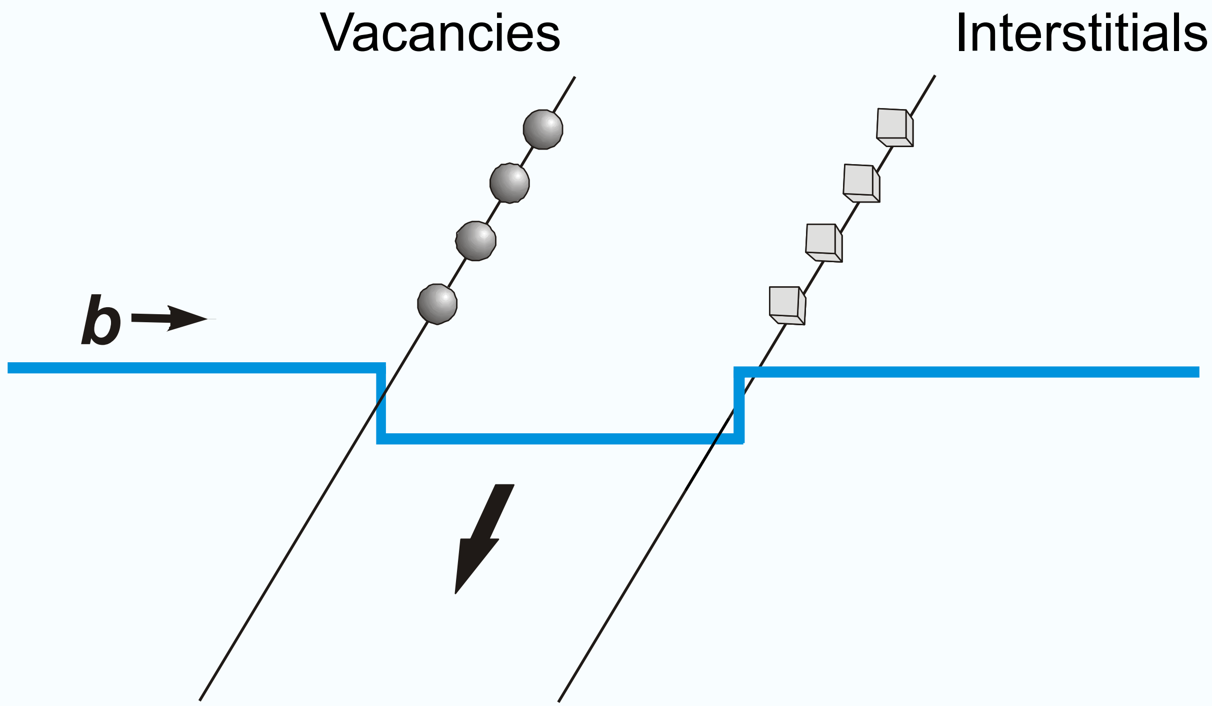
Results of plastic deformation experiments

Positron annihilation/density function tight binding calculations

- Long positron lifetime due to large vacancy agglomerations
- Stable vacancy clusters V_6, V_{10}, V_{14}
- Magic numbers of stable clusters: $n = 4i + 2$, $i = 1, 2, 3, \ldots$

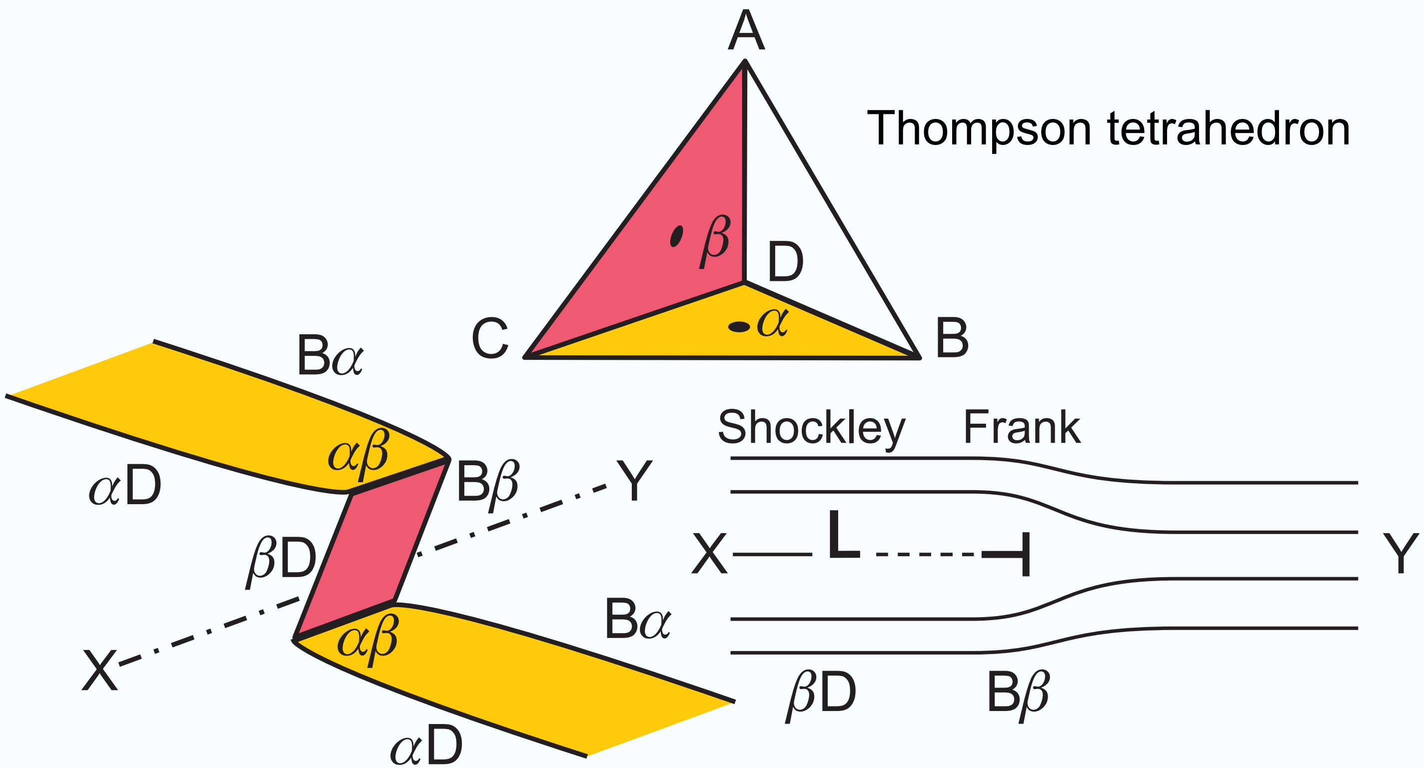


Interstitials



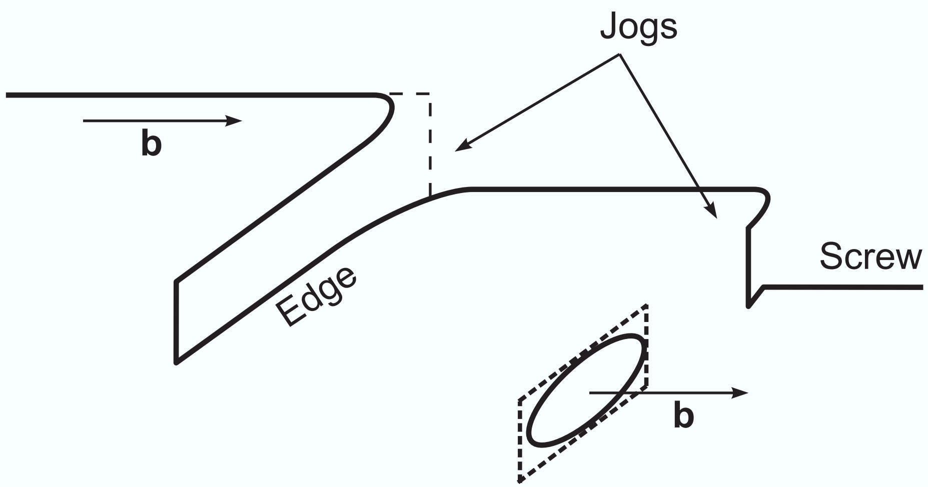
Type of the point defect emitted depends on the sign of the jog

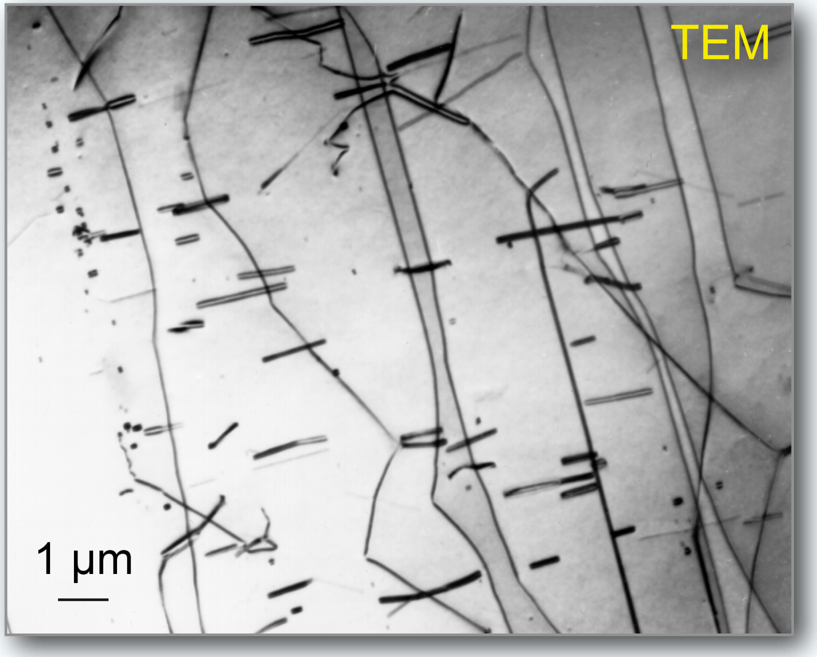
Extended jog



Structure of an extended jog in the acute-angle configuration on the screw **DB**. The X–Y cut illustrates the dissociation of the jog in a Shockley and a Frank partial (Burgers vectors **βD** and **Bβ**). The latter one has a pure edge character and can only follow the glide motion of the screw by emission or absorption of point defects.

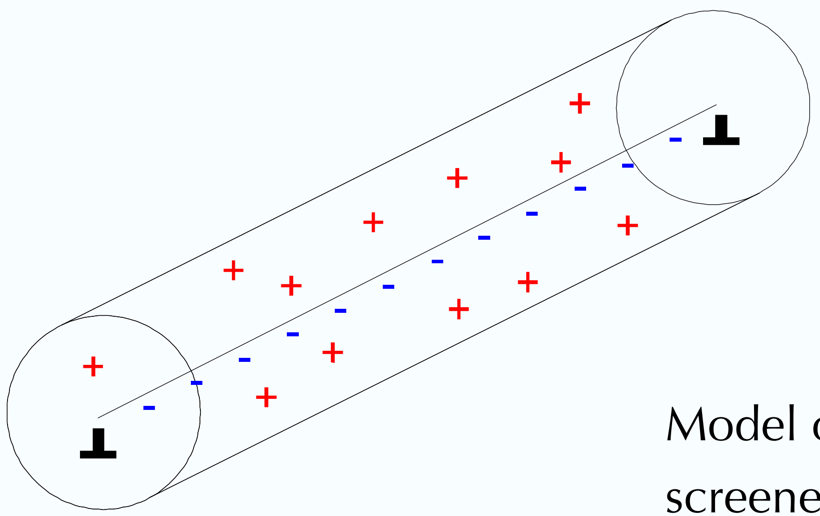
Superjogs





Formation of edge dipoles and prismatic dislocation loops

Interaction with impurities



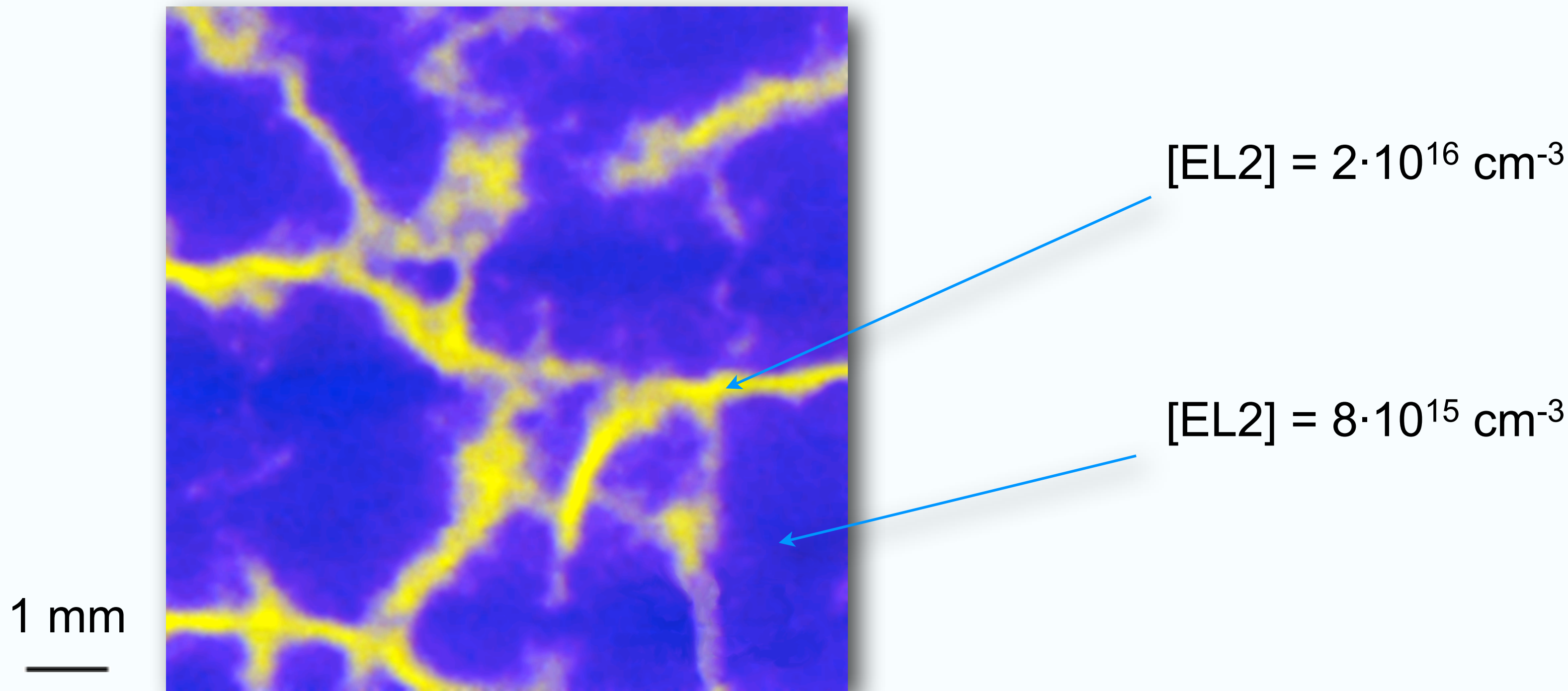
Model of Read (1957): The line charge of the dislocation is screened by a cylindrical space charge region, *i. e.* a negative dislocation is surrounded by positively charged acceptors.

Radius of the Read cylinder

$$R = \frac{1}{\sqrt{a\pi |N_\mathrm{d} - N_\mathrm{a}|}}$$

(a distance between charged core atoms, N_d, N_a donor, acceptor density)

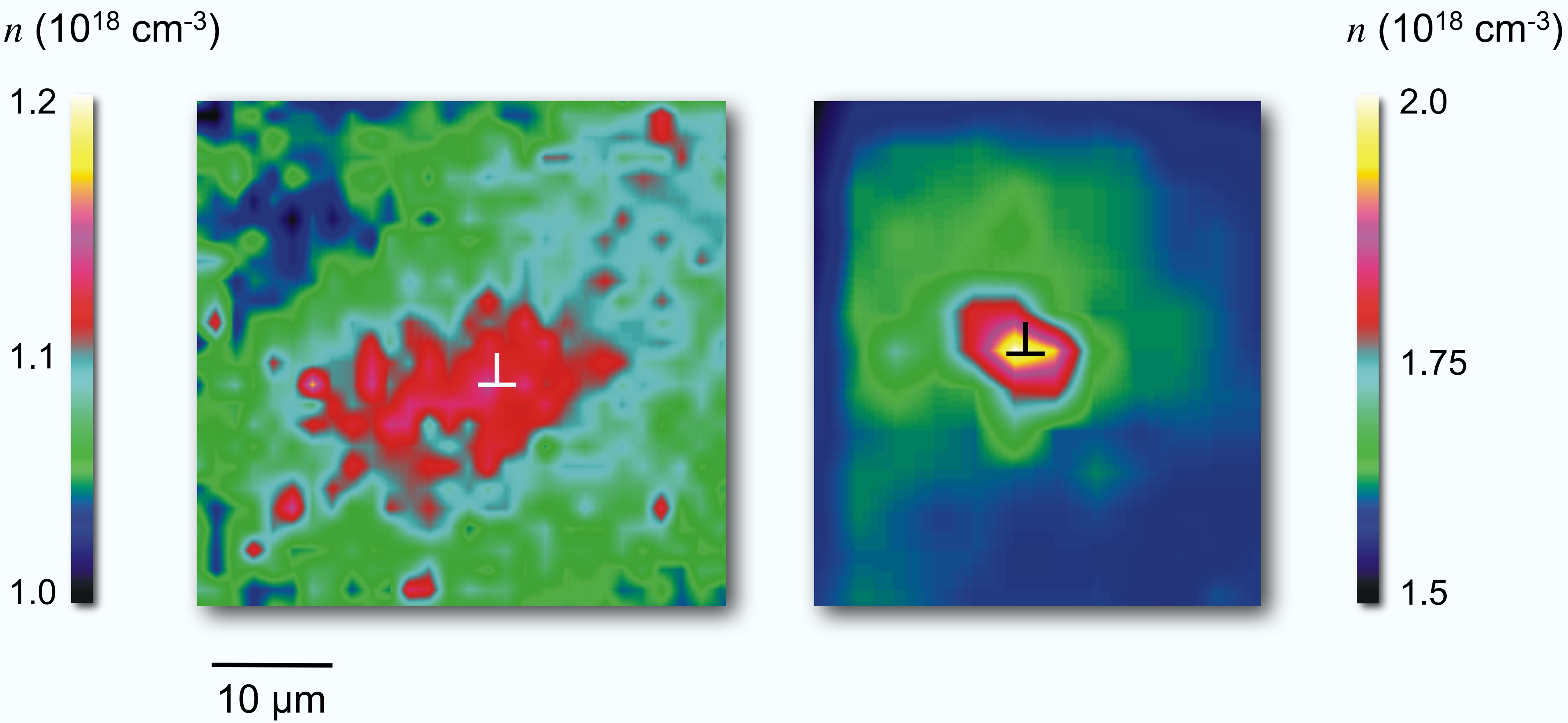
Accumulation of point defects at dislocations



Mesoscopic distribution of EL2 centers in VGF GaAs as seen in optical absorption at 1 μm. The concentration of EL2 distinctly increases at dislocations.

[R Kremer, S Teichert, Comp. Semicond. 2003]

Distribution of carriers



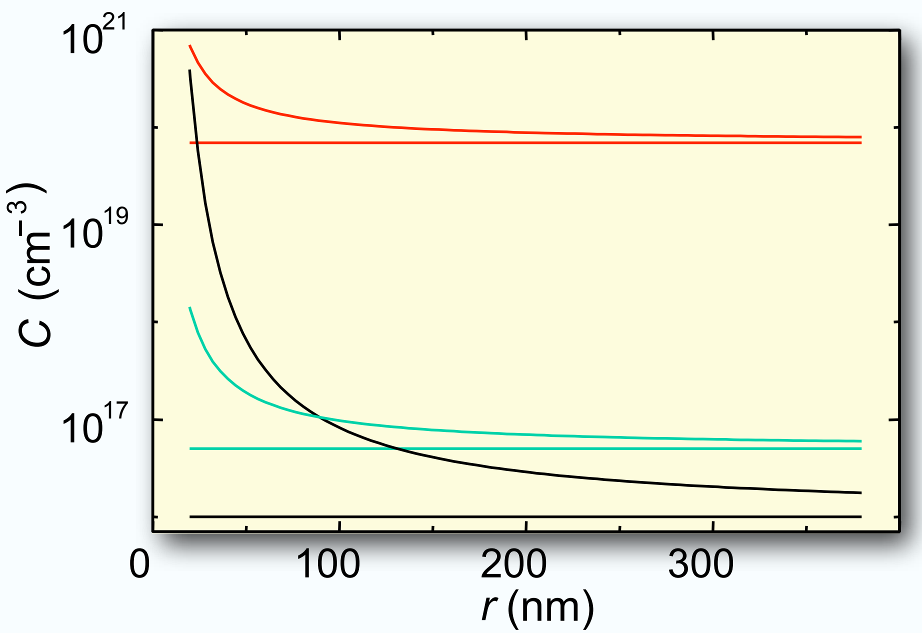
Density of free carriers n measured by confocal Raman microscopy at dislocations in GaAs:Si (*left*) and GaAs:S (*right*)

Cottrell atmosphere

Equilibrium case

Distribution of impurities at an edge dislocation for time $t \to \infty$

$$C(r) = C_{eq} \exp\left(-\frac{\beta \sin\theta}{r k_B T}\right) \qquad \beta = \frac{G b_e}{3\pi} \frac{1+\nu}{1-\nu} \Delta V$$



C_{eq} = $8 \cdot 10^{18}$ cm^{-3} (1373 K)

C_{eq} = $5 \cdot 10^{16}$ cm^{-3} (973 K)

C_{eq} = $1 \cdot 10^{16}$ cm^{-3} (300 K)

Distribution of copper at a 60° dislocation in GaAs for different solubilities C_{eq}

Microscopic processes at dislocations

- Elastic interaction of point defects and dislocations

$$\Phi(r) = -\frac{A}{r}\sin\theta$$

- Diffusion of point defects, *e. g.* via kick-out or vacancy mechanism

$$\mathrm{X_i} \rightleftarrows \mathrm{X_s} + \mathrm{I}$$

- Formation of precipitates

$$\mathrm{X_i} \rightleftarrows \mathrm{p}$$

- Formation of dislocation loops

$$\mathrm{I} \rightleftarrows \ell$$

- Formation of defect complexes

$$\mathrm{X_s} + \mathrm{V} \rightleftarrows \mathrm{X_sV}$$

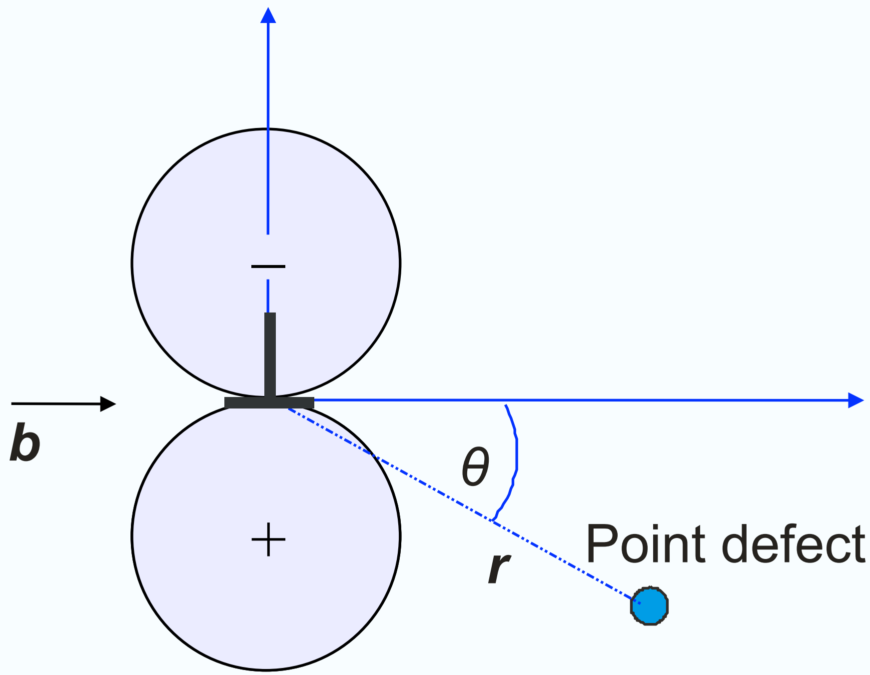
- Fermi-level effect

$$\frac{C_{\mathrm{X}^z}}{C_{n_\mathrm{i}}} = \left(\frac{n}{n_\mathrm{i}}\right)^z$$

↓

Diffusion–drift–aggregation model

Diffusion–drift–aggregation model



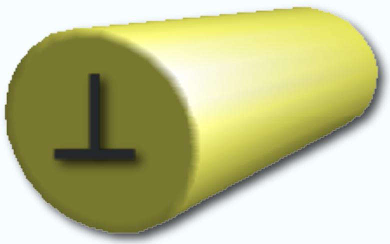
Elastic interaction potential

$$\Phi(r) = -\frac{A}{r}\sin\theta \qquad A = \frac{4}{3}\frac{1+\nu}{1-\nu}Grb\,\varepsilon$$

Diffusion current — Effect of charged point defects — Drift — Precipitation

$$\frac{\partial C(r,t)}{\partial t} = \nabla D\left[\nabla C(r,t) - \frac{C(r,t)}{C_{\mathrm{eq}}(r)}\nabla C_{\mathrm{eq}}(r) + \frac{C(r,t)}{k_{\mathrm{B}}T}\nabla\Phi(r)\right] - \gamma\Psi_{\mathrm{p}}$$

Non-equilibrium atmosphere



Homogeneous formation of precipitates only inside a cylinder with the radius r_0 about the dislocation core

$$\gamma = \begin{cases} 1 & \text{for } r < r_0 \\ 0 & \phantom{\text{for }} r > r_0 \end{cases}$$

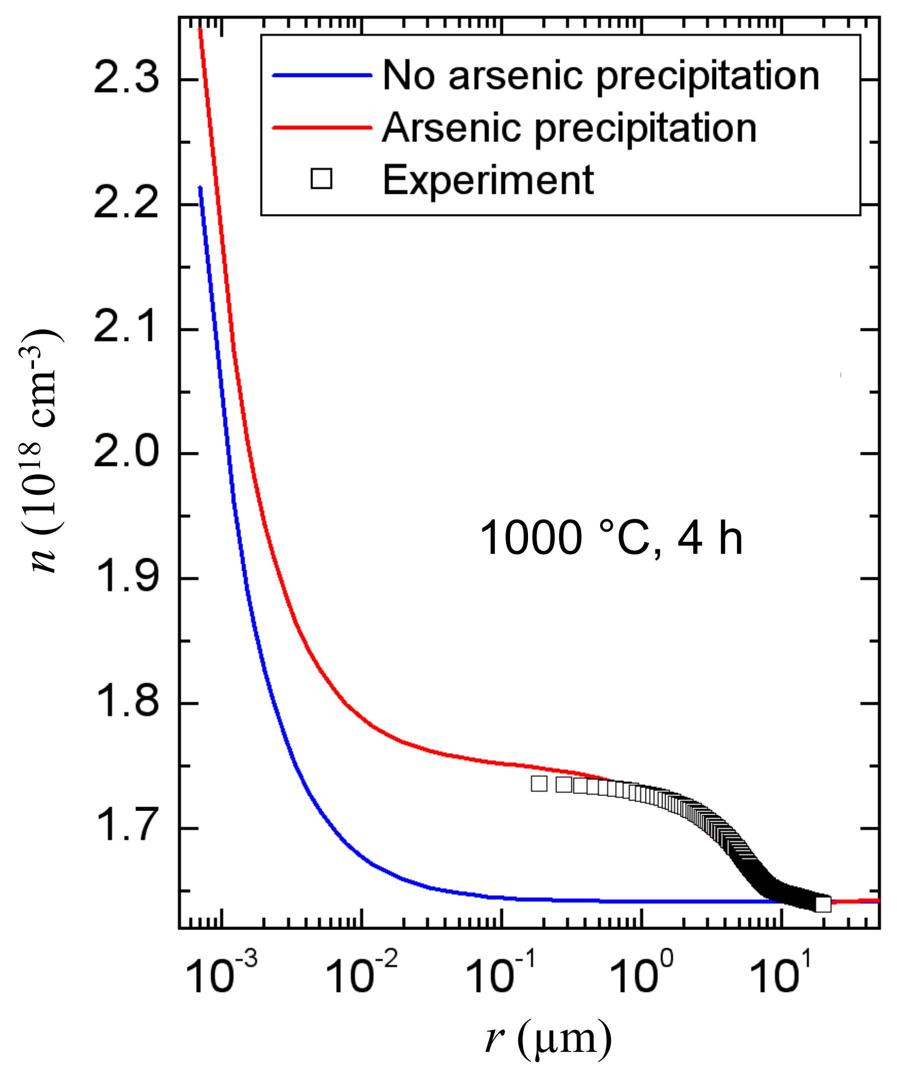
Nucleation rate according to classical nucleation theory in the dislocation region

$$\Psi = 4\pi r_0 C(r,t)^2 D \exp\left(-\frac{16}{3}\frac{\sigma^3 V^2}{k_\mathrm{B} T (k_\mathrm{B} T \ln \Sigma)^2}\right)$$

(σ interface energy, V atomic volume, Σ supersaturation)

Simulation of the distribution of carriers

- From the DDA model: variation of the concentration of defects (interstitials, charged vacancies, impurities, complexes
- Calculation of the local carrier concentration



Distribution of free carriers at a 60° dislocation in GaAs:S without and with consideration of native point defects

Conclusions

- Straight, perfect dislocation line hardly exists
- Complicated set of core defects; interaction with intrinsic defects of the bulk
- Hardly to separate in spectroscopic measurements different types of defects in the bulk, in the strain field of the dislocation, and in the core
- Shuffle set can be stabilized by the interaction with vacancies
- An extended defect zone, characterized by the depletion or enrichment of various point defects, is formed around dislocations.
- Electrical activity of a dislocation is the superposition of core effect, core defects, segregation of impurities in the core, accumulation/depletion of impurities in the strain field

Crashed-car dislocations
[Courtesy J. Rabier]

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References

- W. Shockley: Phys. Rev. **91** (1953) 228.
- W. T. Read: Phil. Mag. **45** (1954) 775.
- R. Kremer, S. Teichert: Comp. Semicond. **9** (2003) 35.