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Interaction of dislocations and point defects

Influence on defect patterning

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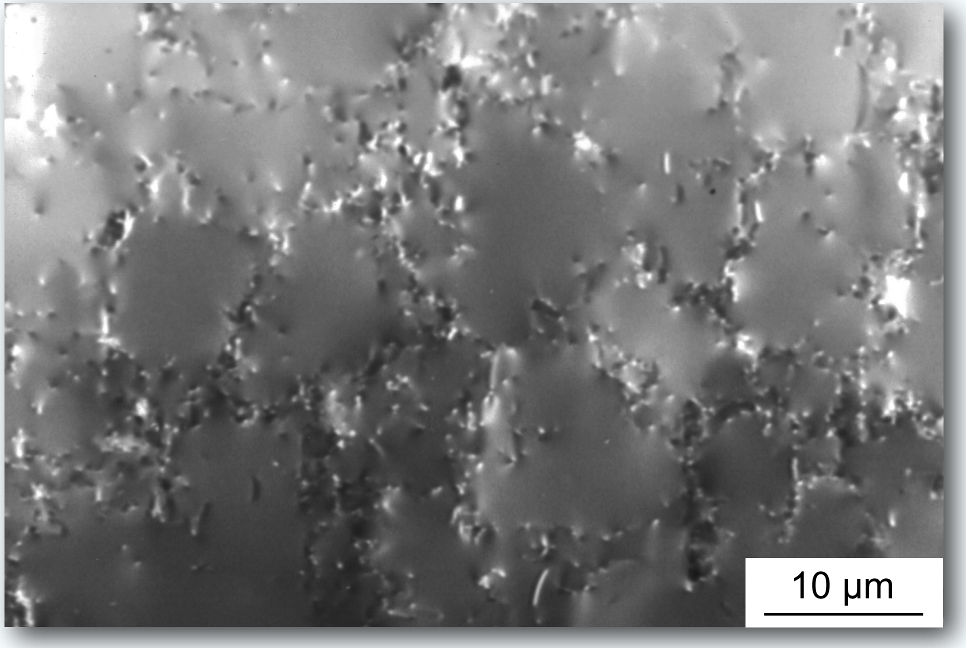
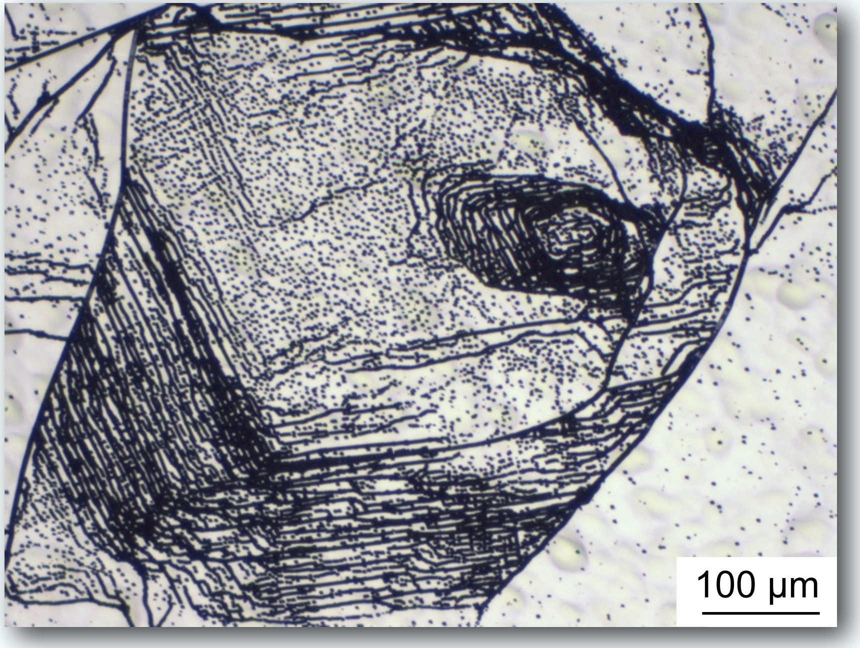
Dislocation patterning



Double-crystal topography of dislocation cells in LEC-grown (001) GaAs. Cu Kα_1 radiation, 511 reflection.
[W. Leitenberger]

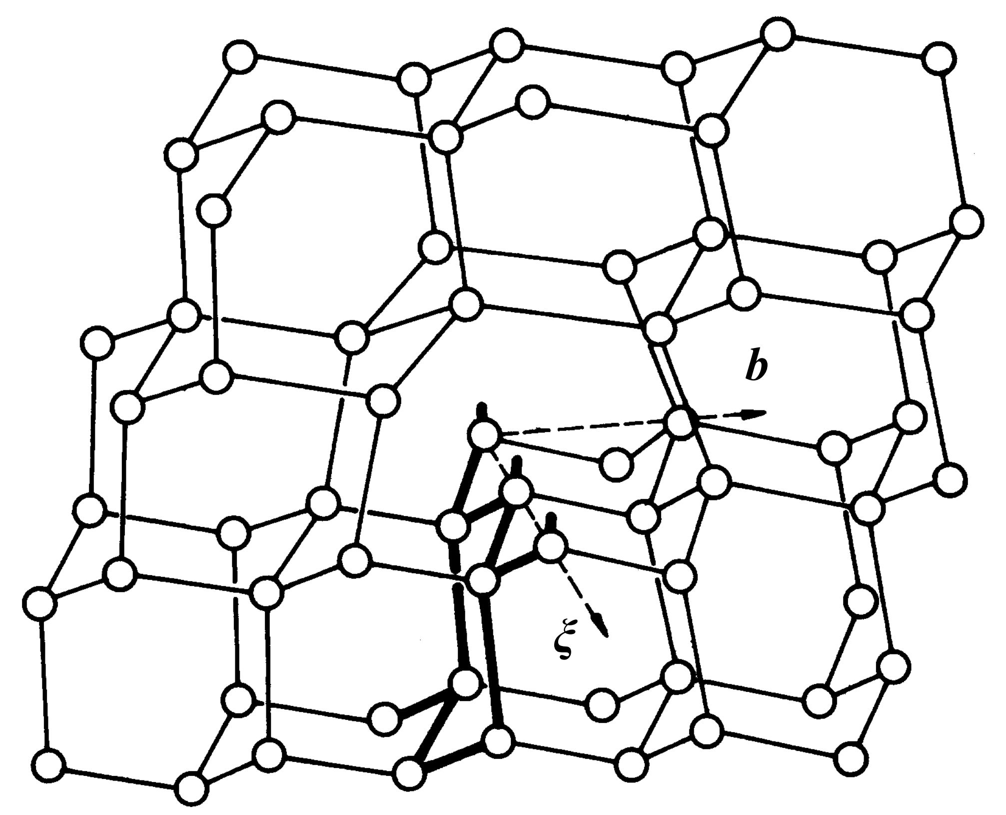


Etch-pit pattern of the dislocation distribution in multi-crystalline silicon
[D. Oriwol]

Dislocation distribution ↔ Variation in electrical/optical properties

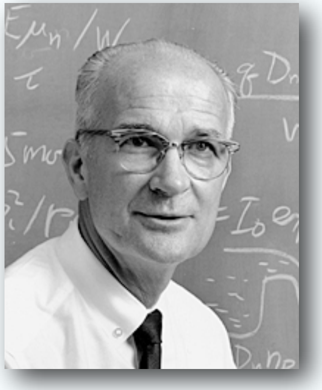
Role of intrinsic point defects and impurities

Core structure of dislocations

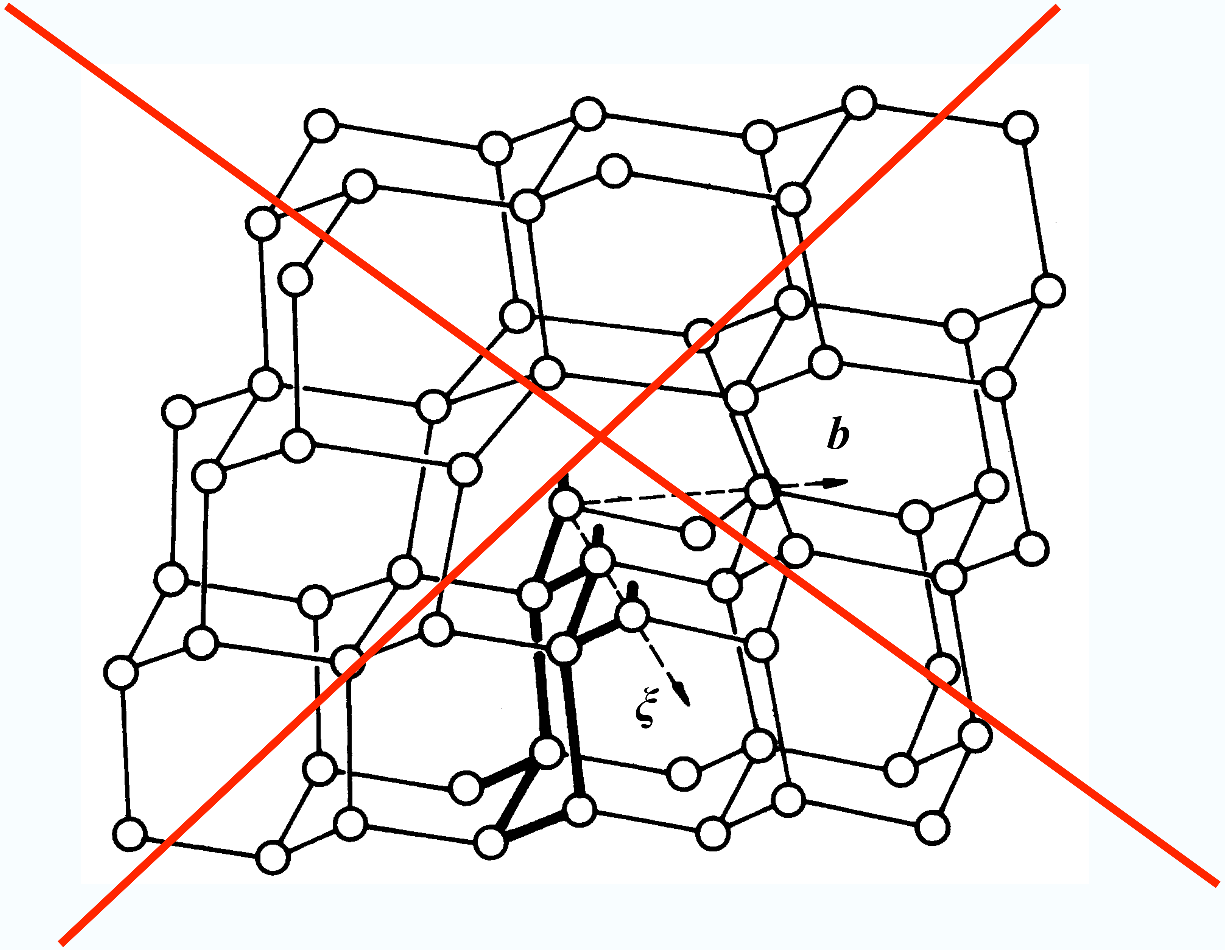


60° dislocation in the diamond structure, $\boldsymbol{b} = \frac{a}{2}\langle 110\rangle$.

[Shockley 1953]



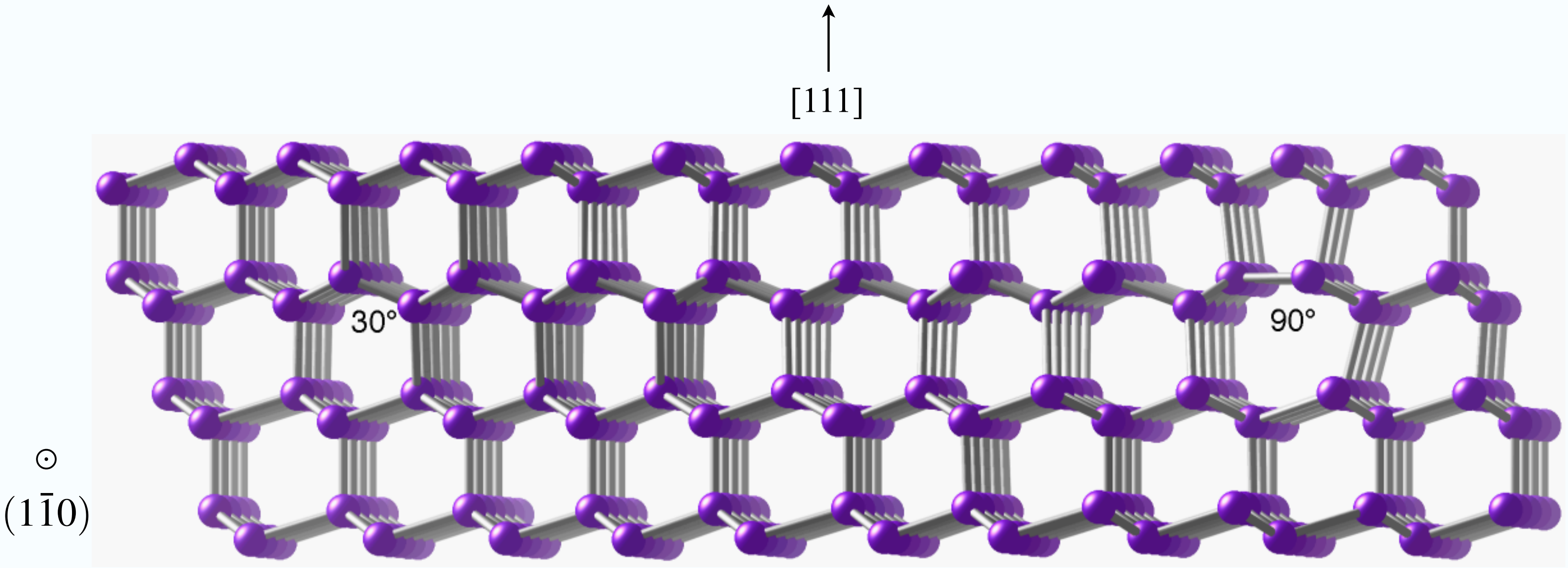
“Ptolemaic” picture of dislocations



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

[Shockley 1953]

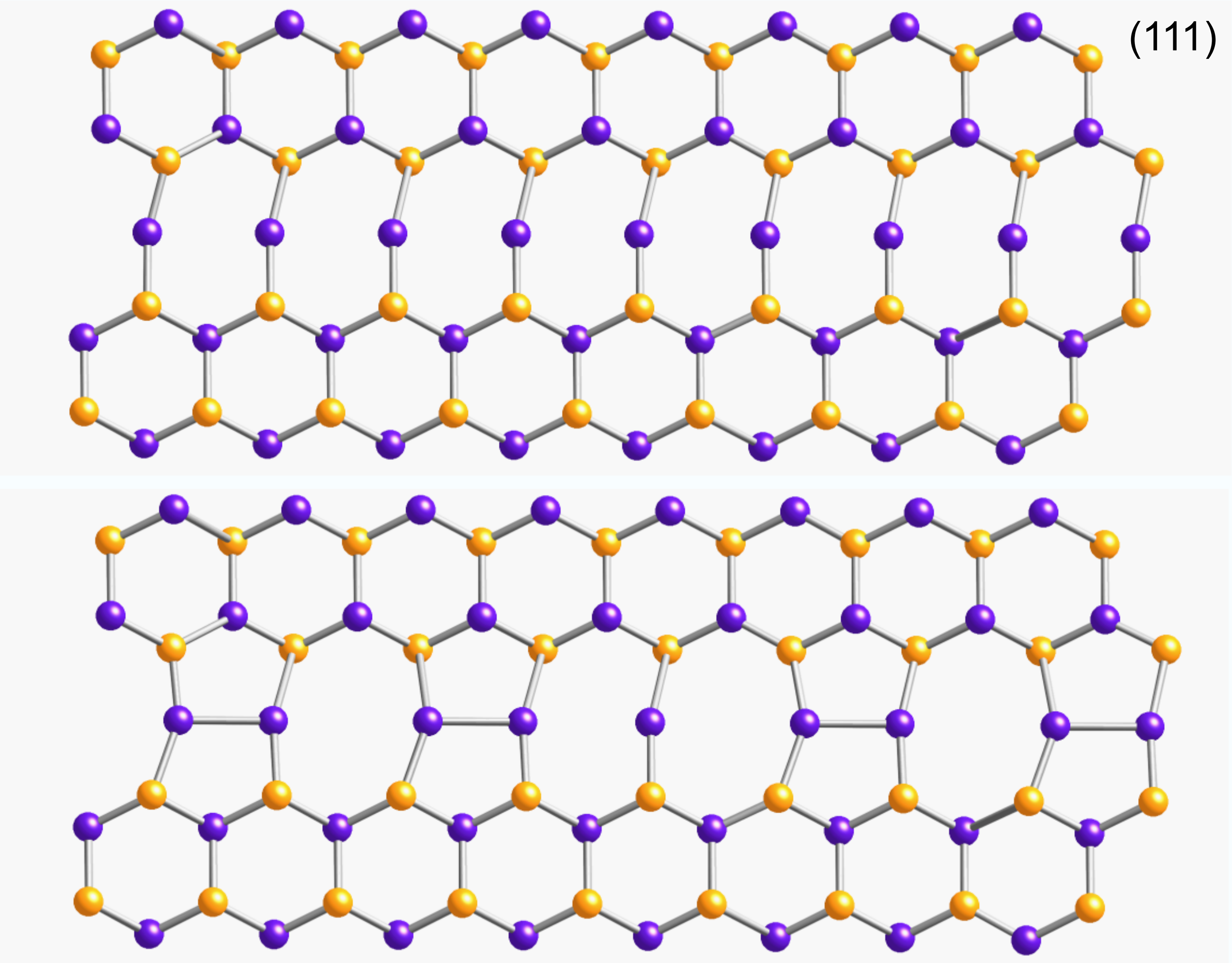
Dissociation



Dissociation of a perfect 60° dislocation in the diamond structure into a 30° and a 90° partial.

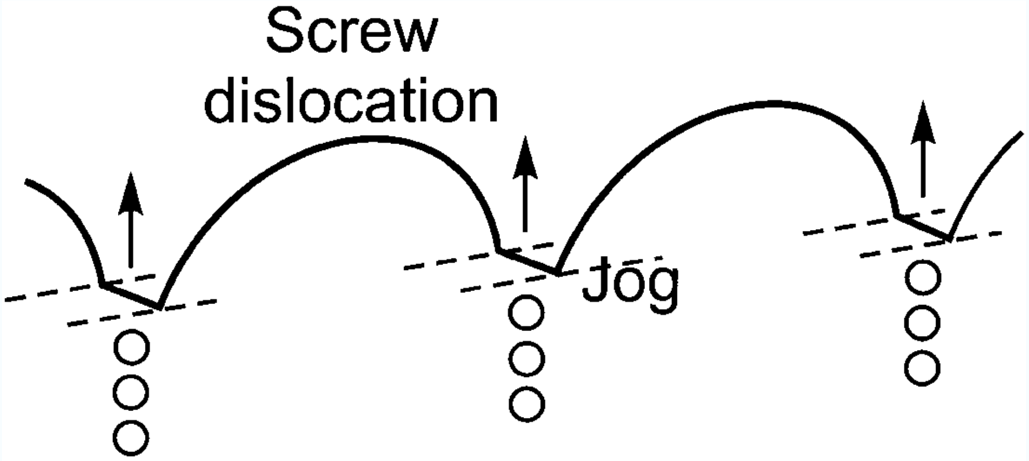
The Shockley partial dislocations, $\boldsymbol{b} = \frac{\boldsymbol{a}}{6}\langle 211\rangle$, are separated by a stacking fault.

Reconstruction



Unreconstructed and reconstructed 30° partial

Jog dragging



Jog dragging at screw dislocations
and point defect emission

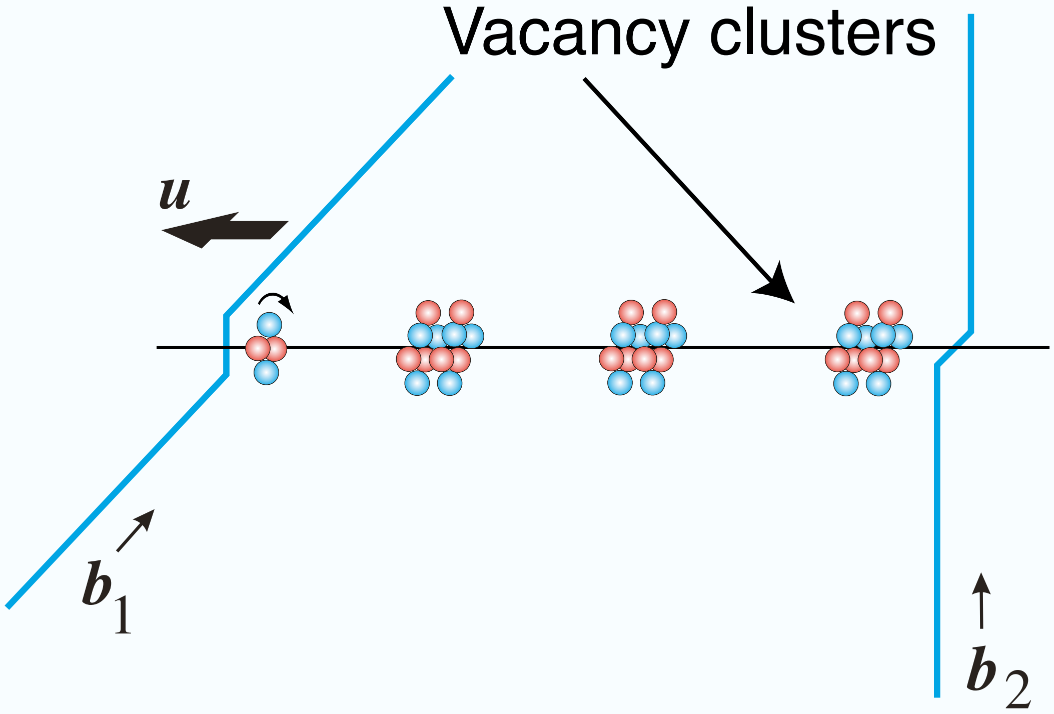
TEM Staab HS Leipner *et al* Phys Rev Lett **83** (1999) 5519

Formation of a trail of vacancy clusters

Number of point defects

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

(per unit step
from the cutting of two screws)

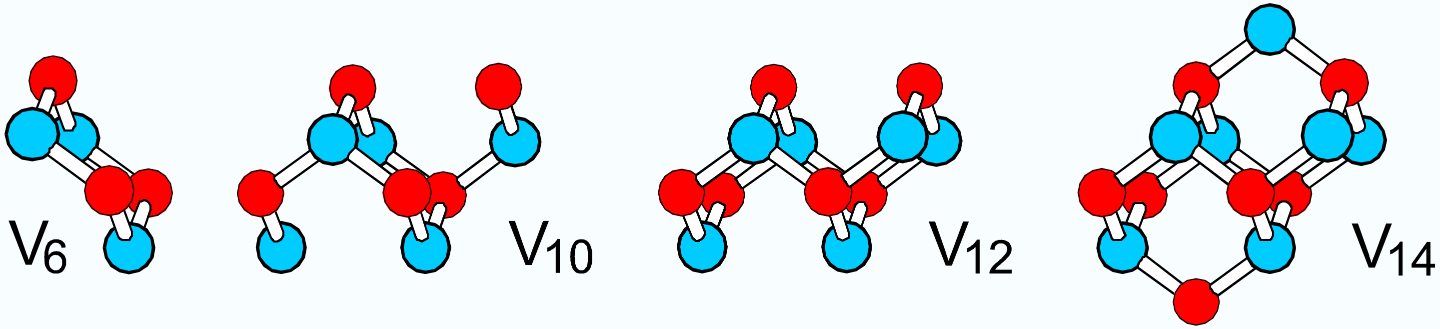


Agglomerations of vacancies as a result
of jog dragging at screw dislocations

Plastic deformation

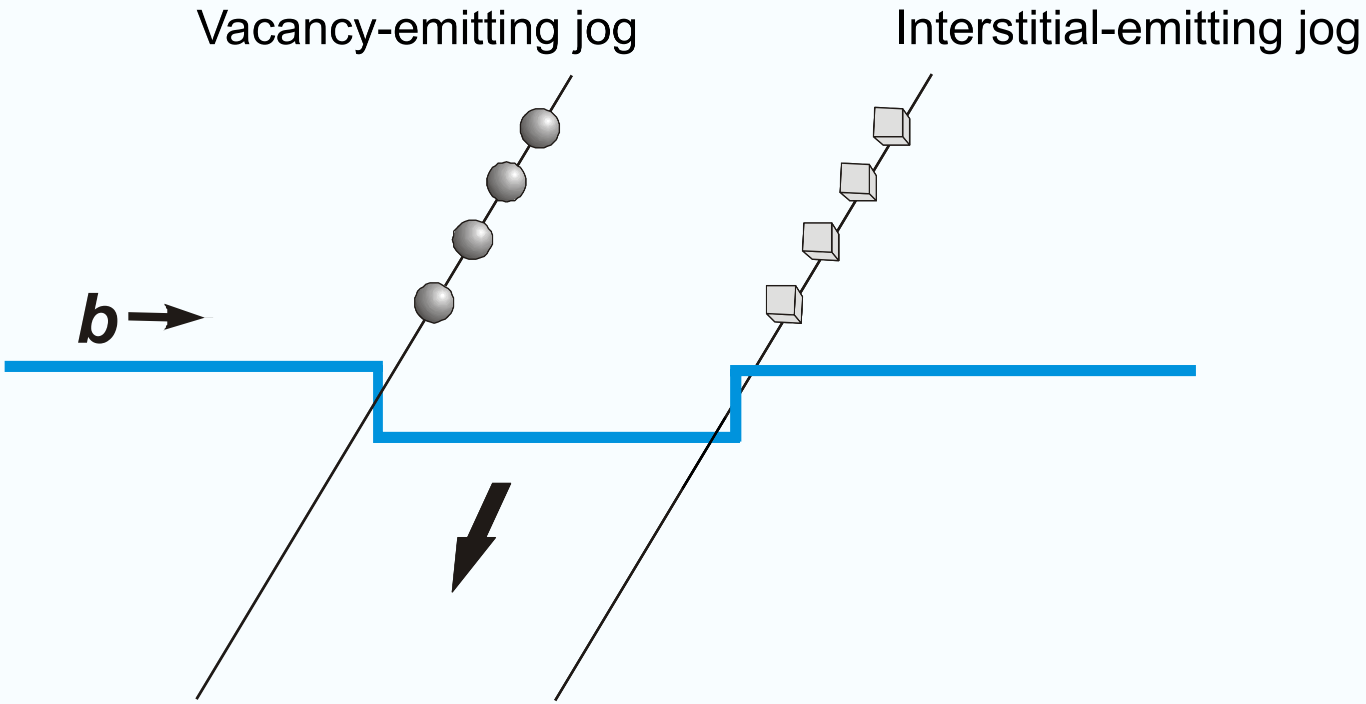
Positron annihilation measurements and density functional tight binding calculations

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



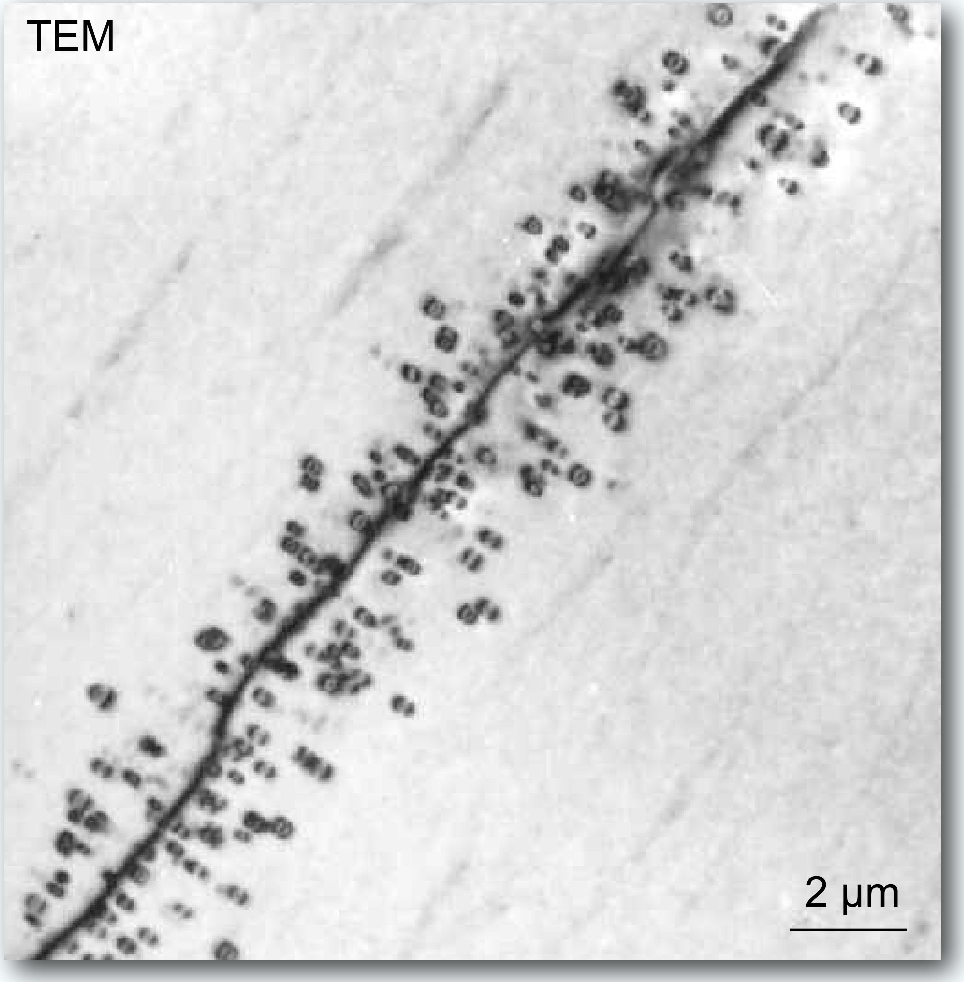
TEM Staab HS Leipner *et al* Phys Rev Lett **83** (1999) 5519

Interstitials



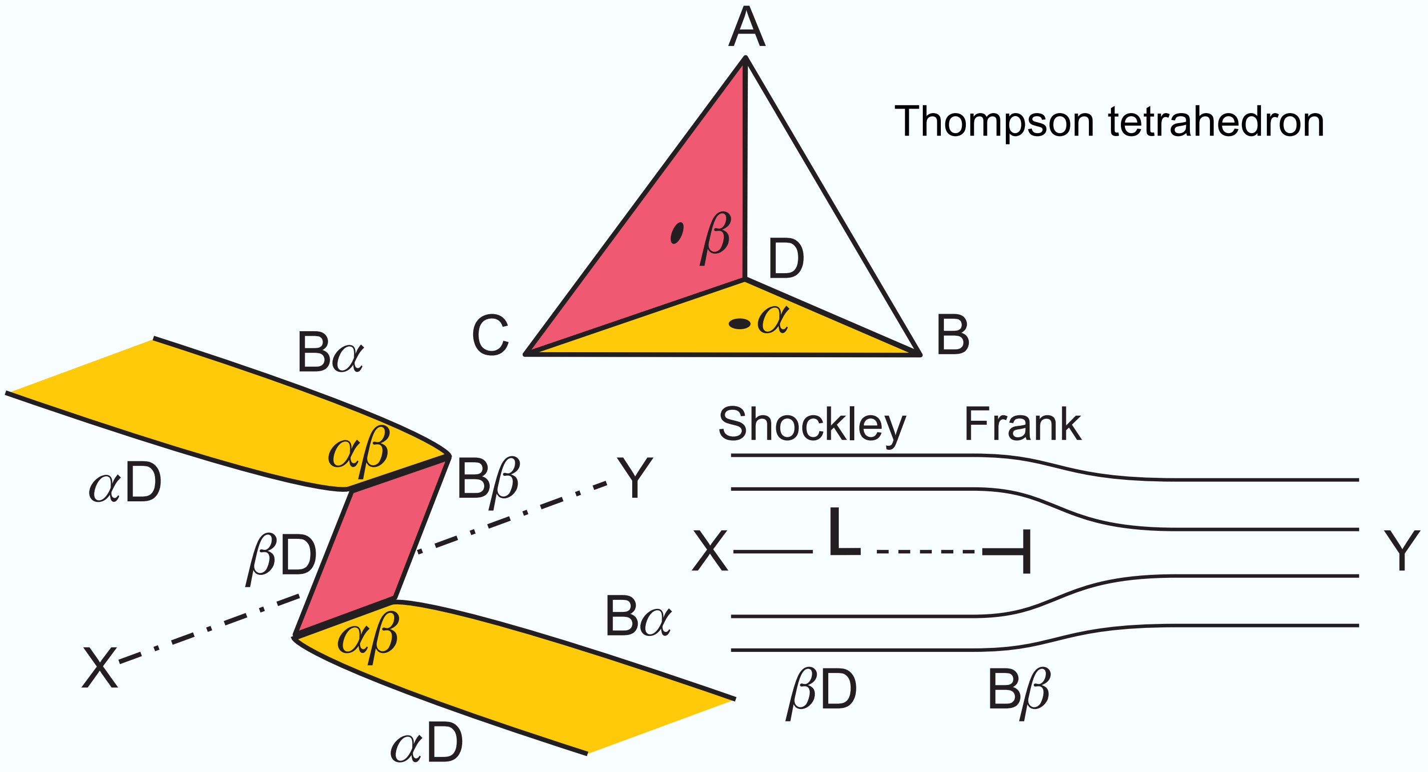
The type of the point defects emitted depends on the sign of the jog

Interstitials



Interstitial loops surrounding a dislocation in GaAs

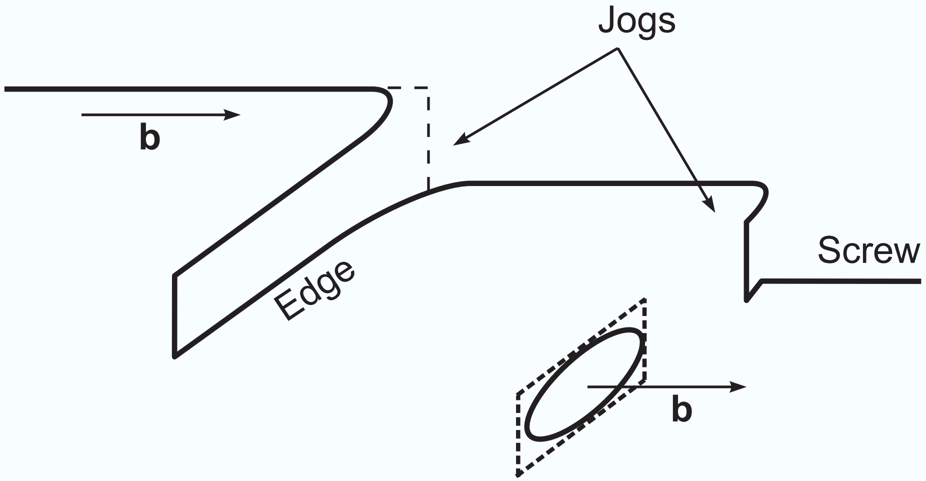
Extended jog

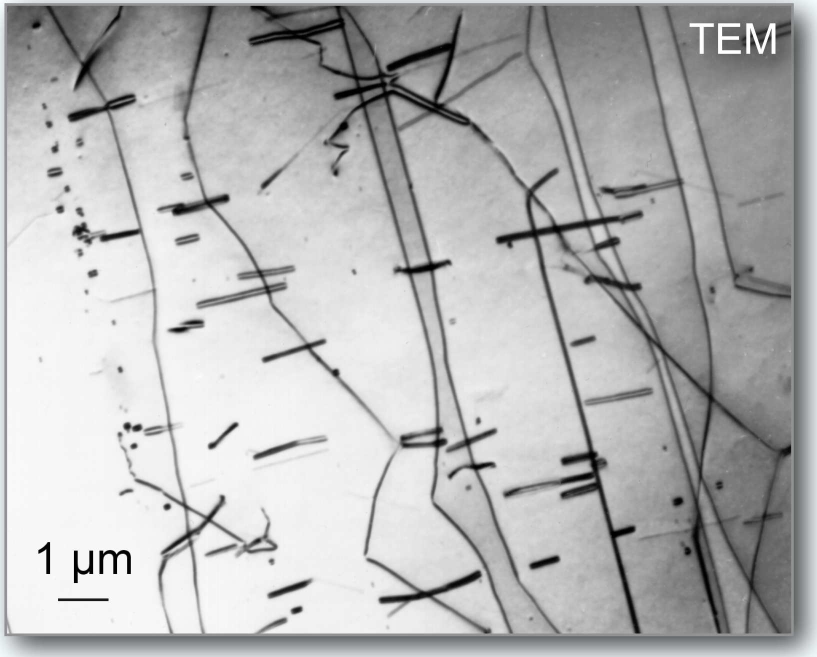


Structure of an extended jog in the acute-angle configuration on the screw **DB**. The X–Y cut illustrates the dissociation of the jog in a Shockley and a Frank partial (Burgers vectors **βD** and **Bβ**). The latter one has a pure edge character and can only follow the glide motion of the screw by the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

HS Leipner *et al* J Phys Cond Mat **12** (2000) 10071

Superjogs





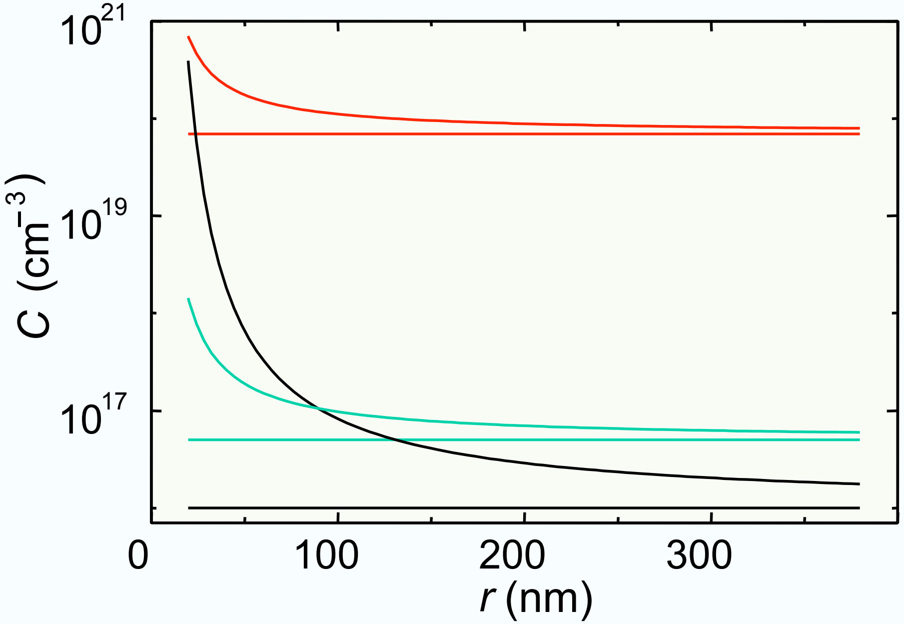
Formation of edge dipoles and prismatic dislocation loops

Cottrell atmosphere of impurities

Equilibrium case from elastic interaction

Distribution of impurities about an edge dislocation for time $t \rightarrow \infty$

$$C(r) = C_{\text{eq}} \exp\left(-\frac{\beta \sin\theta}{r\, k_{\text{B}} T}\right) \qquad \beta = \frac{G b_{\text{e}}}{3\pi} \frac{1+\nu}{1-\nu} \Delta V$$



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

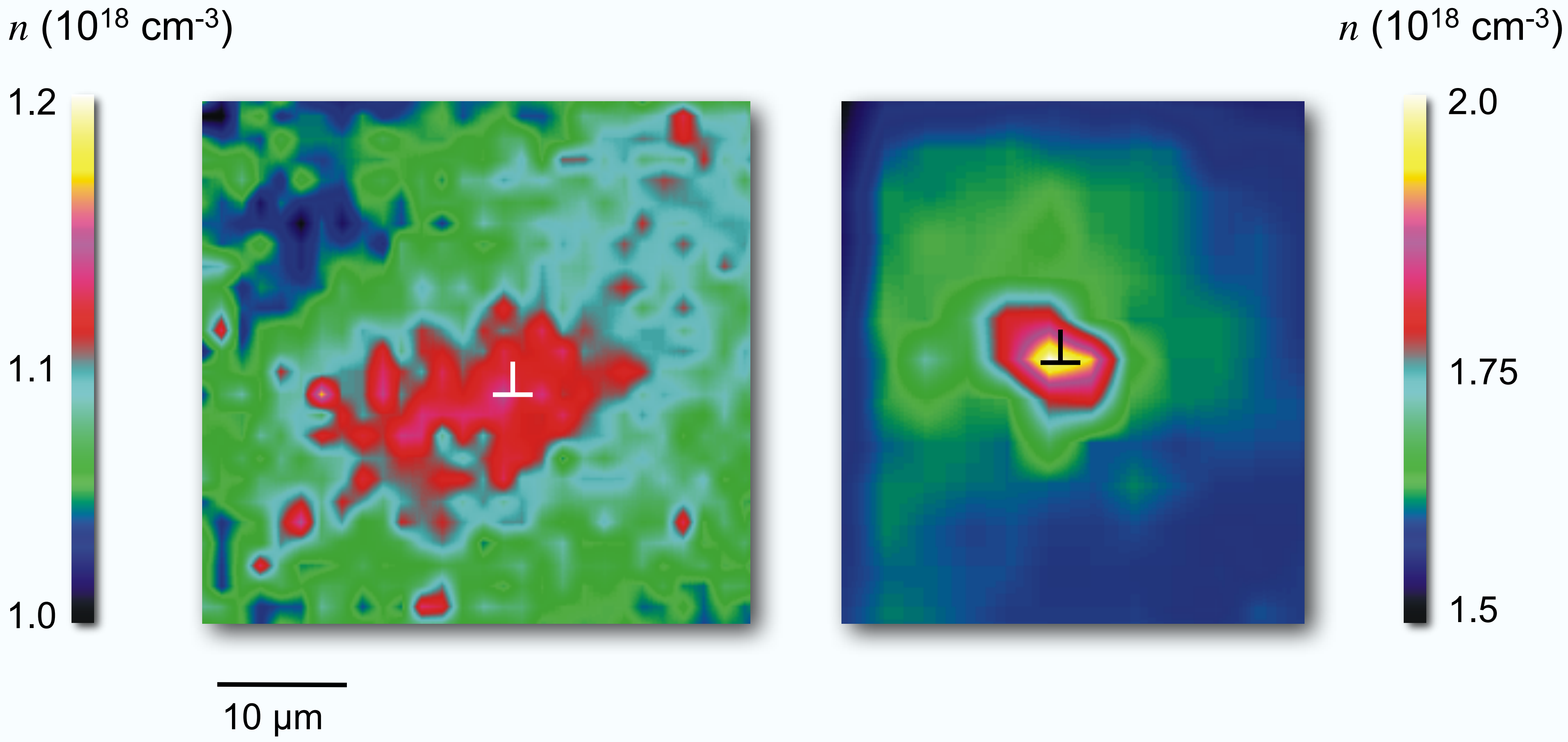
$C_{\text{eq}} = 5 \cdot 10^{16}$ cm^{-3} (973 K)

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

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

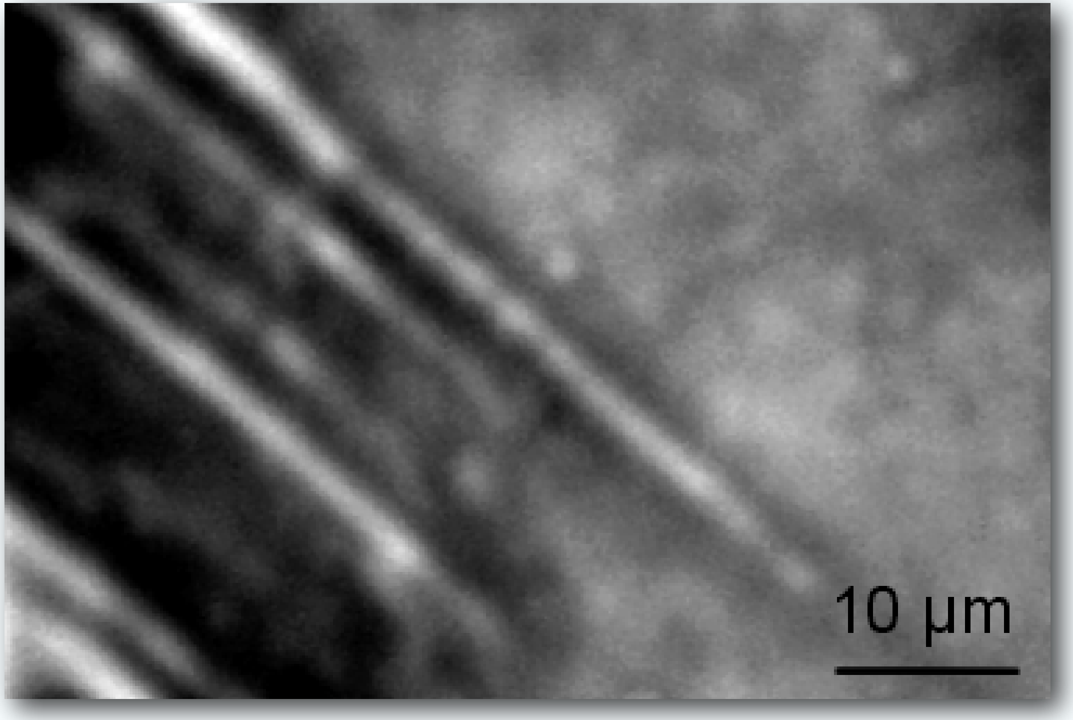
HS Leipner *et al* Phil Mag A **79** (1999) 2785

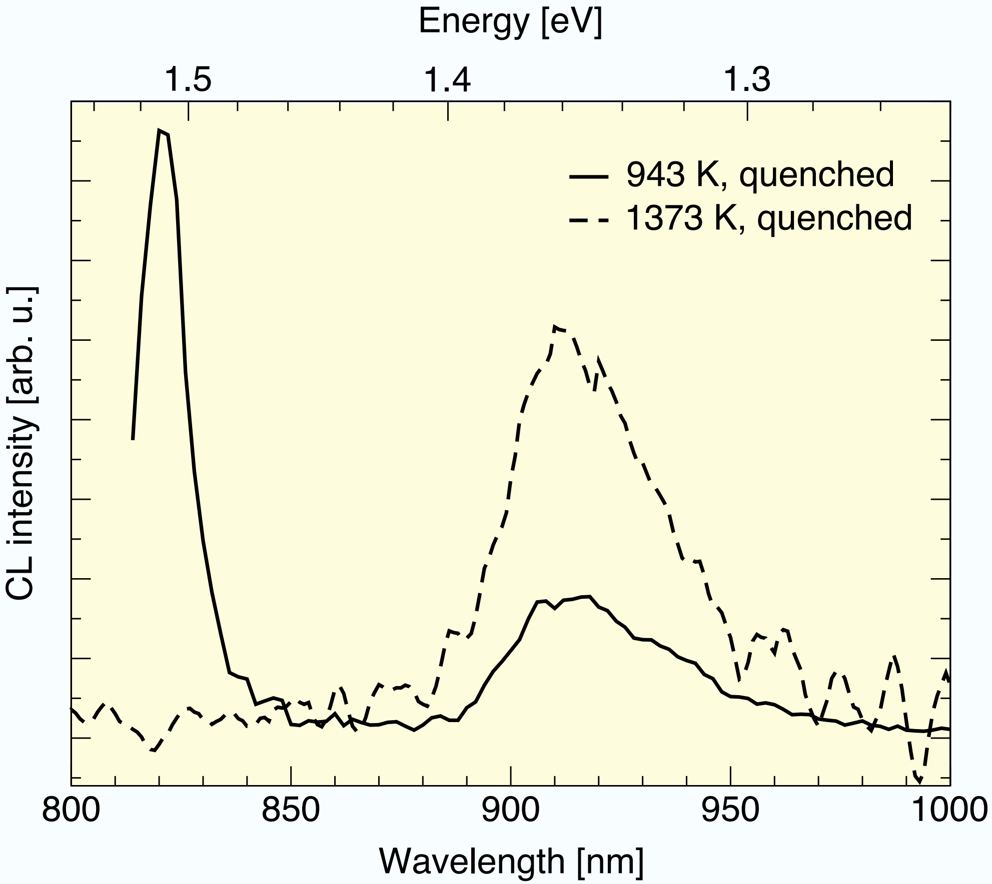
Distribution of charge carriers



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

Decorated dislocations





Decorated dislocations with a bright cathodoluminescence contrast in GaAs after copper in-diffusion. The bright contrast is due to the 1.36 eV emission related to Cu_{Ga} acceptors.

HS Leipner *et al* Mater Sci Eng B **42** (1996) 185

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

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

- Segregation in the core

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

- Formation of dislocation loops from supersaturated point defects

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

- Formation of defect complexes (intrinsic point defects/impurities)

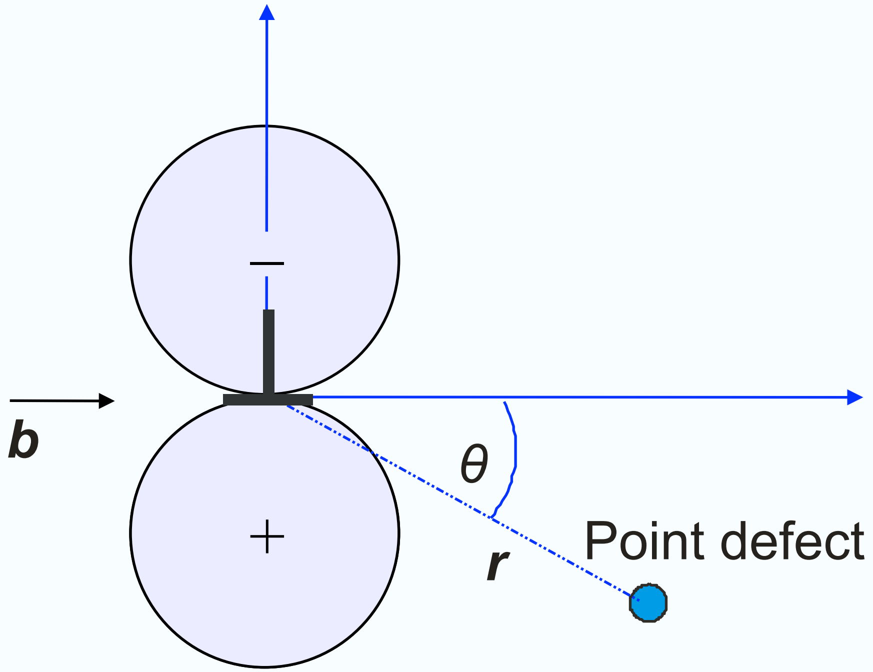
$$\mathrm{X_s} + \mathrm{V} \rightleftarrows \mathrm{X_sV}$$

- Fermi-level effect

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

Diffusion–drift–aggregation (DDA) model

Diffusion–drift–aggregation model



Elastic interaction potential

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

Drift current

Effect of charged point defects

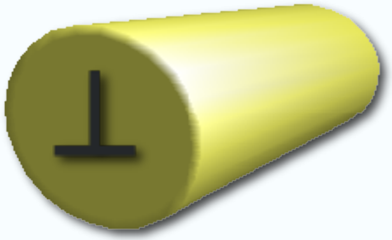
Diffusion

Segregation

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

HS Leipner *et al* Phil Mag A 79 (1999) 2785

Non-equilibrium atmosphere



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

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

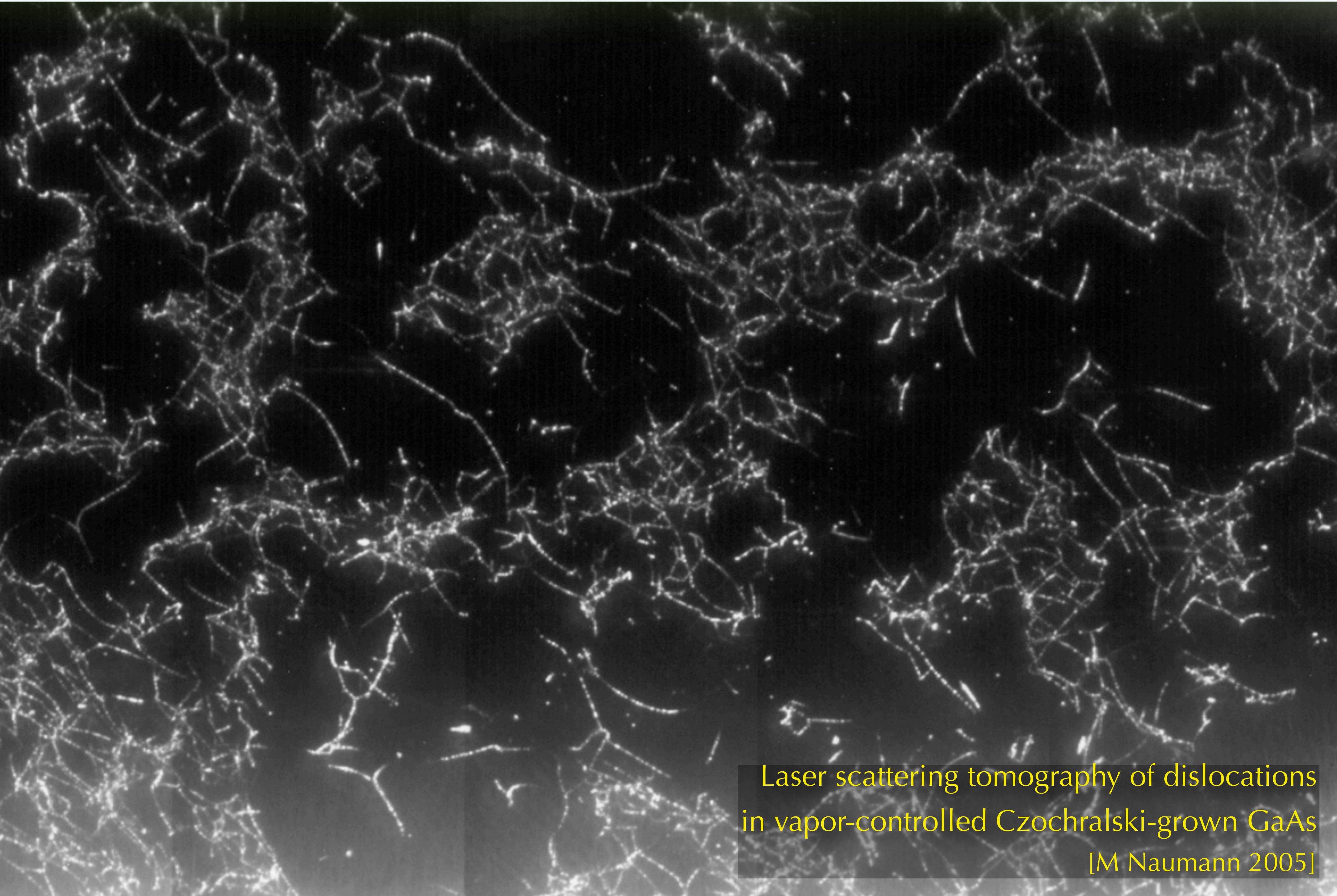
- Nucleation rate according to classical nucleation theory in the dislocation region

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

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

see R Bullough, R Newman Proc Royal Soc A **198** (1962) 209, 266

Arsenic precipitates at dislocations in GaAs

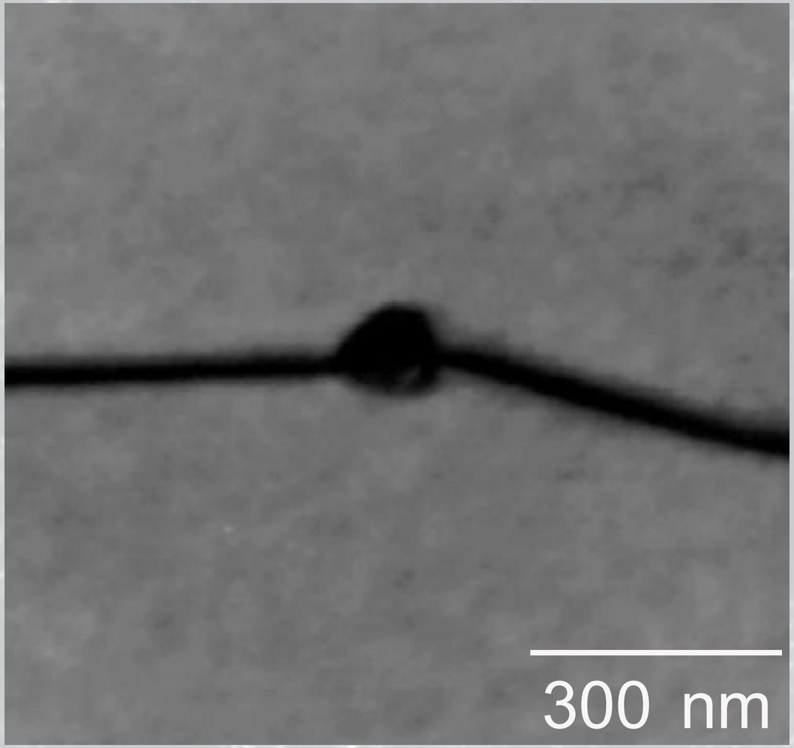


Laser scattering tomography of dislocations in vapor-controlled Czochralski-grown GaAs

[M Naumann 2005]

Arsenic precipitates at dislocations in GaAs

- Arsenic precipitation not homogeneous along the core
- Decoration of the core?

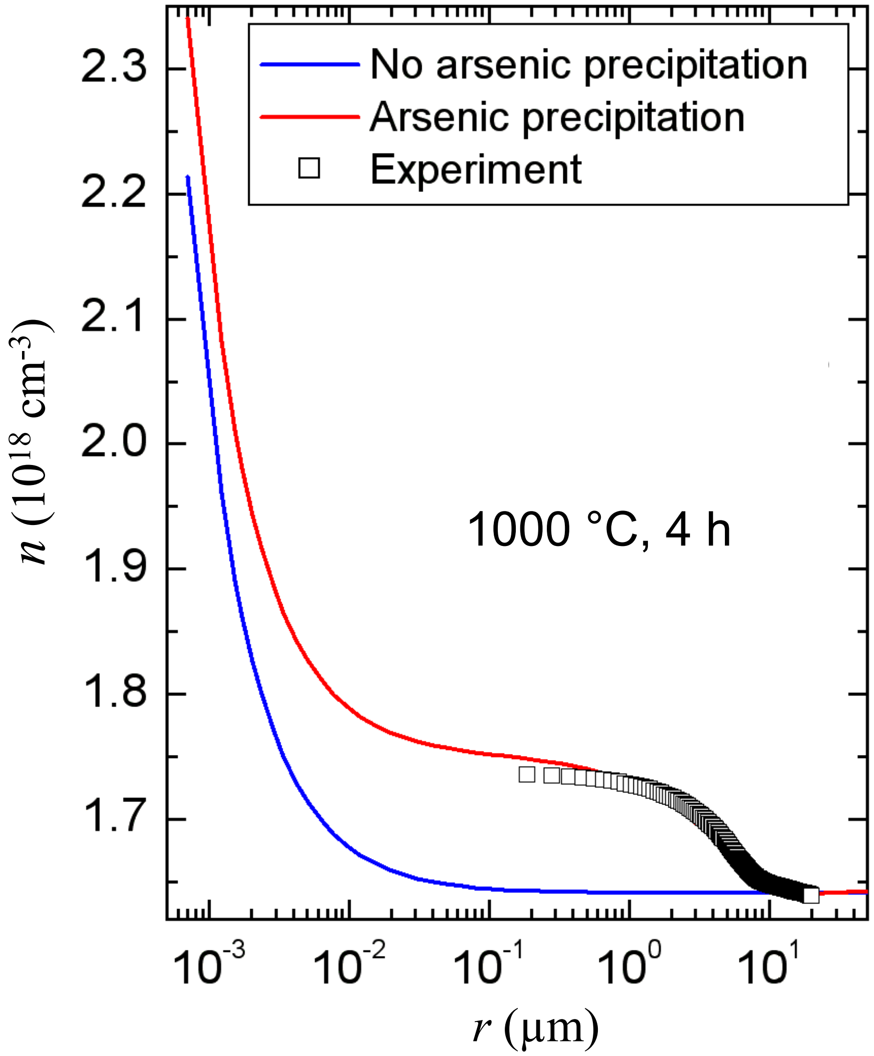


TEM bright field image of a dislocation decorated with an arsenic precipitate

HS Leipner H Lei phys stat sol (c) **2** (2005) 1859

Simulation of the distribution of carriers

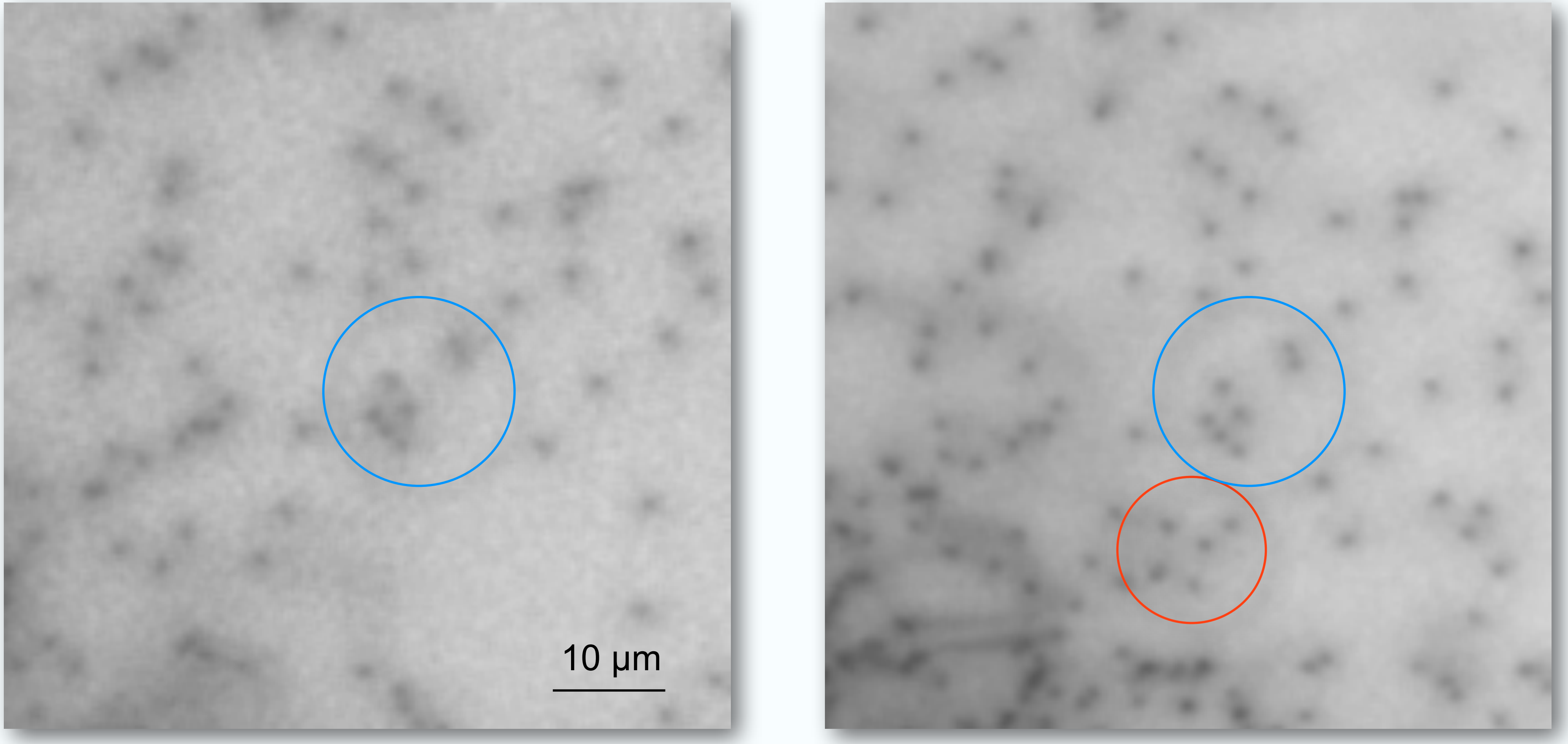
- From the DDA model:
  variation of the concentration of defects (interstitials, charged vacancies, impurities, complexes
- Calculation of the local carrier concentration



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

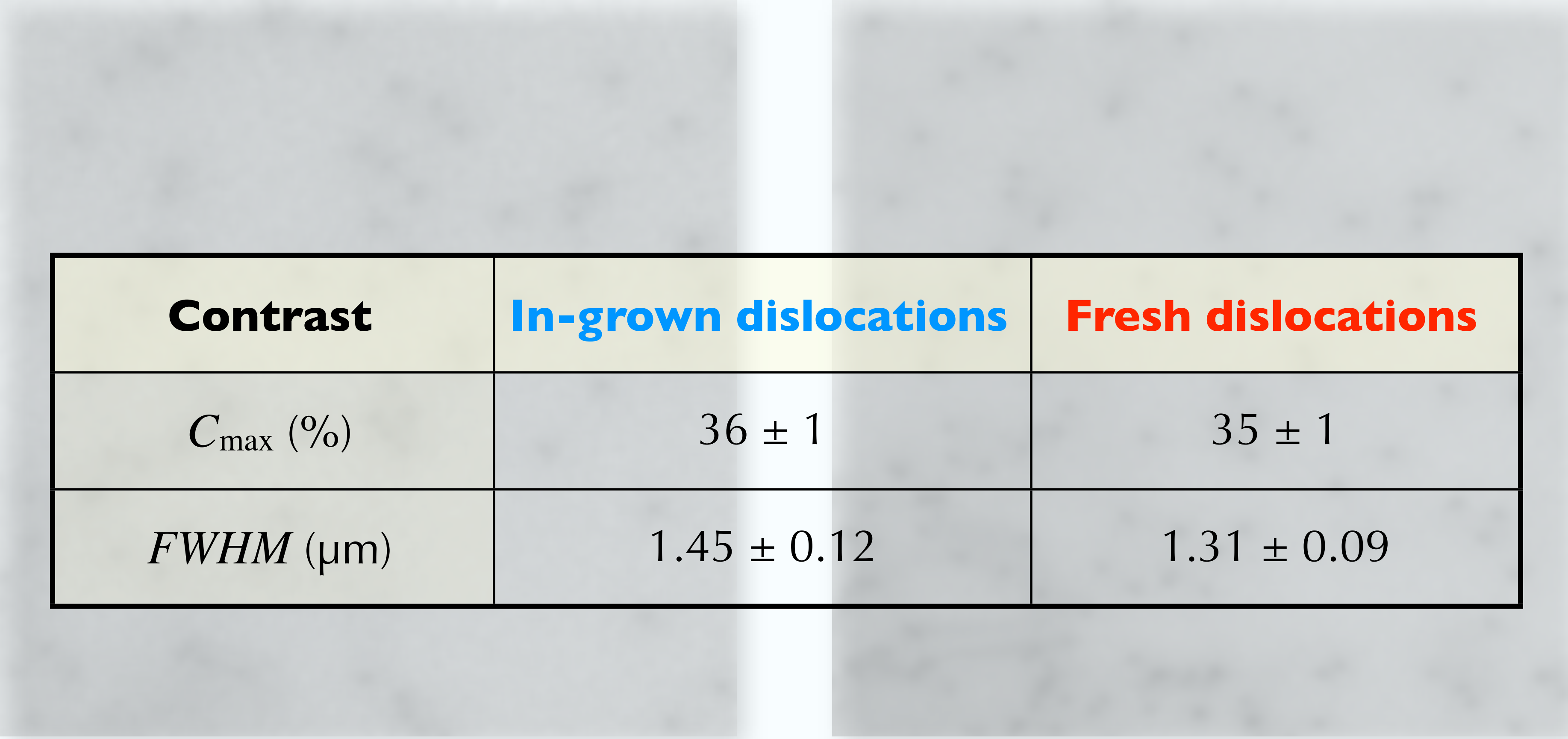
HS Leipner H Lei phys stat sol (c) **2** (2005) 1859

Cathodoluminescence of dislocations in GaN



Cathodoluminescence microscopy ($U_\mathrm{b} = 10$ kV, $I_\mathrm{b} \approx 15$ nA) of in-grown and fresh dislocations in gallium nitride single crystals grown by hydride vapor phase epitaxy

Cathodoluminescence of dislocations in GaN



Contrast	**In-grown dislocations**	**Fresh dislocations**
$C_{\max}$ (%)	36 ± 1	35 ± 1
FWHM (μm)	1.45 ± 0.12	1.31 ± 0.09

Cathodoluminescence microscopy ($U_b = 10$ kV, $I_b \approx 15$ nA) of in-grown and fresh dislocations in gallium nitride single crystals grown by hydride vapor phase epitaxy

Contrast similar but distinct differences in mobility

Conclusions

- Straight, perfect dislocation line hardly exists
- Complicated set of core defects;
  generation of intrinsic point defects
- Hardly to separate in spectroscopic measurements different types of defects in the bulk, in the strain field of the dislocation, and in the core → local analysis necessary
- An extended defect zone, characterized by the depletion or accumulation of various point defects, is formed around dislocations.
- Electrical activity of a dislocation is the superposition of core defects, segregation of impurities in the core, accumulation/ depletion of impurities in the strain field

Thanks to:
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G Leibiger, F Habel, U Gösele, M Jurisch

Deutsche Forschungsgemeinschaft
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Freiberger
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Mit uns wird Sonne Strom.

IKZ

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Interdisziplinäres Zentrum
für Materialwissenschaften

Martin-Luther-Universität Halle–Wittenberg

References

- W Shockley Phys. Rev. **91** (1953) 228.
- W T Read Phil. Mag. **45** (1954) 775.