Spezialistentreffen Versetzungsdynamik
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Experimental study of dislocation dynamics

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Alexander–Haasen model

Helmut Alexander
∗ 1928 Mannheim, † 2009 Brühl

Peter Haasen
∗ 1927 Gotha, † 1993 Göttingen

- Orowan eq. $\dot{\varepsilon} = f b \rho_{\mathrm{m}} \upsilon$

  $\upsilon = \upsilon(T, \tau, \rho_{\mathrm{m}}), \rho_{\mathrm{m}} = \mathrm{f}(T, \tau)$

- Dislocation multiplication $\mathrm{d}\rho_{\mathrm{m}} = K \tau_{\mathrm{eff}} \rho_{\mathrm{m}} \mathrm{d}x$
- Effective stress $\tau_{\mathrm{eff}} = \tau - A\sqrt{\rho_{\mathrm{m}}}$
- Dislocation velocity $\upsilon = B \tau_{\mathrm{eff}}^{m} \exp(-\frac{Q}{k_{\mathrm{B}} T})$

Determination of the dislocation density

Density of *mobile* dislocations

- System of coupled differential eqs. for the ongoing deformation in a volume element

$$\frac{\mathrm{d}\varepsilon_{\mathrm{pl}}(t)}{\mathrm{d}t} = fBb\rho(t)\exp(-\frac{Q}{k_{\mathrm{B}}T})(\sigma_{\mathrm{elast,res}} - A\sqrt{\rho})^{m}$$

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = KB\rho(t)\exp(-\frac{Q}{k_{\mathrm{B}}T})(\sigma_{\mathrm{elast,res}} - A\sqrt{\rho})^{(m+1)}$$

- Calculation for all slip systems separately
- Dislocation density by integration over the growth time
- Numeric solution

Empirical parameters

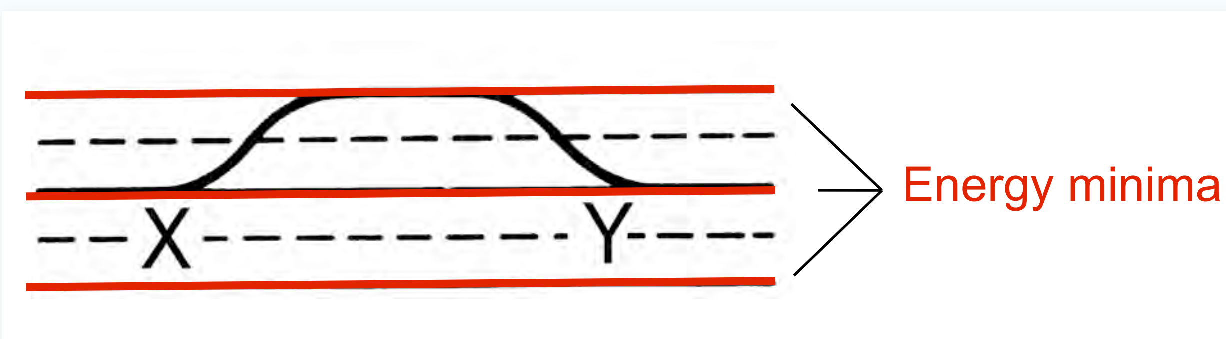
Material	Type	B (m/s MPa^{-m})	m	Q (eV)	T/T_m (K/K)
Si	60°	$1.0 \cdot 10^4$	1.0	2.20	0.52…0.63
	Screw	$3.5 \cdot 10^4$	1.0	2.35	
GaAs	α	$1.9 \cdot 10^3$	1.7	1.00	0.38…0.61
	β	$5.9 \cdot 10^1$	1.6	1.30	
	Screw	$1.2 \cdot 10^2$	1.8	1.40	
InP	α	$4.0 \cdot 10^4$	1.4	1.60	0.51…0.78
	β	$5.0 \cdot 10^5$	1.8	1.70	
	Screw	$4.0 \cdot 10^4$	1.7	1.70	

[Sumino, Yonenaga 1993; Alexander, Gottschalk 1989]

Dislocation velocity ↔ Double kinks

- Activation energy $Q = W_{\mathrm{m}} + F_{\mathrm{k}}$
- What is higher: Kink formation energy or kink migration energy?
- Silicon (90° partial dislocation):

  $W_{\mathrm{m}} = 1.2$ eV, $F_{\mathrm{k}} = U_{\mathrm{k}} - TS = 0.7$ eV



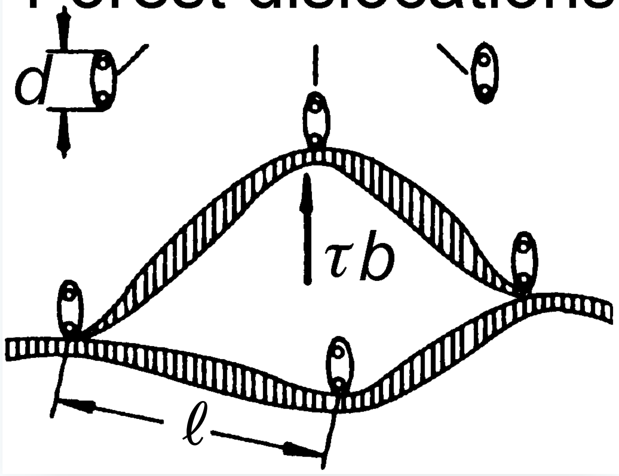
Schoeck formalism

- Plastic deformation rate as a function of the Gibbs energy to overcome a glide obstacle

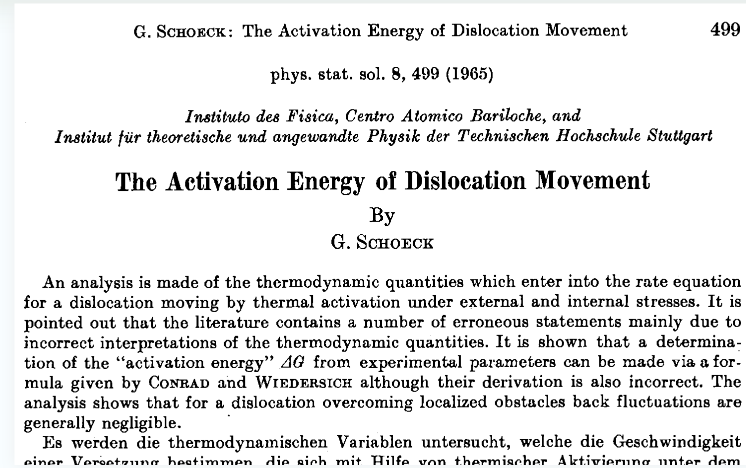
$$\dot{\varepsilon} = \dot{\varepsilon}_0 \exp\left[-\frac{\Delta G(\tau_{\text{eff}}, T)}{k_B T}\right]$$

- Activation energy depends on the shear stress, $\Delta G = \Delta G_0 - V\tau_{\text{eff}}$
- Activation volume $V = bd\,\ell$

Forest dislocations



Comparison of models


G. Schoeck: The Activation Energy of Dislocation Movement 499

phys. stat. sol. 8, 499 (1965)

Instituto des Fisica, Centro Atomico Bariloche, and
Institut für theoretische und angewandte Physik der Technischen Hochschule Stuttgart

The Activation Energy of Dislocation Movement

By

G. Schoeck

An analysis is made of the thermodynamic quantities which enter into the rate equation for a dislocation moving by thermal activation under external and internal stresses. It is pointed out that the literature contains a number of erroneous statements mainly due to incorrect interpretations of the thermodynamic quantities. It is shown that a determination of the "activation energy" ΔG from experimental parameters can be made via a formula given by Conrad and Wiedersich although their derivation is also incorrect. The analysis shows that for a dislocation overcoming localized obstacles back fluctuations are generally negligible.

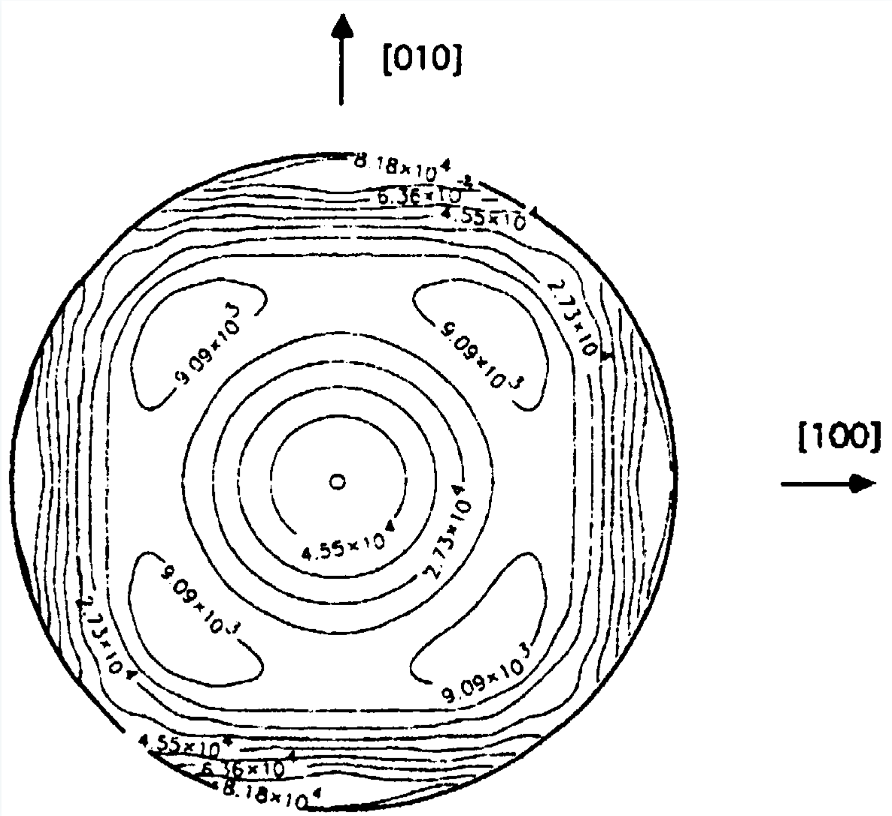
Es werden die thermodynamischen Variablen untersucht, welche die Geschwindigkeit einer Versetzung bestimmen, die sich mit Hilfe von thermischer Aktivierung unter dem

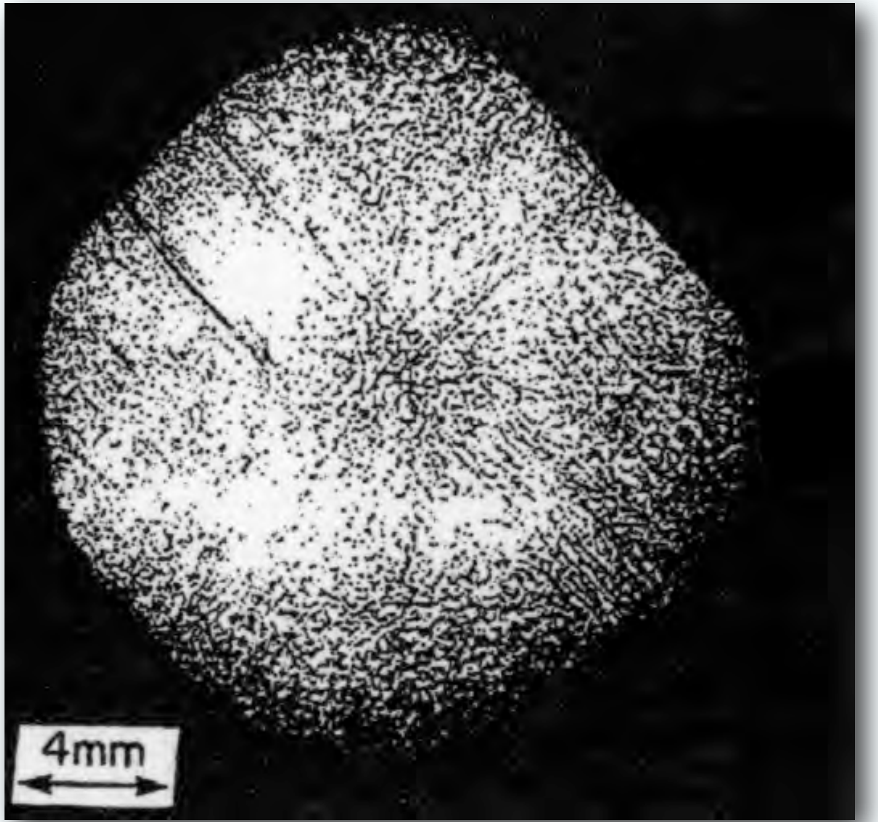
- Empirical description of A–H represents better the experimental findings in high-purity semiconductors
- Schoeck model adequate at high temperatures or for materials with a low Peierls barrier
- No physical meaning of parameters B, K, m
- Stress relaxation experiments provide

$$V = k_{\mathrm{B}} T \left(\frac{\partial \ln \dot{\varepsilon}}{\partial \tau} \right)_T \qquad 2 + m = \left(\frac{\partial \ln \dot{\varepsilon}}{\partial \ln \tau} \right)_T$$

Stress exponent m not a constant, but in relation to the multiplication mechanism of dislocations

Dislocation pattern





Total dislocation density (in cm^{-2}) in an (001) GaAs wafer summed up over all 12 slip systems. The picture shows a wafer after KOH etching.

[Tsai 1993/Jordan 1980]

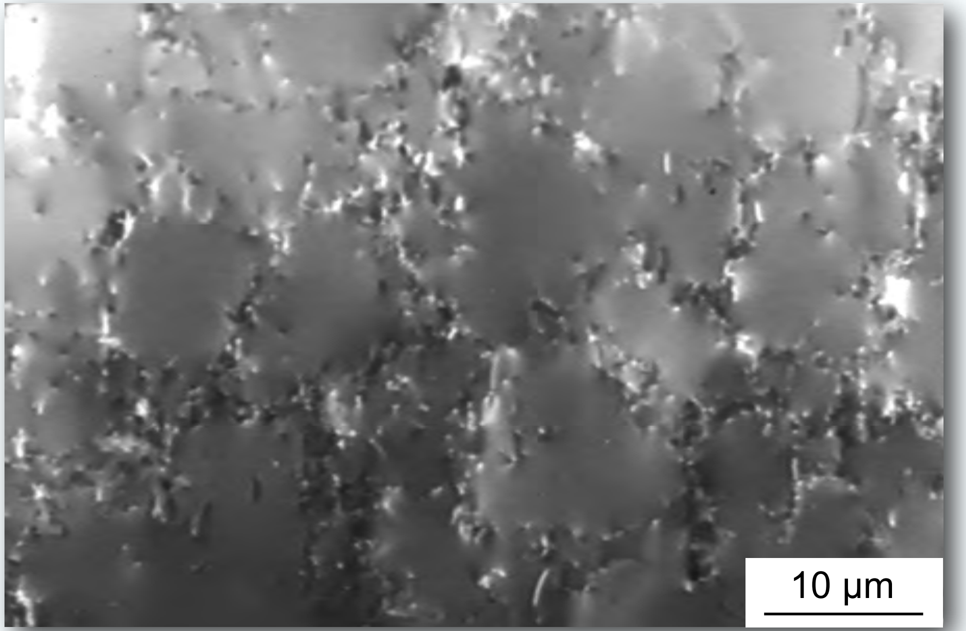
Empirical models

- Insufficient theoretical justification of empirical parameters
- Problems of thermoelastic properties at high temperatures
- Precise determination of the stress/strain in the crystal requires a 3D thermo-*plastic* model including the dynamics of growth and deformation

Plasticity as a non-equilibrium process

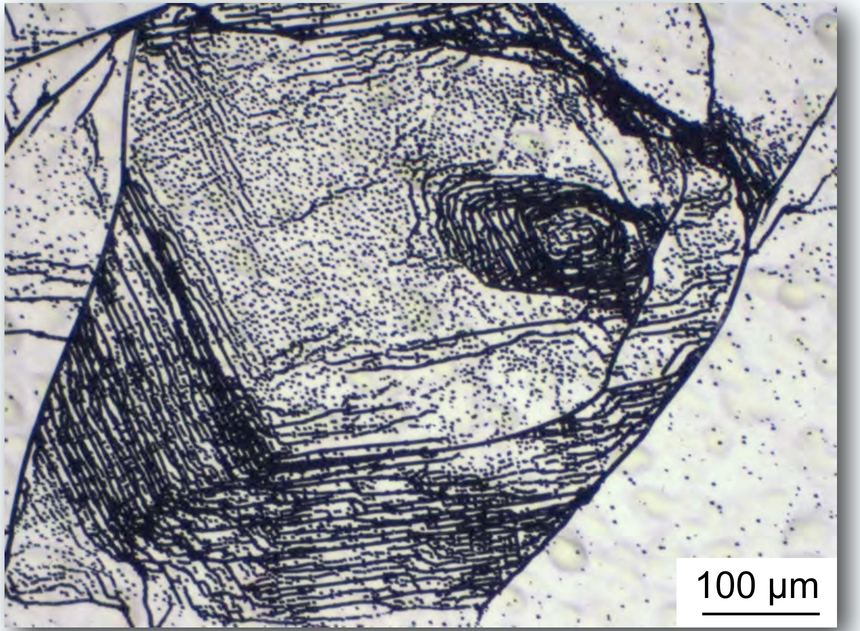
- There is no reversible, quasi-static plastic deformation.
- Dislocation dynamic unstable, dissipative, away from equilibrium
- Highly hierarchical with structure elements on different scales in time and space
- Dislocations can be influenced externally in a limited way due to microscopic instabilities (fluctuations in the friction forces, Frank–Read sources, defects in the dislocation core, grain boundaries).
- The microstructure of dislocations does not result from the minimization of a generalized potential, but from the dyn. equilibrium between reaction and transport processes.

Dislocation patterning



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

[Leitenberger]



Etch-pit pattern of the dislocation distribution in multi-crystalline silicon

[Oriwol]

Dislocation distribution ↔ Variation in electrical/optical properties

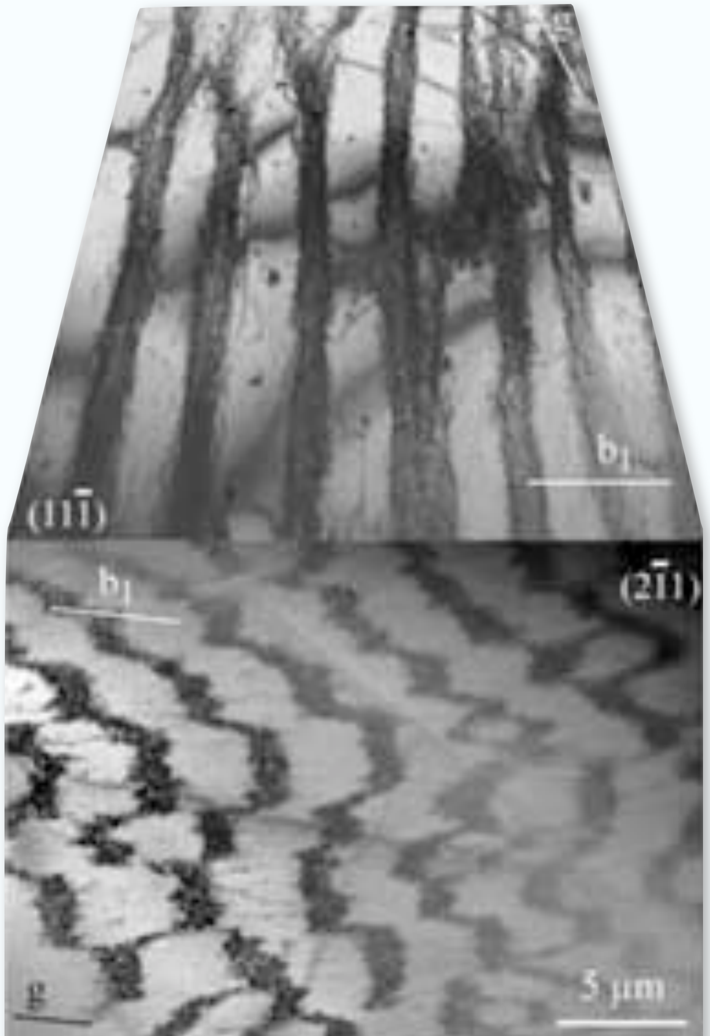
Role of intrinsic point defects and impurities

Dislocation cells

TEM of the dislocation structure in plastically deformed molybdenum, $\varepsilon = 12$ %.

[Luft 1970]

Fatigue investigations of silicon



Dislocation structures in silicon after fatigue at high temperatures

[Legros 2002]

Collective behavior of dislocation evolution

Ghoniem *et al.*, Walgraef *et al.*, Kratochvil *et al.*:

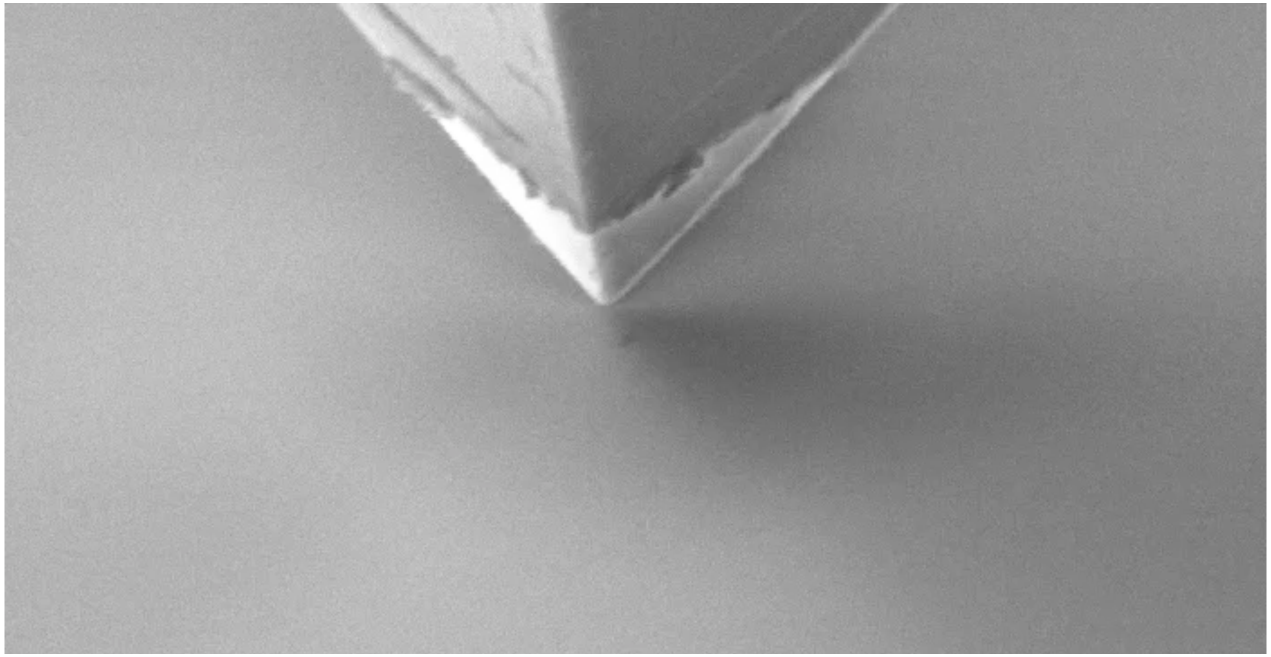
- Dislocation population divided in static and mobile dislocations
- Coupled rate equations for densities ρ_s and ρ_m
- Densities from Orowan relation $\dot{\varepsilon} = f b \rho_m \upsilon$
  and internal stress $\sigma_i = \dfrac{Gb}{2\pi d} + \alpha G b \sqrt{\rho_s}$
- Characteristic quantities of the models: dislocation mobility (thermal diffusion or climb), interaction between dislocations (multiplication, annihilation, immobilization)

$$\partial_t \rho_{s,m} = f(\Delta_{\mathbf{r}} \rho_{s,m})$$

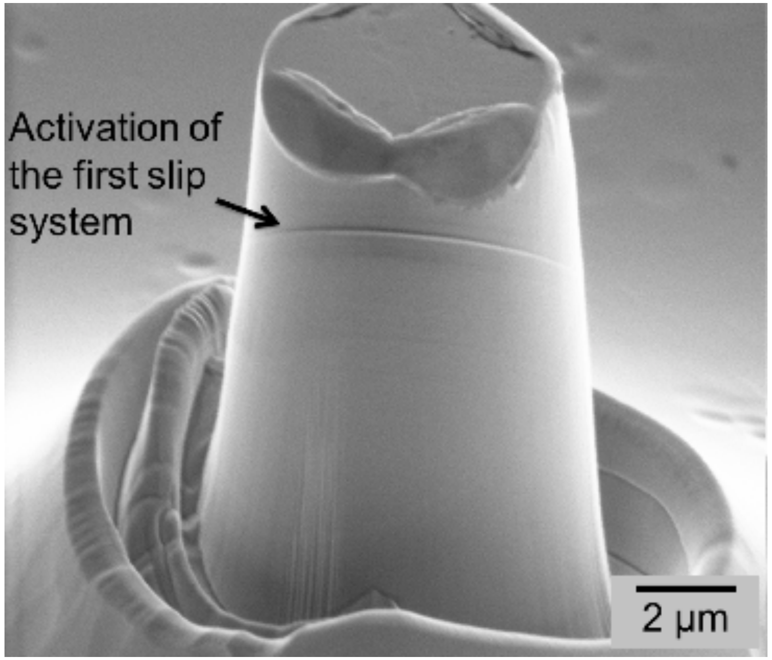
[*cf.* Walgraef 2003]

Local mechanical testing experiments

- Local probes of the dynamics of dislocations in the interaction with glide obstacles
- Deformation under constrained conditions: indentation tests, *in-situ* experiments with nanopillars
- Onset of dislocation motion (nanoindentation pop-in)



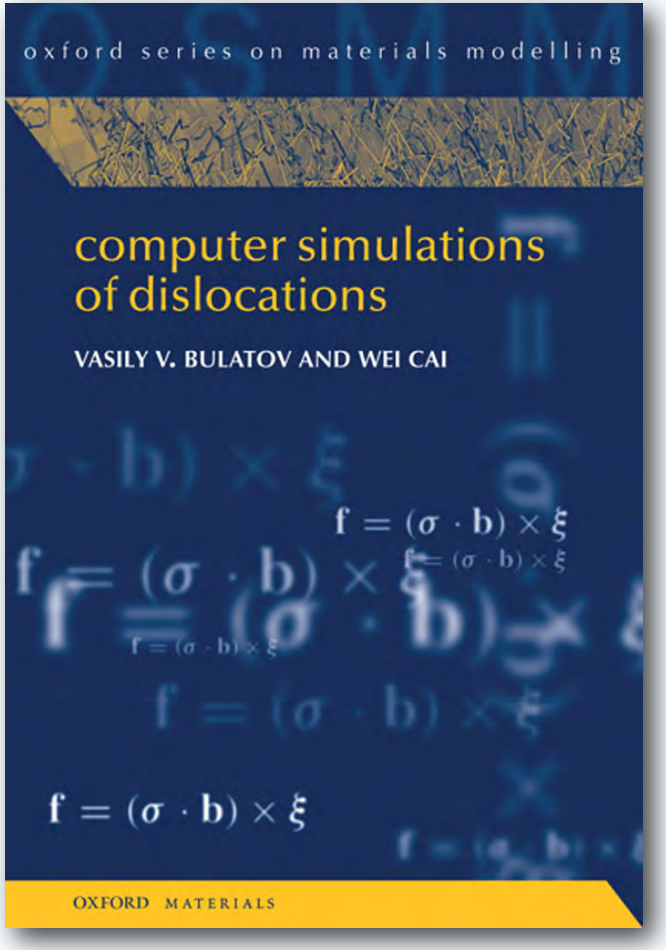
[Ratschinski 2011]



[Kheradmand 2012]

Kink dynamics

- Structure and dynamics of kinks crucial for the velocity of dislocation glide
- Multitude of possible kink structures with/without dangling bonds
- Reaction with reconstruction defects, *e. g.* LK + RD $\rightleftarrows$ LC, RK + RD $\rightleftarrows$ RC
- *Ab initio* calculations provide different formation and migration energies of the different configurations.
- Further complications: Interaction with incorporated vacancies, impurities, charge effects



Conclusions

- Quantitative description of plastic deformation requires a precise knowledge about the behavior of the ensemble of mobile and static dislocations (not characterized by a single density no.) under stress (explore!).
- Different scales of the description (space/time) must be applied in a coordinated way.
- Highest expectations/biggest problems: connection of atomistic and mesoscopic models

Thanks to:

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