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Title: INCORPORATION OF DISLOCATION CLIMB IN CRYSTAL PLASTICITY MODELS

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Incorporation of dislocation climb in crystal plasticity models

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This work presents an improved plasticity model for single crystals deforming by a combination of dislocation glide and climb. A constitutive framework based on dislocation densities has been implemented in a viscoplastic self-consistent (VPSC) formulation. Accounting for the explicit evolution of edge and screw dislocations densities enables the instantaneous determination of the climb tensor, which depends on the average character of the mobile dislocations. Mobilities of dislocations accommodating deformation by climb and glide, which depend on their interaction with point defects, are determined using kinetic Monte Carlo simulations.

Incorporation of Dislocation Climb in Crystal Plasticity Models

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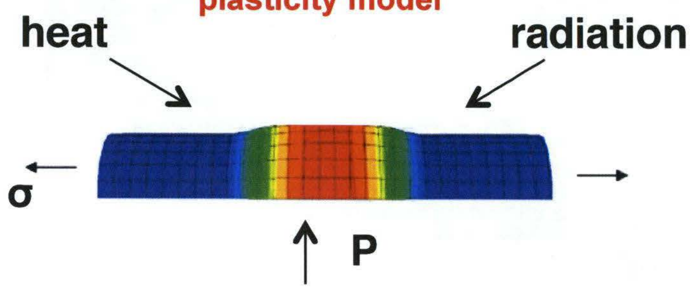
Overview

1. **Thermal creep – incorporation of dislocation climb in polycrystal crystal plasticity code VPSC**
2. **Material parameters based on atomistic simulations and kinetic Monte Carlo simulations**

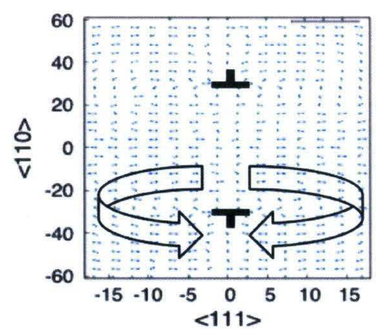
Continuum model connects with atomistics

clad mechanical behavior - crystal plasticity model

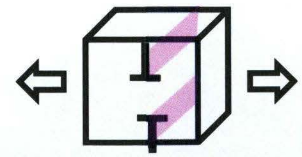


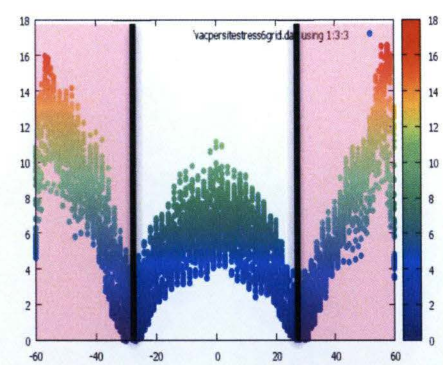
$$\dot{\varepsilon} = \rho_d b v_c \Leftrightarrow \dot{\varepsilon} = A\sigma^n \exp\left(-Q/k_B T\right)$$

The presence of the strain field of an edge dislocation affects vacancy diffusion. Off lattice kMC takes this effect into account.



Stress applied normal to this plane changes the vacancy profile concentration, affecting the flux to dislocations and therefore the climb rate





Motivation

Schmid tensor

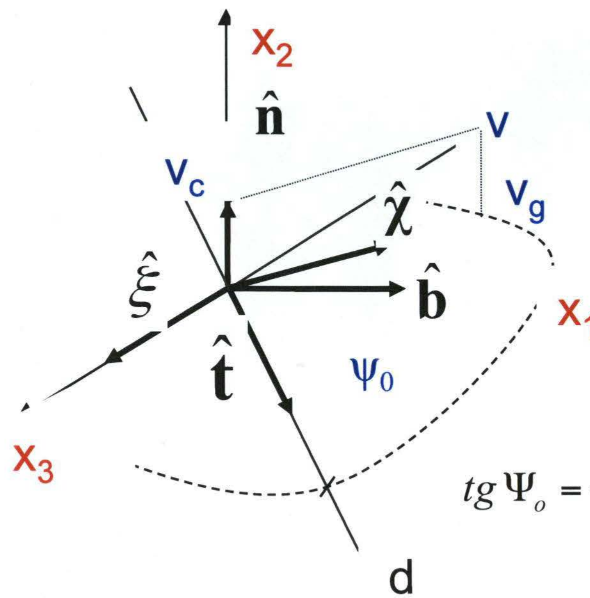
$$\dot{\varepsilon} = \dot{\gamma}_o \sum_s m^s \left(\frac{|m^s : \sigma'|}{\tau^s} \right)^n \mathrm{sgn}\left(m^s : \sigma'\right) \quad \mathbf{+}$$

CRSS

Point defect generation, interaction with dislocations, grain boundaries

$$\tau^s = \mu b \sqrt{\rho} \quad ; \quad \dot{\rho} = \alpha\sqrt{\rho} - k\rho$$

dislocation density ; **dislocation density evolution (production, interaction, annihilation)**



$$tg\,\Psi_o = \frac{\rho_{edge}}{\rho_{screw}}$$

Strain-rate as a function of stress:

$$\dot{\varepsilon}_{ij} = \dot{\gamma}_o \sum_s k_{ij}^{d,s} \left(\frac{\left| k^{d,s} : \sigma' + \sigma_{ch} \right|}{\sigma_{o,c}^s} \right)^{n_c} \times \mathrm{sgn}(\bullet)$$

"Climb" P-K force**:

$$f_c = -|\mathbf{b}|\,\sigma' : \left(\hat{\mathbf{b}} \otimes \hat{\chi}\right) - |\mathbf{b}| \left[-\frac{k_B T}{\alpha |\mathbf{b}|^3} \log\left(x_v / x_v^{o,PT}\right) \right] \left(\hat{\mathbf{b}} \otimes \hat{\chi}\right)$$

If the local concentration of vacancies is instantaneously restored into the equilibrium concentration:

$$x_v = x_v^{o,PT}, \quad |\mathbf{b}| \left[-\frac{k_B T}{\alpha |\mathbf{b}|^3} \log\left(x_v / x_v^{o,PT}\right) \right] \left(\hat{\mathbf{b}} \otimes \hat{\chi}\right) = 0$$

(*) Lebensohn et al. , Phil. Mag. 2010

(**) J. Weertman: "The Peach-Koehler Equation for the Force on a Dislocation, Modified for Hydrostatic Pressure". Phil Mag. 114, 1217 (1964).

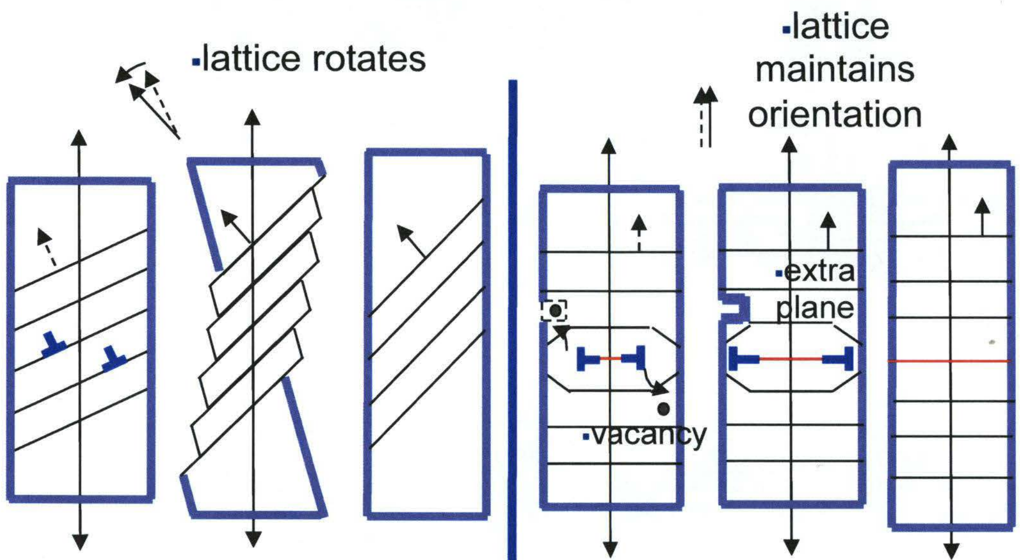
Climb and glide

$$\dot{\varepsilon} = \dot{\gamma}_o \sum_s \left(\frac{\left| m^s : \sigma' \right|}{\tau^s_{o,g}} \right)^{n_g} \times \mathrm{sgn}(\ ) + \left(\frac{\left| k^{d,s} : \sigma' + \sigma_{ch} \right|}{\tau^s_{o,c}} \right)^{n_c} \times \mathrm{sgn}(\ )$$

Glide **Climb**

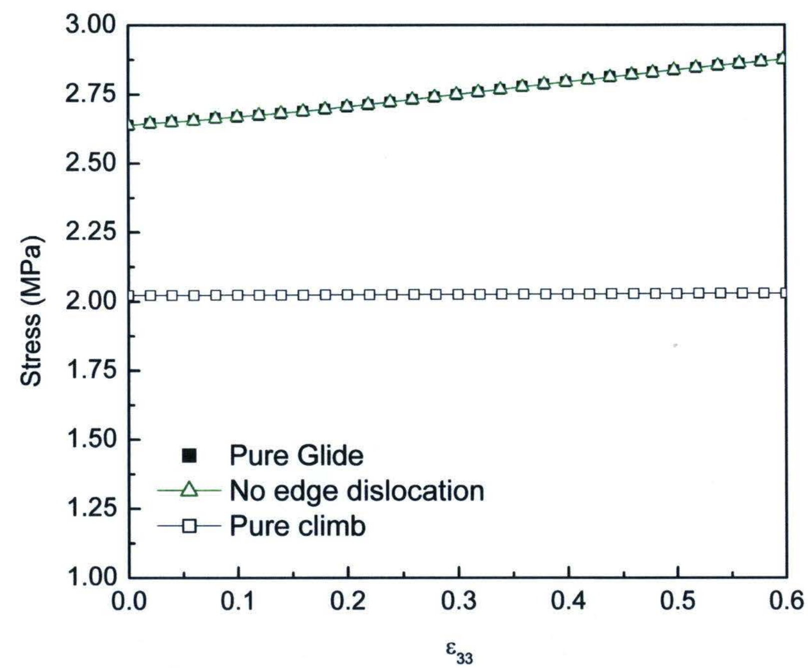
* Lebensohn et al, Phil Mag (2010)

Glide vs. climb in terms of stress-strain response

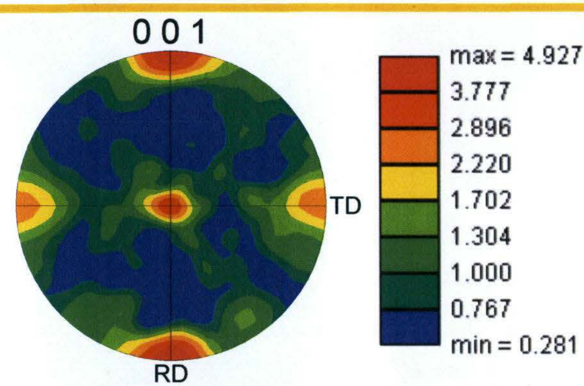


single crystal extension accommodated by glide: involves lattice reorientation

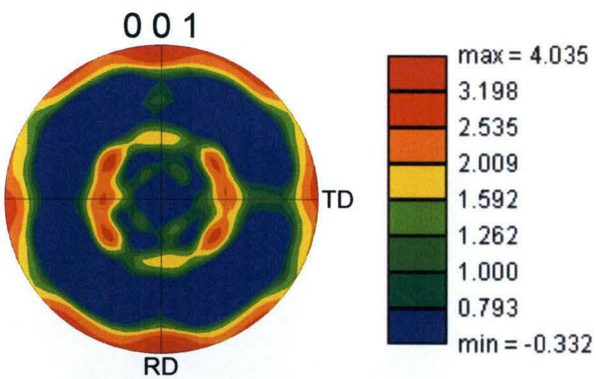
single crystal extension accommodated by climb of edge dislocations: no lattice reorientation



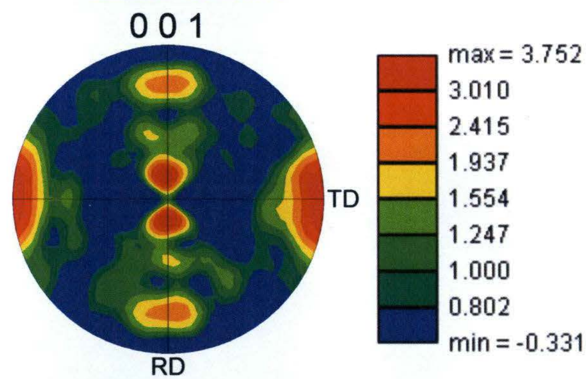
Simulations of uniaxial compression – glide vs. glide + climb



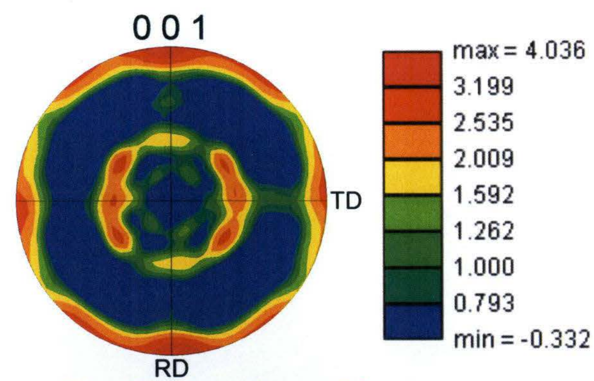
Initial texture



Uniaxial compression of fcc polycrystal, pure glide, 948 crystallites, 90 % reduction

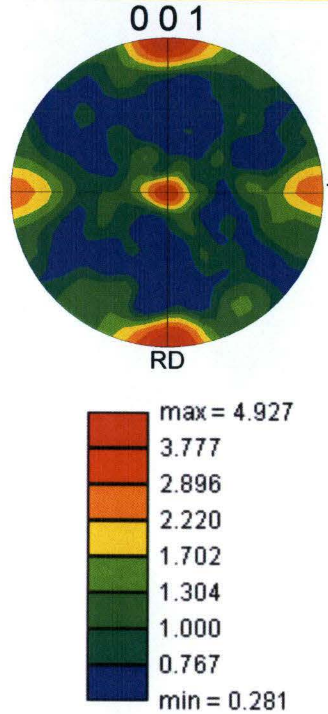


Glide + climb

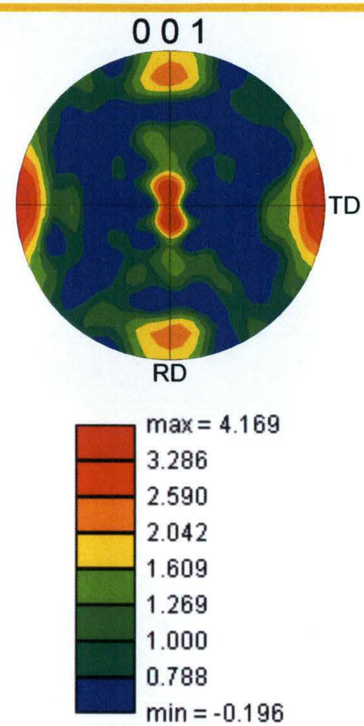


No climb activated by means of having no edge dislocations

Simulations of uniaxial compression – effect of edge dislocation content on equilibrium concentration of vacancies

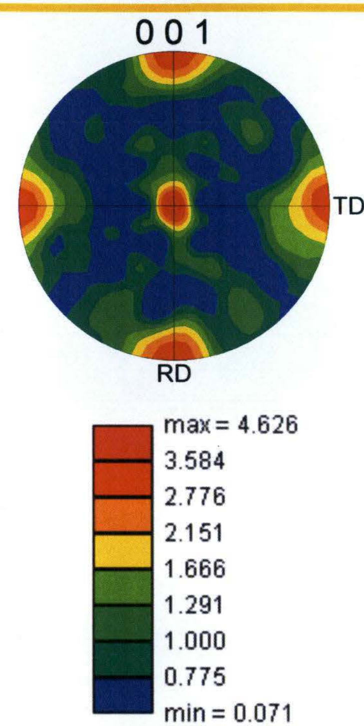


Initial texture



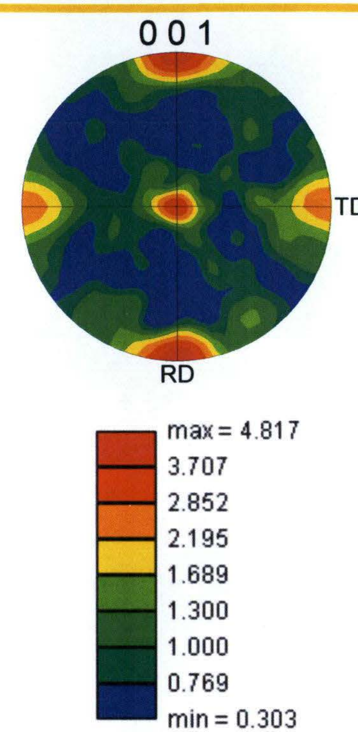
$$\Psi_o = tg^{-1}\left(\frac{\rho_{edge}}{\rho_{screw}}\right) = 0.7853$$

ρ_{edge} = 50 %, 90 % thickness reduction, $\langle\sigma_{ch}\rangle$=0.12 $\sigma_{0,c}$



$$\Psi_o = tg^{-1}\left(\frac{\rho_{edge}}{\rho_{screw}}\right) = 0.8500$$

ρ_{edge} = 53 %, 90 % thickness reduction, $\langle\sigma_{ch}\rangle$=0.41 $\sigma_{0,c}$

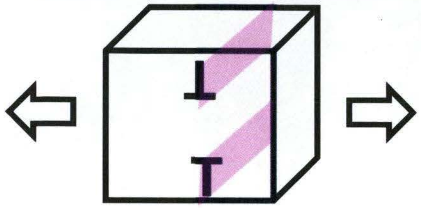


$$\Psi_o = tg^{-1}\left(\frac{\rho_{edge}}{\rho_{screw}}\right) = 0.9500$$

ρ_{edge} = 58 %, 90 % thickness reduction, $\langle\sigma_{ch}\rangle$=0.53 $\sigma_{0,c}$

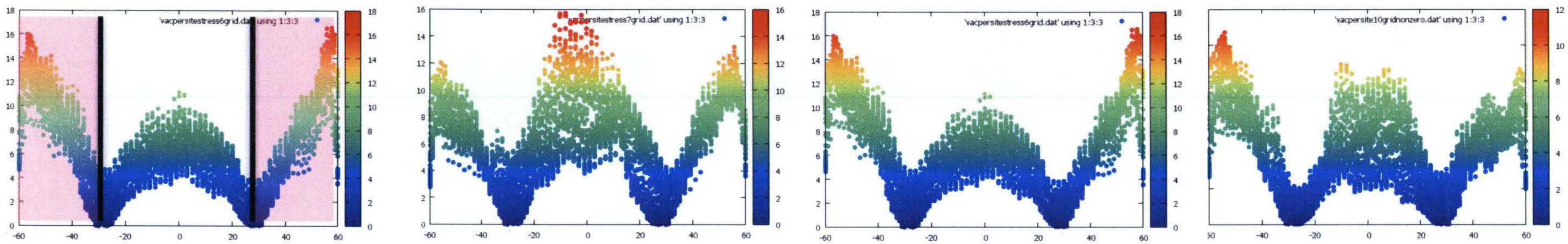
Simulations for creep rate and stress exponent

The simulations show vacancy profile around dislocations core as a function of applied stress. The number in the legend are representatives of number density of vacancies.



Temperature = 500 K

$$v_c = kh/N_y \qquad \dot{\varepsilon} = \rho_d b v_c \Leftrightarrow \dot{\varepsilon} = A\sigma^n \exp(-Q/k_B T)$$

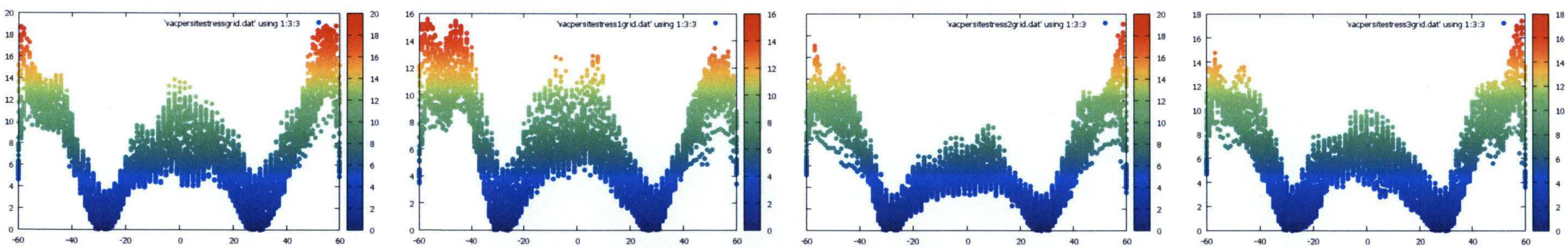


Stress is applied normal to this plane

-2 GPa

-1 GPa

0 GPa



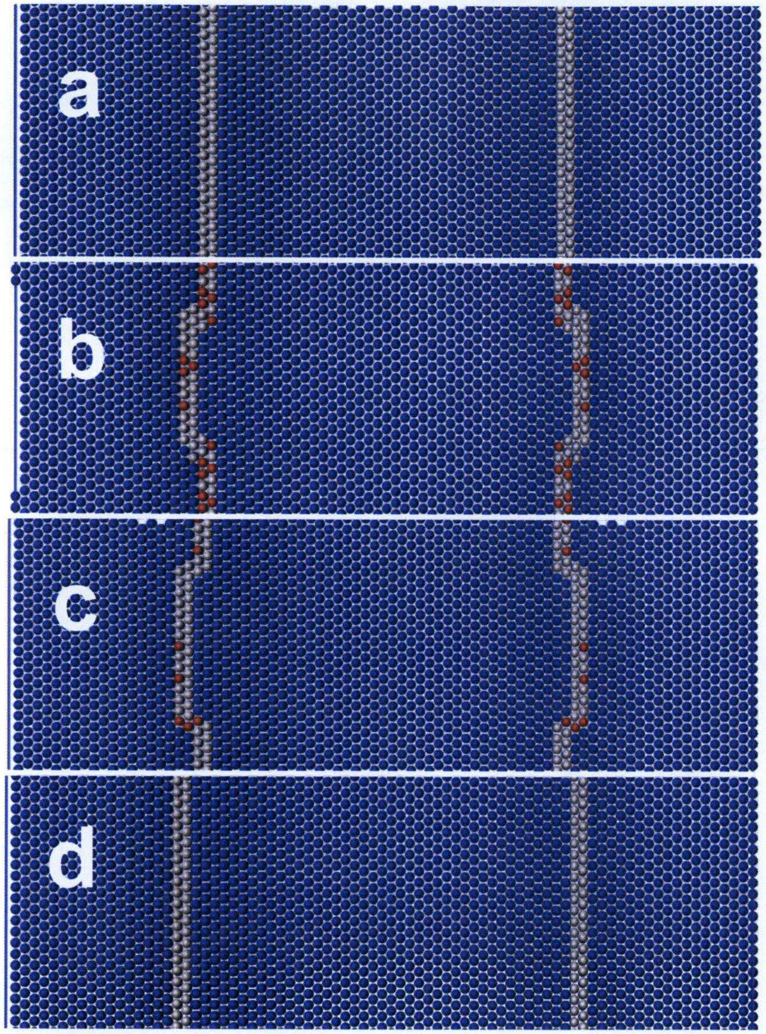
1 GPa

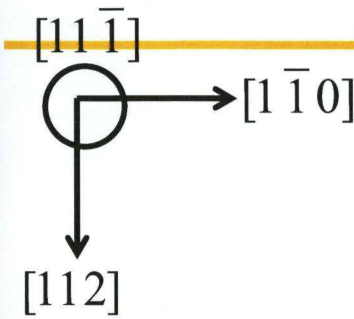
2 GPa

3 GPa

4 GPa

The atomic scale - Essence of dislocation climb



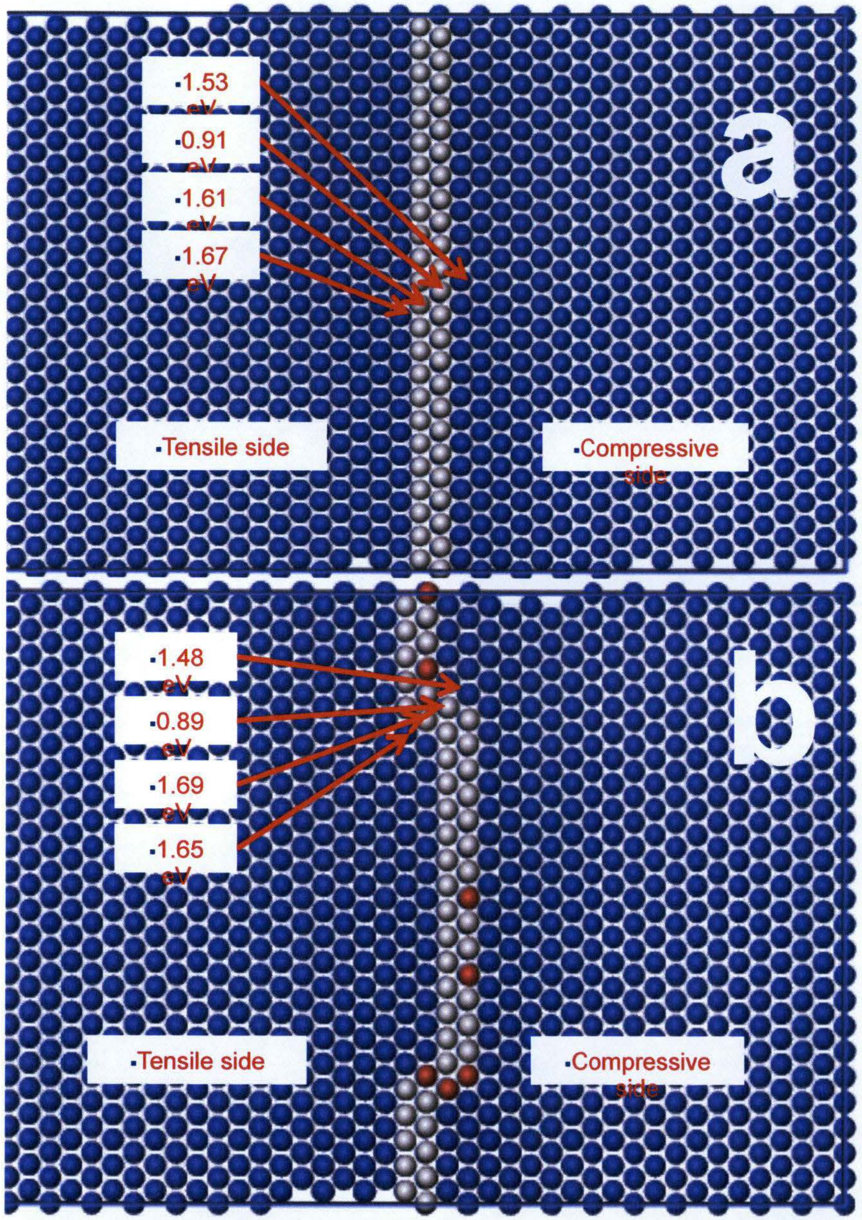


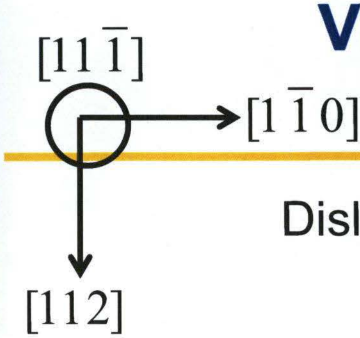
- By absorption/emission of interstitials/ vacancies, dislocations nucleate jogs, propagate them, and do climb
- a- an edge dislocation dipole in Fe; climb direction is (1-10) along x-axis, Burger vector direction is (111) is perpendicular to the figure.
- b- addition of vacancies to the dislocation cores creates a jog pair
- c- additional vacancies move the jog pair increasing the length of the climbed portion of the dislocation
- d- with a sufficient number of vacancies, the dislocation climbes a full step along (1-10)

$$\dot{\varepsilon}_{gc} = \sum_{\alpha=1}^{N} \dot{\varepsilon}^{\alpha} = \sum_{\alpha=1}^{N} \dot{\varepsilon}^{\alpha}_{rs} = \sum_{\alpha=1}^{N} \alpha^{\alpha} b^{\alpha}_{r} b^{\alpha}_{s}$$

“Anisotropy” of climb

Case	% ΔL_x	% ΔL_y	% ΔL_z	ΔV_x $(\mathring{A}^3)$	ΔV_y $(\mathring{A}^3)$	ΔV_z $(\mathring{A}^3)$
Jog created on dislocation	-0.014770	0.00177	0.00594	-579.10	6.94	23.30
Jog moved along a dislocation	-0.043330	0.004294	-0.001719	-169.70	16.82	-6.73
Dislocation climbs	-0.032090	0.007721	0.007823	-1258.00	30.28	30.68
Vacancy far away between dislocation dipoles	0.000216	-0.000334	-0.000255	0.85	-1.31	-1.00
Vacancy in bulk	-0.003590	-0.003590	-0.003590	-0.84	-0.84	-0.84





Vacancy energetics

Dislocations are natural traps for point defects

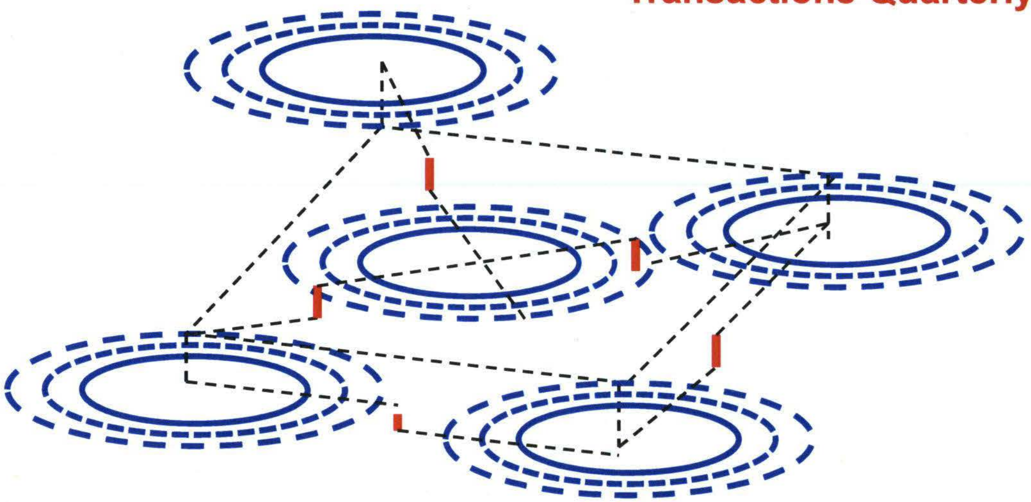
(a) along a segment of a straight dislocation, vacancy formation energies clearly show the preferential tendency to sit at the core on the compressive side

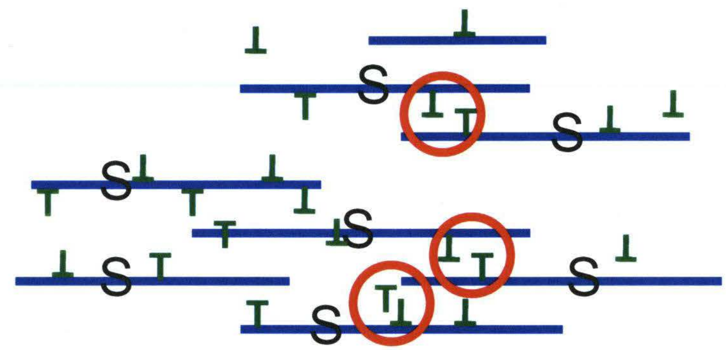
(b) in the presence of a jog, trapping energies are even lower

Glide accounts for total strain and climb accounts for creep rate

In creep, both glide and climb of dislocations take place.

"almost all of the creep strain is produced by glide motion of dislocations". J. Weertman, ASM Transactions Quarterly, 61(1968), p. 681





$$\dot{\varepsilon}_{ij}^{c} = \sum_{s=1}^{N_s} k_{ij}^{s}\,\rho^{s}\,b\,v^{s} = \sum_{s=1}^{N_s} k_{ij}^{s}\,\rho^{s}\,b\left[\mu^{c}\left(k^{s}:\sigma^{*}b\right)\right] = \sum_{s=1}^{N_s} k_{ij}^{s}\,\rho^{s}\,b^{2}\,\mu^{c}\,k^{s}:\sigma^{*}$$

Plastic strain rate due to climb

climb mobility (per unit length)

climb force (per unit length)

Summary

- Phenomenological model of climb and glide
- Dependence of crystallographic orientation on the chemical stress
- Molecular dynamics simulations for understanding "unit process" of climb – movement of jogs along dislocation line
- Implementation into a kinetic Monte Carlo setup

Thank you for your kind attention !