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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

Alankar Alankar, Alfredo Caro and Ricardo Lebensohn

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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.

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Jan. 03, 2012

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San Juan, PR,

Motivation

- **Standard crystal plasticity models do not account explicitly for the mechanisms involved in metal deformation in elevated temperatures e.g. phenomena of creep**
- **In general, these phenomena are modeled via phenomenological description and the models thus developed are not well informed by intrinsic microstructure evolution e.g. dislocation climb**
- **At high temperatures, the mechanical response of a metal is governed by coupled microstructure activities e.g. creep is accounted by coupled glide and climb of dislocations**

▪Single crystal plastic deformation geometry (glide only)

Schmid tensor

$$\dot{\varepsilon} = \dot{\gamma}_0 \sum_s m^s \left(\frac{\left| m^s : \sigma' \right|}{\tau^s} \right)^n \operatorname{sgn}\left(m^s : \sigma' \right)$$

CRSS

\+

Continuum (physically-based) hardening theory

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

dislocation density

dislocation density evolution (production, interaction, annihilation)

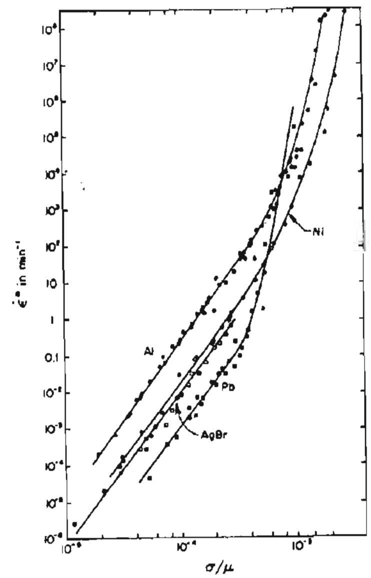
\+

Point defect generation, interaction with dislocations, grain boundaries

Different constitutive formulations for creep rate and their limitations

When the grain size is fairly large, pure metals stressed in the stress range $10^{-5}\,\mu$ to $10^{-3}\,\mu$ follow the Power law creep as shown below. n = 3 – 6. *A* is temperature dependent. The equation gives a good fit as shown in the picture . This model assumes that climb occurs to circumvent the obstacles e.g. immobile dislocations in pure metals. Bailey 1930, Norton 1929

$$\dot{\varepsilon} = A\sigma^n$$



At higher stress levels than $10^{-3}\,\mu$ the power law does not predict the creep rates correctly. The experimental observations show a steeper trend. μ is the shear modulus

A is resolved into a constant and temperature dependent part. *Q* is the activation energy for steady state creep and is almost equal to that of self diffusion. (Dorn 1954). This equation also assumes generation of immobile dislocations.

$$\dot{\varepsilon} = A\sigma^n \exp(-Q/kT)$$

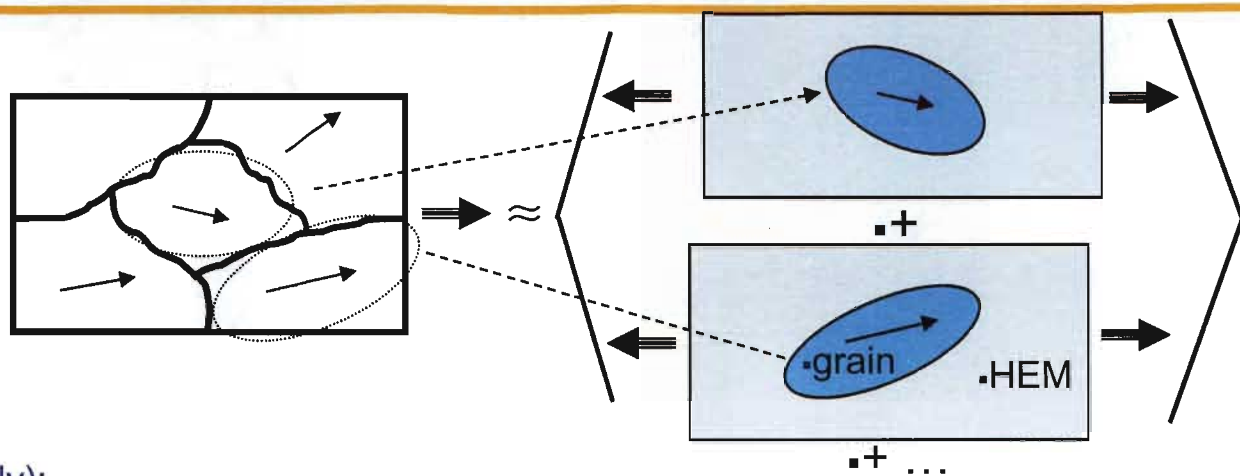
Weertman, 1955

$$\dot{\varepsilon} = A(\sigma^n/kT)\exp(-Q/kT)$$

If the production is immobile dislocations is not considered, Weertman 1957. This is proposed for high stresses.

$$\dot{\varepsilon} = A\sigma^n \sinh(B\sigma^{n'}/kT)\exp(-Q/kT)*$$

Self consistent formulation for viscoplastic deformation of polycrystals via glide + climb*



VPSC (glide only):

Grain (r): $\dot{\varepsilon} = \dot{\gamma}_0 \sum_s m^s \left(\frac{|m^s : \sigma'|}{\tau_0^s} \right)^n \times \mathrm{sgn}(\ ) \Rightarrow \dot{\varepsilon} \cong M^r : \sigma' + \dot{\varepsilon}^{or}$ HEM: $\dot{E} = M : \Sigma' + \dot{E}^0$

linearization

VPSC (climb and glide):

Grain (r):

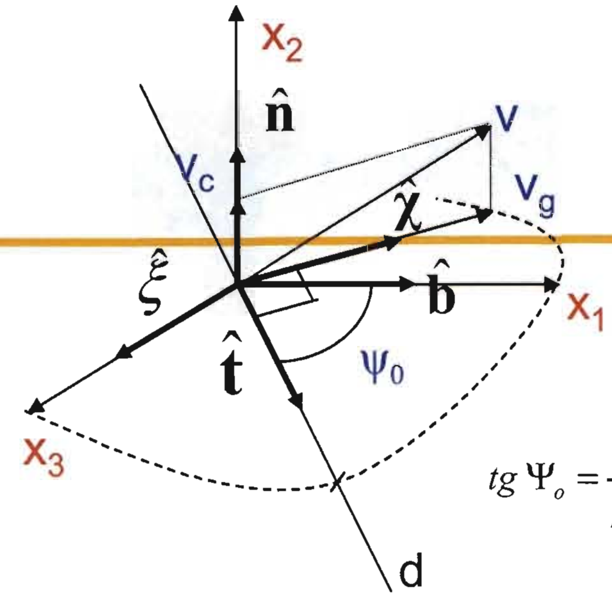
$$\dot{\varepsilon} = \dot{\gamma}_o \sum_s \left(\frac{|m^s : \sigma'|}{\tau_{o,g}^s} \right)^{n_g} \times \mathrm{sgn}(\ ) + \left(\frac{|k^{d,s} : \sigma'|}{\tau_{o,c}^s} \right)^{n_c} \times \mathrm{sgn}(\ ) \Rightarrow \dot{\varepsilon} \cong M^r : \sigma' + \dot{\varepsilon}^{or}$$

linearization

HEM: $\dot{E} = M : \Sigma' + \dot{E}^0$

* Lebensohn et al, Phil Mag (2010)

Peach-Koehler (P-K) force



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

$$\mathbf{f} = (\sigma \cdot \mathbf{b}) \times \hat{\mathbf{t}}$$

"Glide" and "climb" components of the P-K force:

$$f_g = \left[(\sigma \cdot \mathbf{b}) \times \hat{\mathbf{t}}\right] \cdot \hat{\chi} = (\sigma \cdot \mathbf{b}) \cdot \left(\hat{\mathbf{t}} \times \hat{\chi}\right) = |\mathbf{b}|\, \sigma : \left(\hat{\mathbf{b}} \otimes \hat{\mathbf{n}}\right) = |\mathbf{b}|\, \sigma' : \left(\hat{\mathbf{b}} \otimes \hat{\mathbf{n}}\right)$$

$$f_c = \left[(\sigma \cdot \mathbf{b}) \times \hat{\mathbf{t}}\right] \cdot \hat{\mathbf{n}} = (\sigma \cdot \mathbf{b}) \cdot \left(\hat{\mathbf{t}} \times \hat{\mathbf{n}}\right) = -|\mathbf{b}|\, \sigma : \left(\hat{\mathbf{b}} \otimes \hat{\chi}\right)$$

Weertman's modified expression for the P-K force (*)

$$\mathbf{f} = (\sigma' \cdot \mathbf{b}) \times \hat{\mathbf{t}} + \left[-\frac{k_B T}{\alpha |\mathbf{b}|^3} \log\left(x_v / x_v^{o,PT}\right) \right] \mathbf{b} \times \hat{\mathbf{t}}$$

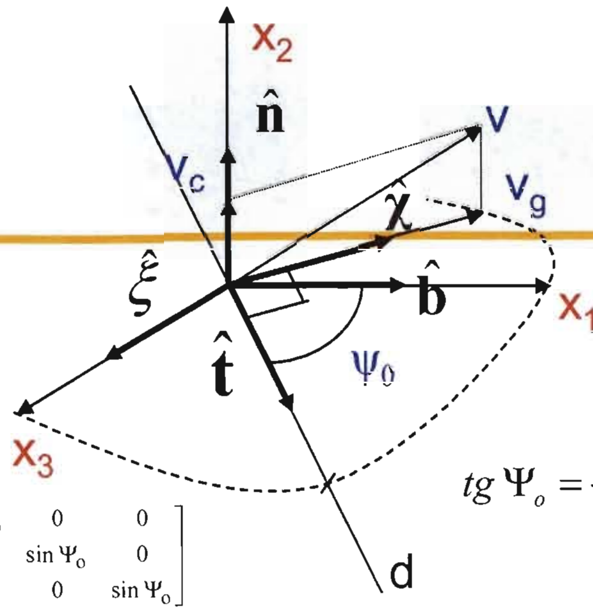
"Glide" and "climb" components of Weertman- modified P-K force

$$f_g = |\mathbf{b}|\, \sigma' : \left(\hat{\mathbf{b}} \otimes \hat{\mathbf{n}}\right)$$

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

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

Geometry of climb



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

Climb tensor (*): $C^s_{ij} = \chi^s_i \, b^s_j$ In general $\chi \perp b \Rightarrow C^s_{kk} \neq 0$

Decomposition (*): $C^s_{ij} = k^{d,s}_{ij} + k^{h,s}_{ij} + \kappa^s_{ij}$ (dev + hyd + antisym)

In 'dislocation' coordinates (*): $k^{d,s}_{ij} = \frac{1}{6}\begin{bmatrix} 4\sin\Psi_o & 0 & 0 \\ 0 & -2\sin\Psi_o & 0 \\ 0 & 0 & -2\sin\Psi_o \end{bmatrix}$ $\kappa^s = \frac{1}{2}\begin{bmatrix} 0 & 0 & \cos\Psi_o \\ 0 & 0 & 0 \\ -\cos\Psi_o & 0 & 0 \end{bmatrix}$ $k^{h,s}_{ij} = \frac{1}{3}\begin{bmatrix} \sin\Psi_o & 0 & 0 \\ 0 & \sin\Psi_o & 0 \\ 0 & 0 & \sin\Psi_o \end{bmatrix}$

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

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

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

Plastic spin associated with climb:

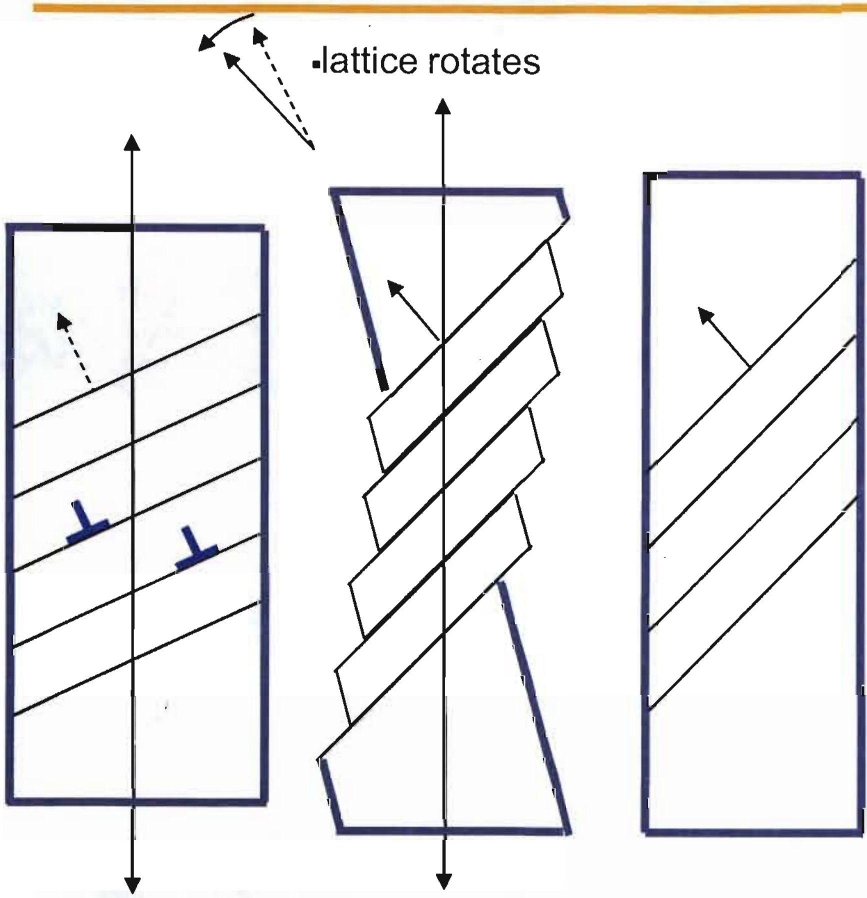
$$\dot{\omega}^p_{ij} = \dot{\gamma}_o \sum_s \kappa^s_{ij}\,\dot{\beta}^s$$

$$\rightarrow edge\ dislocations: \ \kappa^s_{ij} = 0 \Rightarrow \dot{\omega}^p_{ij} = 0\,!$$

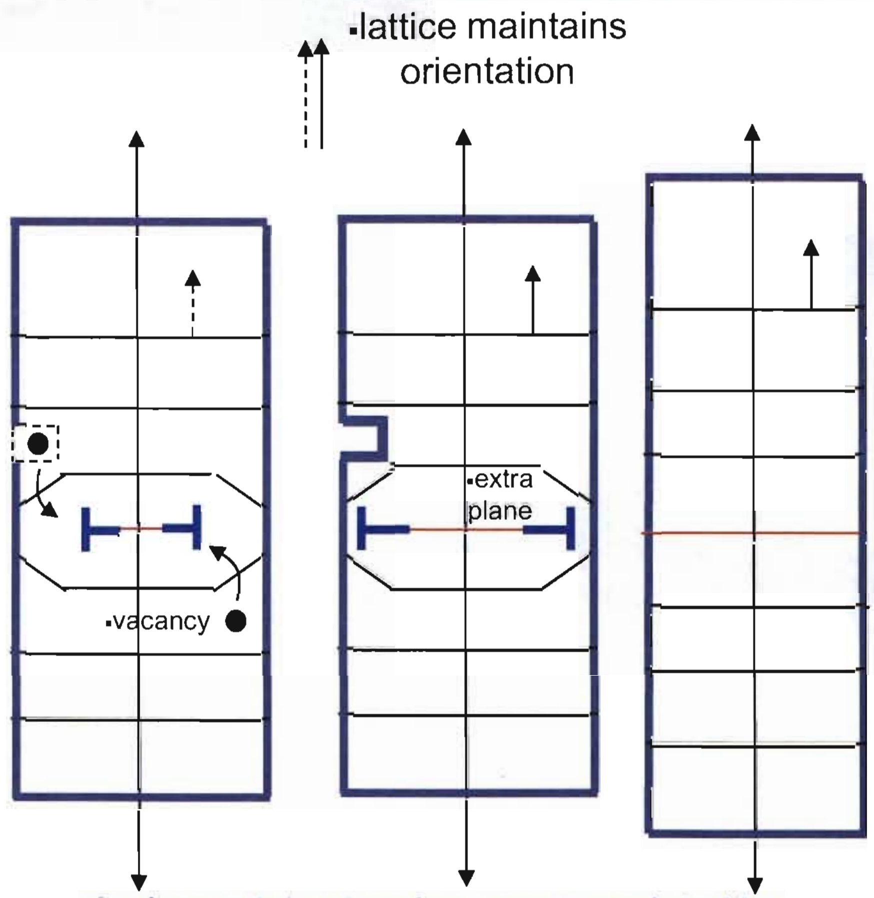
Strain-rate (climb-rate): $\dot{\varepsilon}_{ij} = k^{d,s}_{ij}\,\dot{\beta}^s$ Strain-rate: $$\dot{\beta}^s = \dot{\gamma}_o \left(\frac{\left|k^{d,s} : \sigma'\right|}{\sigma^s_{o,c}}\right)^{n_c} \times \mathrm{sgn}\left(k^{d,s} : \sigma'\right)$$

Single crystal's strain-rate as a function of stress: $$\dot{\varepsilon}_{ij} = \dot{\gamma}_o \sum_s k^{d,s}_{ij} \left(\frac{k^{d,s} : \sigma'}{\sigma^s_{o,c}}\right)^{n_c} \times \mathrm{sgn}\left(k^{d,s} : \sigma'\right)$$

Glide vs. climb in terms of crystal reorientation

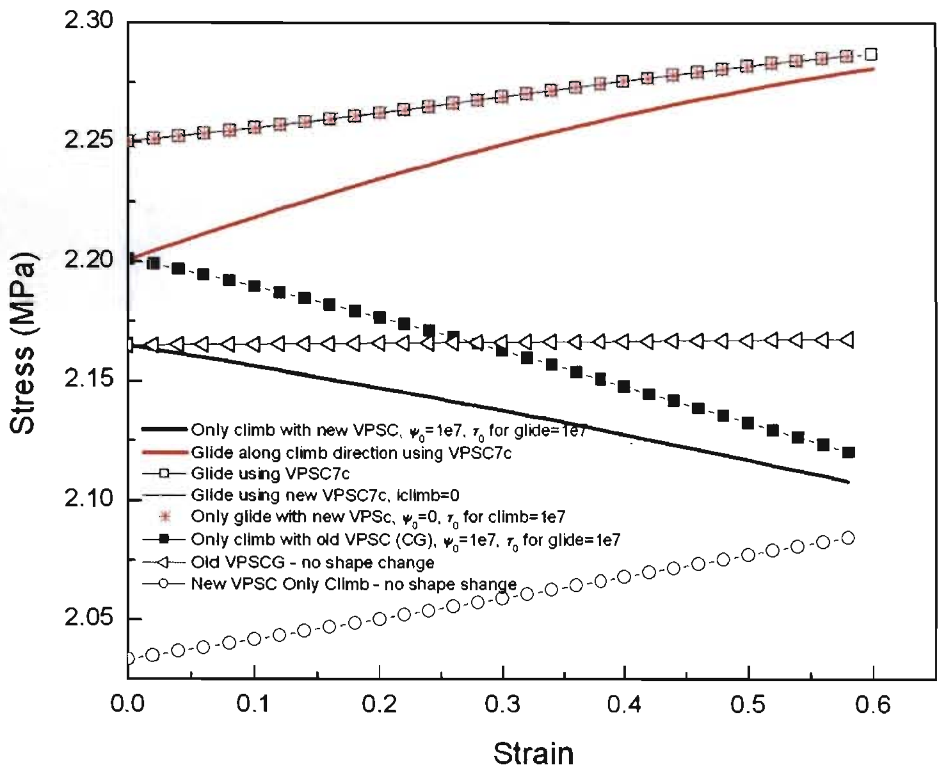


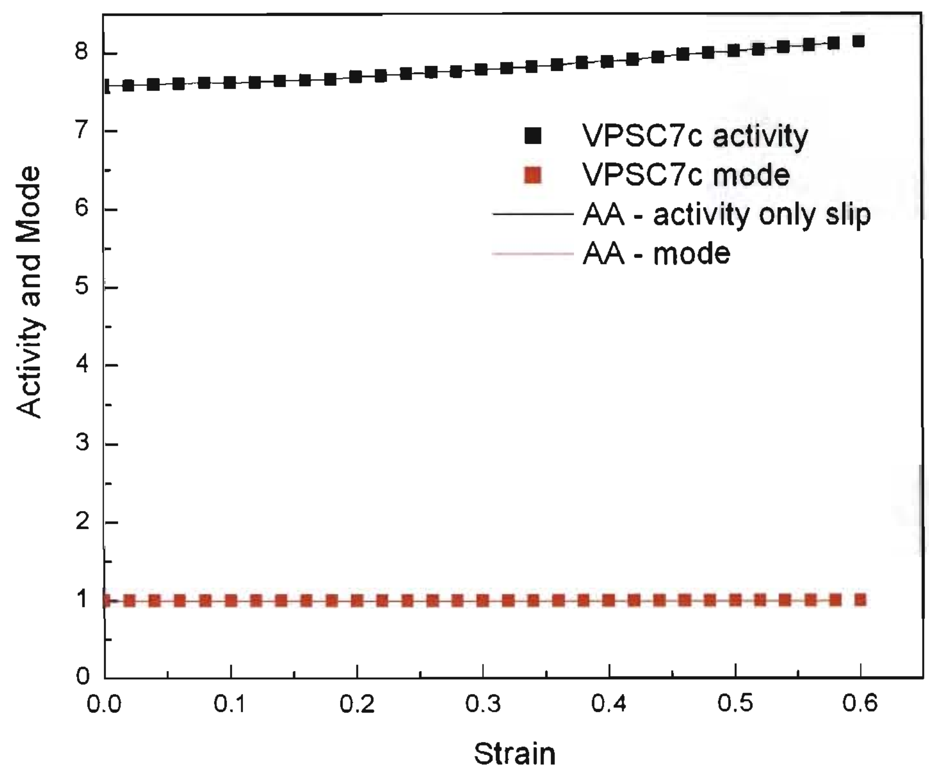
single crystal extension accommodated by glide:
involves lattice reorientation



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

Simulations – glide vs. glide + climb





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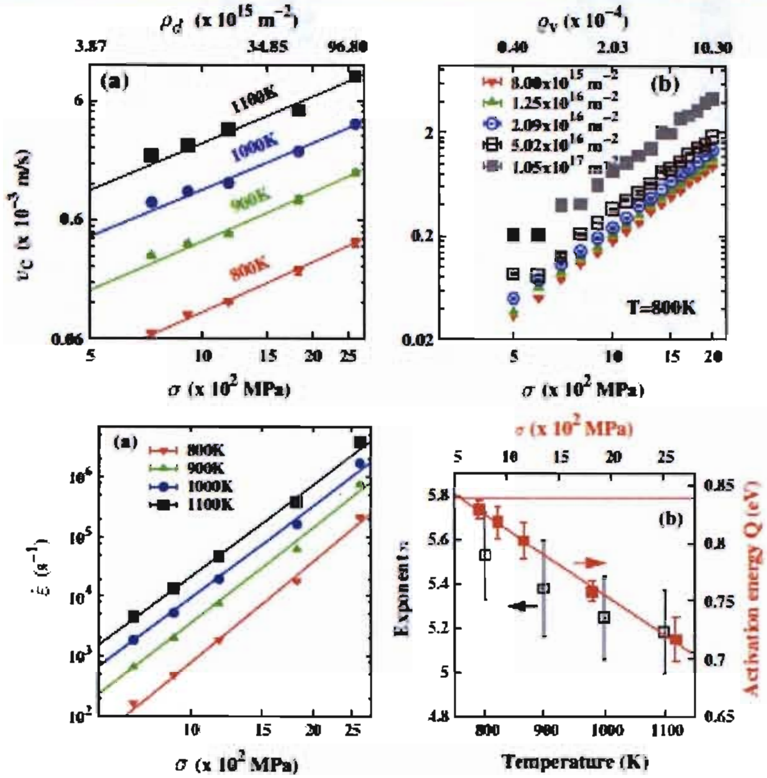
Climb velocity, creep rate and stress exponent – inputs from Kinetic Monte Carlo Simulations



$$\sigma = \alpha\mu b\sqrt{\rho_d} \quad v_c = kh/N_y$$

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

The values of *n* given by the above equation for the appropriate stress range is ~ 3 like many other creep models and is lower than as found in the literature, by Cadek and Milicka, Acta Metall., 1969 and Davies et al., Mat. Sci., 1969.

Kabir et al. (2010) were able to achieve *n* value close to what is determined from experiments but for a 1e4 – 1e5 times higher dislocation density.

The primary reason is that all the models so far consider only climb as the creep governing process. However, it has been suggested that in creep, both glide and climb of dislocations take place.

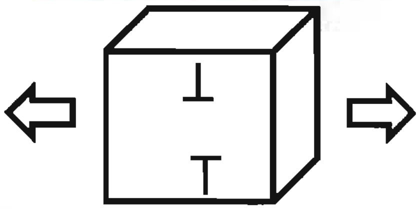
"almost all of the creep strain is produced by glide motion of dislocations". J. Weertman, ASM Transactions Quarterly, 61(1968), p. 681

Only climb can take place when glide is disabled to some constraints e.g. geometric constrains. In pure iron, this is not the case.

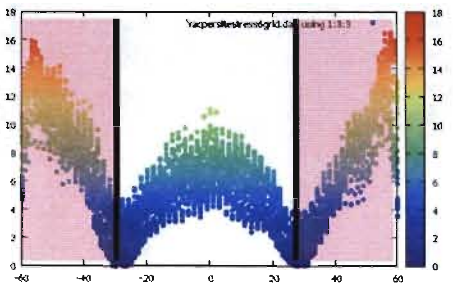
Edelin and Poirier, Phil. Mag., 28 (1973) p.1203

Hafiz et al., Met. Mat. Tran. B., 4(1973) p. 1275

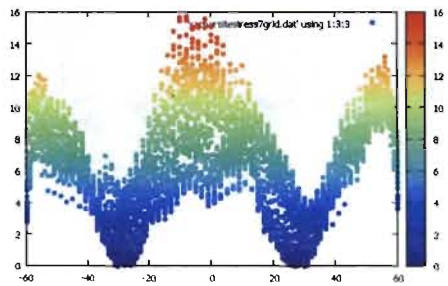
Our calculations of creep rate and stress exponent



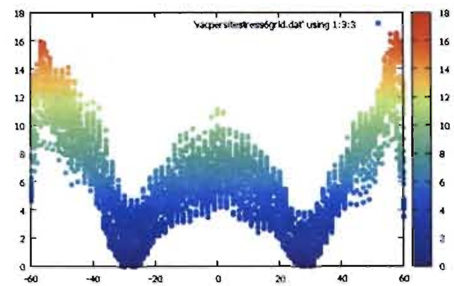
$$v_c = kh/N_y \qquad \dot{\varepsilon} = \rho_d b v_c \qquad \dot{\varepsilon} = A\sigma^n \exp(-Q/k_B T)$$



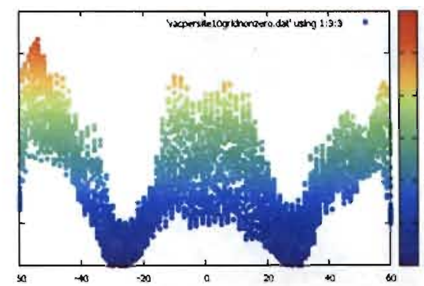
Stress is applied normal to this plane



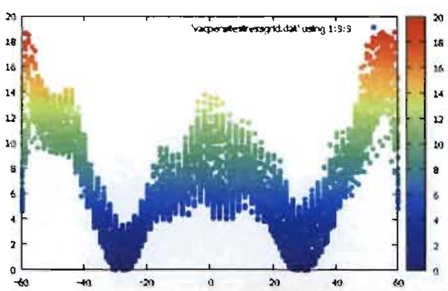
-2 GPa



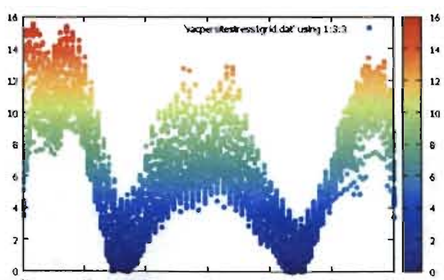
-1 GPa



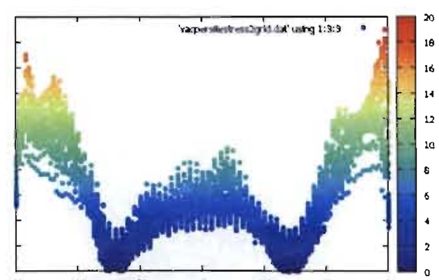
0 GPa



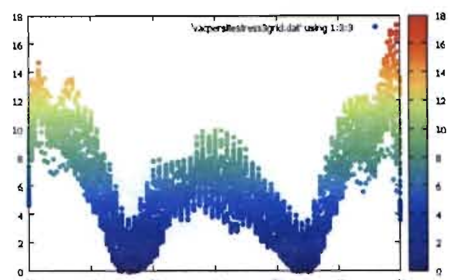
1 GPa



2 GPa

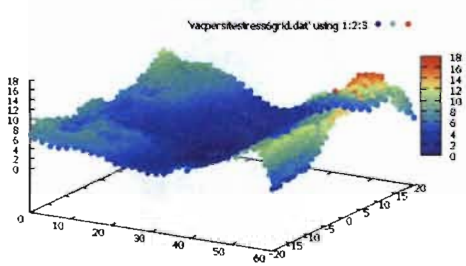


3 GPa

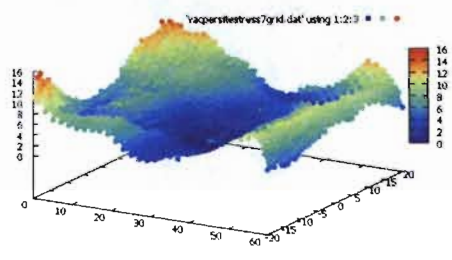


4 GPa

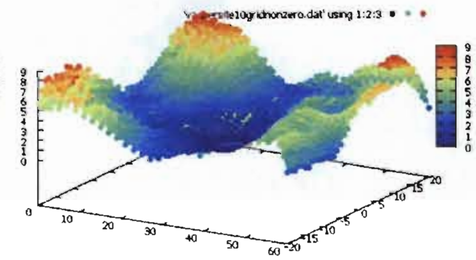
Our calculations of creep rate and stress exponent



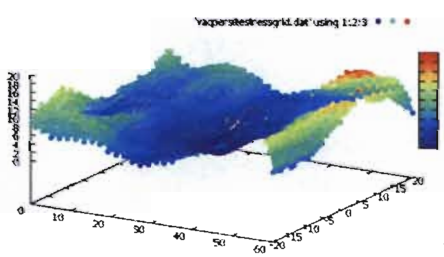
-2 GPa



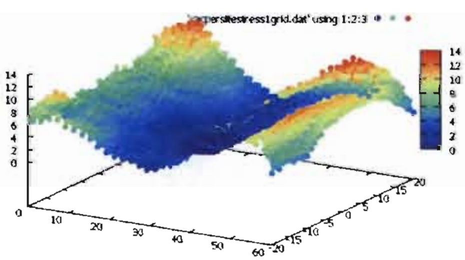
-1 GPa



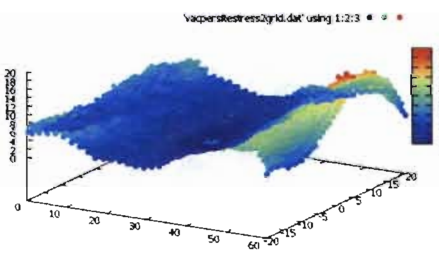
0 GPa



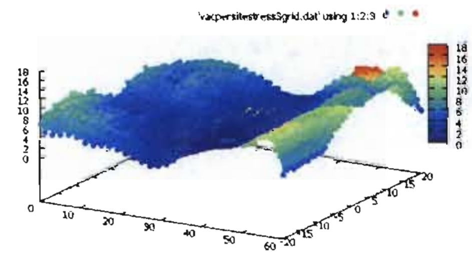
1 GPa



2 GPa



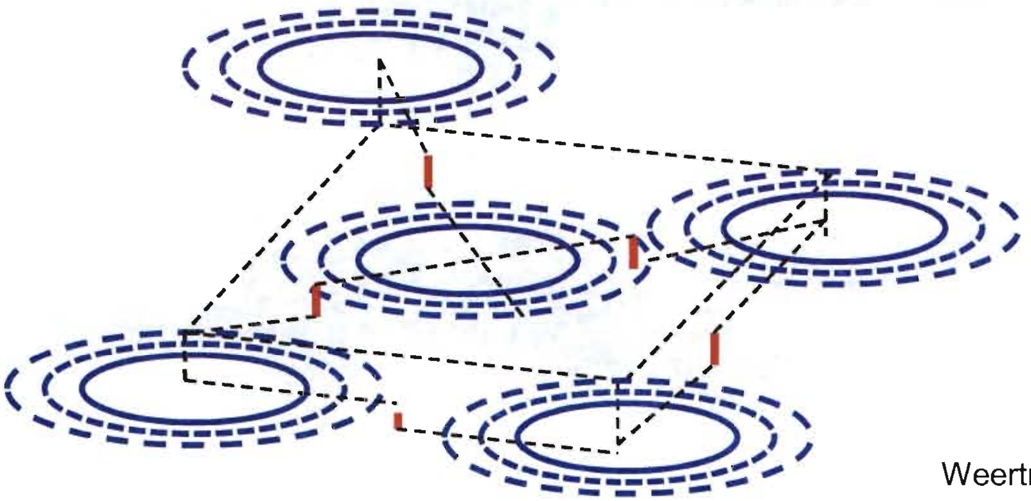
3 GPa

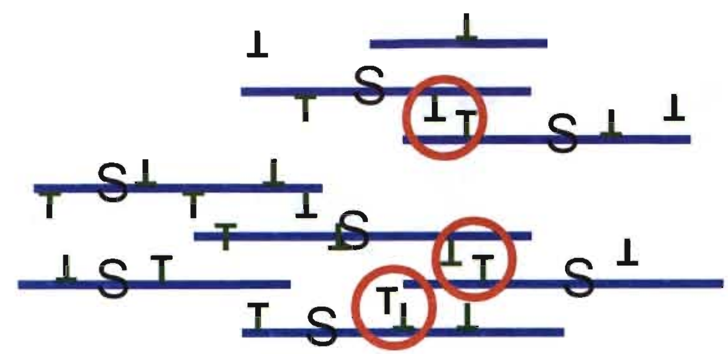


4 GPa

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

Glide accounts for total strain and climb for creep rate





Weertman, 1968

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

Plastic strain rate due to climb

climb mobility (per unit length)

climb force (per unit length)

Summary

- Connection established between P-K force (glide component) and Schmid law
- Climb component of P-K force used to define “climb” tensor (v.g. Schmid tensor)
- Single-crystal plasticity extended to consider climb-and-glide geometry
- Rate-sensitivity constitutive equation for glide extended to climb
- C+G single-crystal constitutive equation implemented in VPSC for the prediction of polycrystal deformation in the C+G regime
- C+G VPSC model can explain differences in texture evolution in Al deformed at high T and different strain-rates.
- Initial version of the single-crystal C+G model (thermal creep only) assumed vacancy concentration instantaneously restored into the equilibrium concentration (at P and T).
- Single-crystal C+G model (thermal creep) extended beyond the instantaneous restoration of equilibrium concentration of vacancies → requires an adjustable phenomenological parameter, a “chemical” stress due to local non-equilibrium concentration of vacancies.\
- Improved single-crystal C+G model for thermal creep extended to irradiation creep → due to super-saturation of vacancies and interstitials, dislocations can only absorb point-defects to climb → model can consider different sink strengths for vacancies and interstitials and swelling → polarity, analogous to twinning.
- strain = strain(glide), strain rate = climb rate
- Important : glide of dislocations is affected by formation of jogs and that is affecting by vacancy supersaturation
- Also, note that activation energy for vacancy diffusion in iron is different for paramagnetic and ferromagnetic temperature ranges