Effects of Non-Glide Stresses on Plastic Flow and Failure Mechanisms arising from Non-Planar Dislocation Core Structures:

Multiscale Simulations of Non-Associated Flow

J. L. Bassani and V. Racherla

Mechanical Engineering and Applied Mechanics

V. Vitek and R. Groger

Materials Science and Engineering

University of Pennsylvania

Penn Engineering

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Mechanics of Materials

Multiscale Simulations of Non-Associated Plastic Flow

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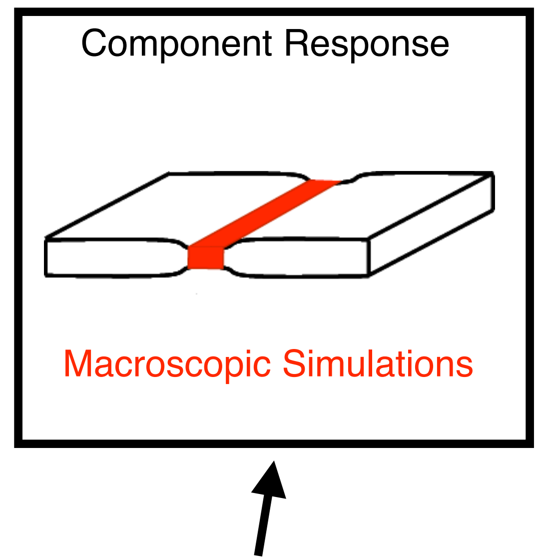
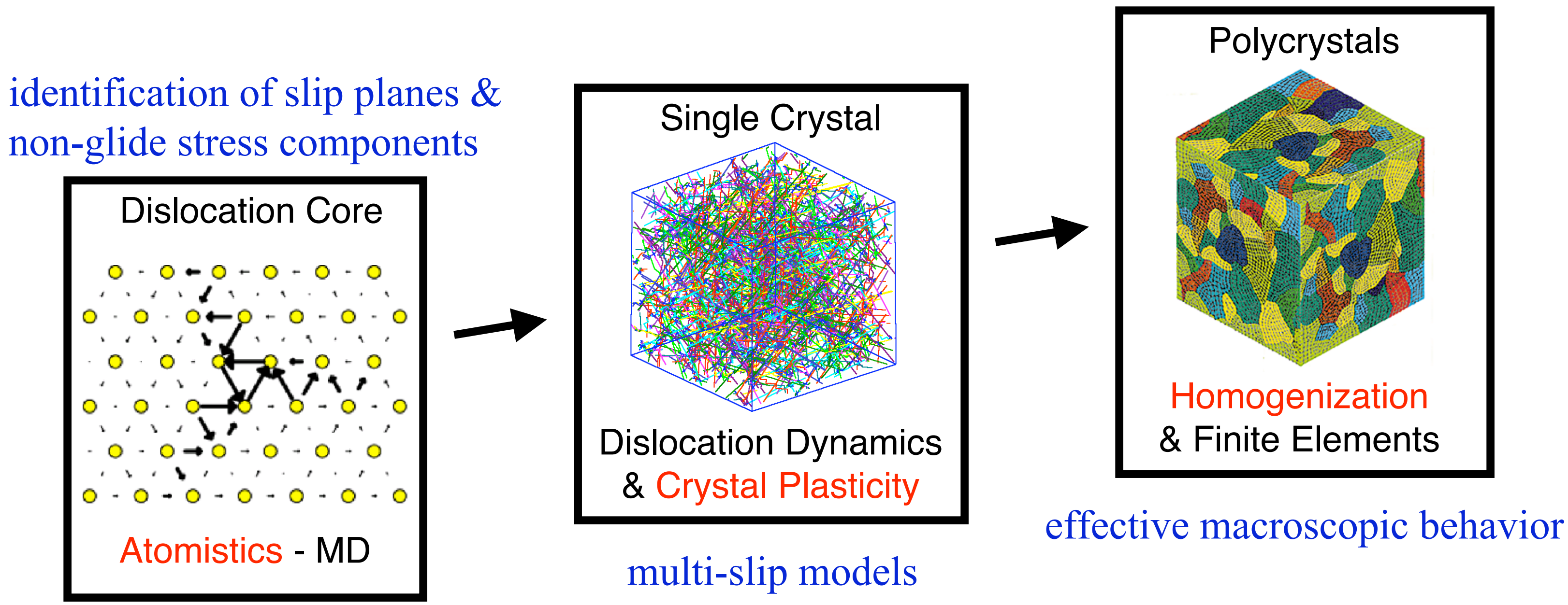
- Our strategy is to pass only the most essential information on to higher length scales.



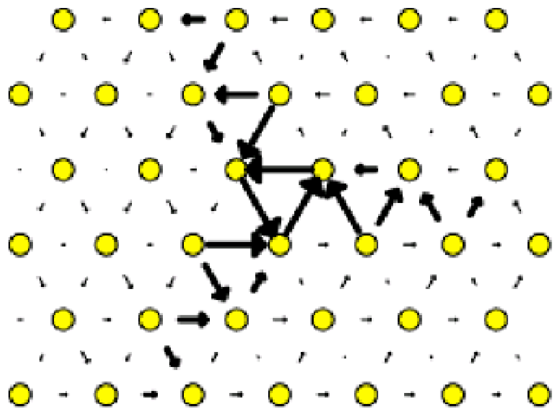


OVERVIEW

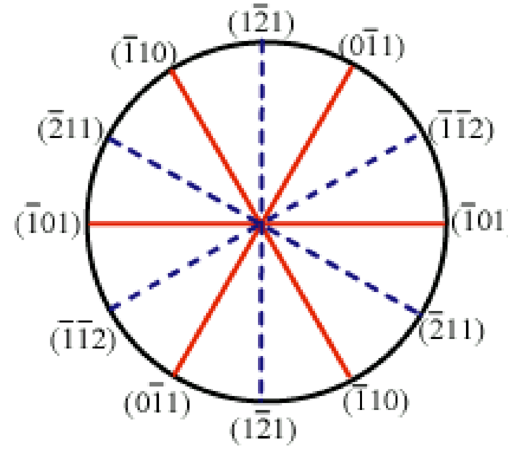
Using accurate potentials to describe the atomic interactions of BCC metals and intermetallic compounds we have:

- **studied the influence of the stress state, on the motion of a screw dislocation from atomistic simulations**
- **developed yield criteria for dislocation motion – effects of non-glide stresses on the Peierls barrier**
- **developed multi-slip constitutive equations for single crystals**
- **calculated yield surfaces and flow potentials for polycrystals**
- **derived yield and flow functions for use in *non-associated flow* continuum models of polycrystals**
- **studied implications of non-associated flow on bifurcation modes, forming limits, and cavitation instabilities**

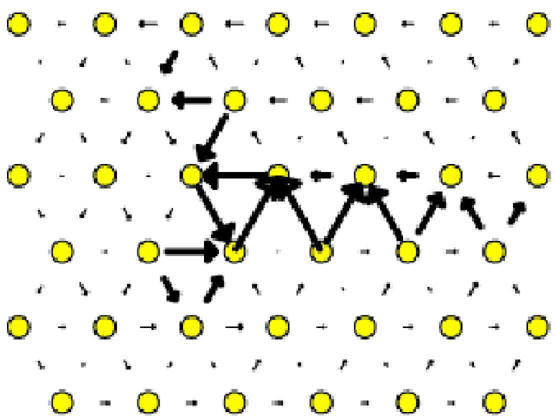
1/2[111] Screw Dislocation Core in Mo: Transformations under Applied Stress



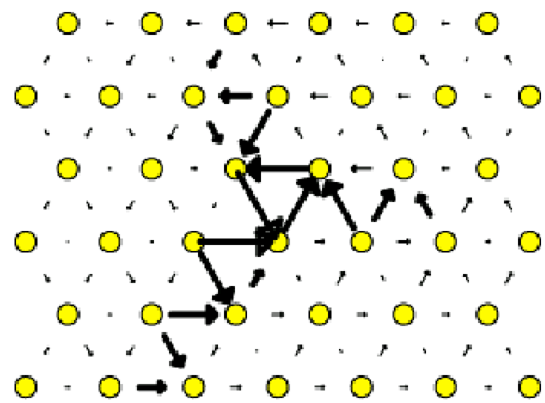
Relaxed Structure: 3-fold symmetry



Planes belonging to the [111] zone



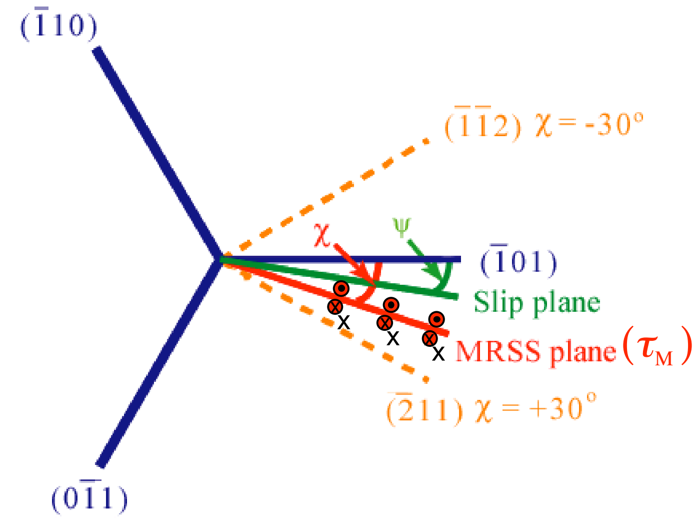
Core under pure shear on $(\bar{1}\,\bar{1}\,2)$ plane in [111] direction ($\chi = -30^o$)



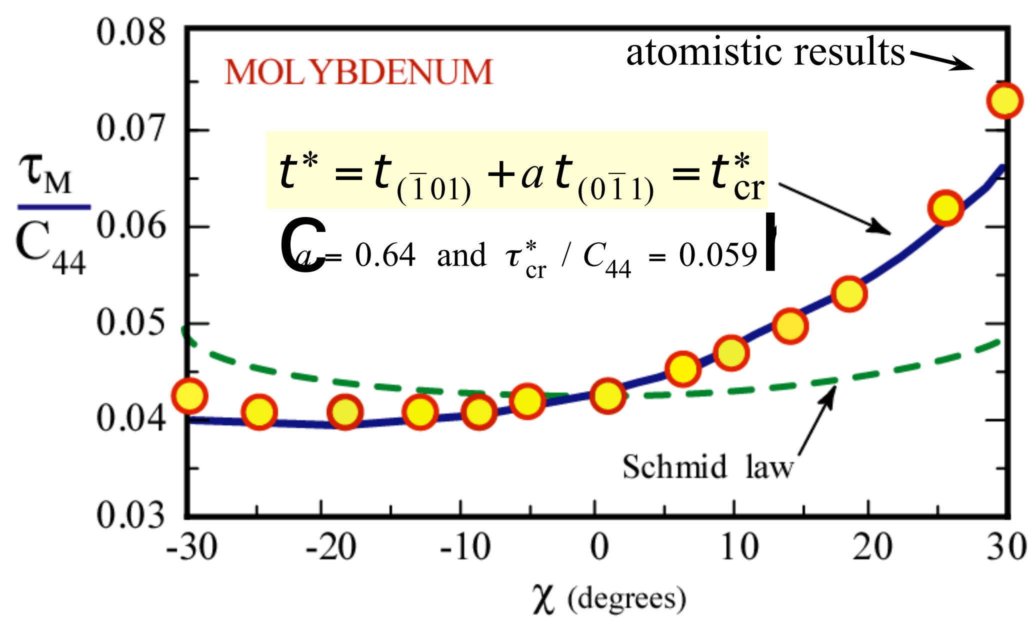
Core under pure shear perpendicular to Burgers vector – alone this stress cannot move the dislocation

Screw Dislocation under Shear Stress on MRSS Plane

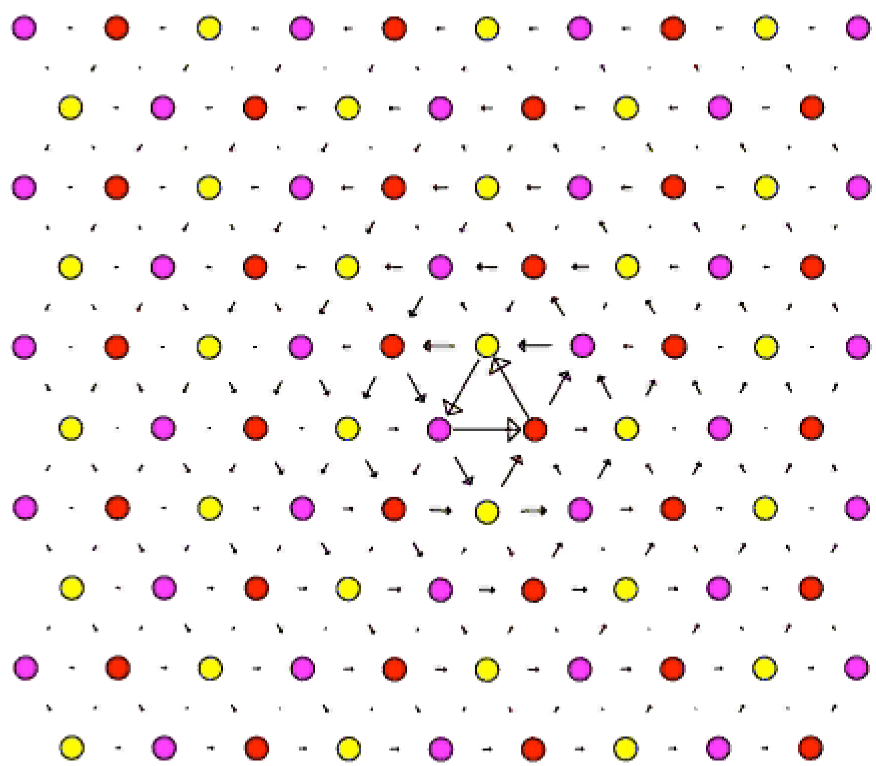
Molybdenum: for $-30 < \chi < 30$ the dislocation moves on the $(\bar{1}01)$ plane at an a applied stress (on the MRSSP), but the atomistic results (circles) do not follow Schmid's law: –

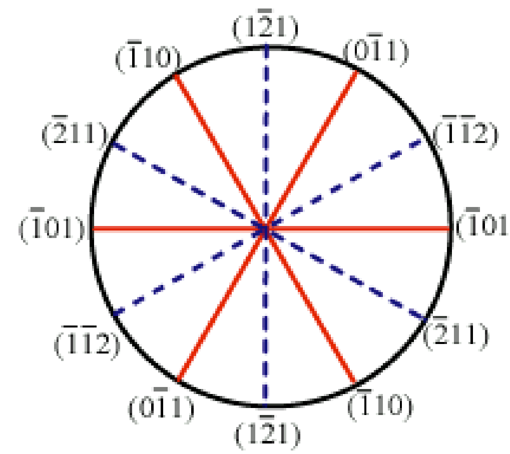


Other components of shear stress parallel to the Burgers vector affect the dislocation motion, and these can be expressed as a linear combination of the Schmid stress and one other shear stress, e.g., –



Motion of a Screw Dislocation in an Infinite Medium Using Bond Order Potentials





Yield Criteria with non-Glide Stresses

stress tensor

Schmid stress on slip system α :

(thermodynamic stress)

slip plane normal

slip direction

non-glide stress components:

identified from atomistic simulations

where $\mathbf{n}_{\eta}^{\alpha}$ and $\mathbf{m}_{\eta}^{\alpha}$ are crystallographic vectors that resolve each of the η =1,N$_{ng}$ non-glide stress components that **transform dislocation core structures** (both shear and pressure).

yield criteria:

(slip system α)

effective hardness

non-glide stress yield parameters

effective yield (Peierls) stress

Slip Systems for BCC Crystals: the effects of non-glide shear stresses parallel and perpendicular to the Burgers vector

Slip System	Slip Direction	Slip plane	Non-Glide Stress Plane	Slip System	Slip Direction	Slip plane	Non-Glide Stress Plane
α	$\mathbf{m}^{\alpha}$	$\mathbf{n}^{\alpha}$	$\mathbf{n}_1^{\alpha}$	α	$\mathbf{m}^{\alpha}$	$\mathbf{n}^{\alpha}$	$\mathbf{n}_1^{\alpha}$
1	111	$01\bar{1}$	$\bar{1}10$	13	$\bar{1}\bar{1}\bar{1}$	$01\bar{1}$	$10\bar{1}$
2	111	$\bar{1}01$	$0\bar{1}1$	14	$\bar{1}\bar{1}\bar{1}$	$\bar{1}01$	$\bar{1}10$
3	111	$1\bar{1}0$	$10\bar{1}$	15	$\bar{1}\bar{1}\bar{1}$	$1\bar{1}0$	$0\bar{1}1$
4	$\bar{1}11$	$0\bar{1}1$	101	16	$1\bar{1}\bar{1}$	$0\bar{1}1$	$\bar{1}\bar{1}0$
5	$\bar{1}11$	$\bar{1}0\bar{1}$	$\bar{1}\bar{1}0$	17	$1\bar{1}\bar{1}$	$\bar{1}0\bar{1}$	$01\bar{1}$
6	$\bar{1}11$	110	$01\bar{1}$	18	$1\bar{1}\bar{1}$	110	101
7	$\bar{1}\bar{1}1$	101	011	19	$11\bar{1}$	101	$1\bar{1}0$
8	$\bar{1}\bar{1}1$	$0\bar{1}\bar{1}$	$1\bar{1}0$	20	$11\bar{1}$	$0\bar{1}\bar{1}$	$\bar{1}0\bar{1}$
9	$\bar{1}\bar{1}1$	$\bar{1}10$	$\bar{1}0\bar{1}$	21	$11\bar{1}$	$\bar{1}10$	011
10	$1\bar{1}1$	$10\bar{1}$	110	22	$\bar{1}1\bar{1}$	$10\bar{1}$	$0\bar{1}\bar{1}$
11	$1\bar{1}1$	011	$\bar{1}01$	23	$\bar{1}1\bar{1}$	011	110
12	$1\bar{1}1$	$\bar{1}\bar{1}0$	$0\bar{1}\bar{1}$	24	$\bar{1}1\bar{1}$	$\bar{1}\bar{1}0$	$\bar{1}01$

yield criteria:

Schmid stress:

non-glide stresses:

Multiple Slip in Single Crystals with Non-Glide Stress Effects

yield criteria:

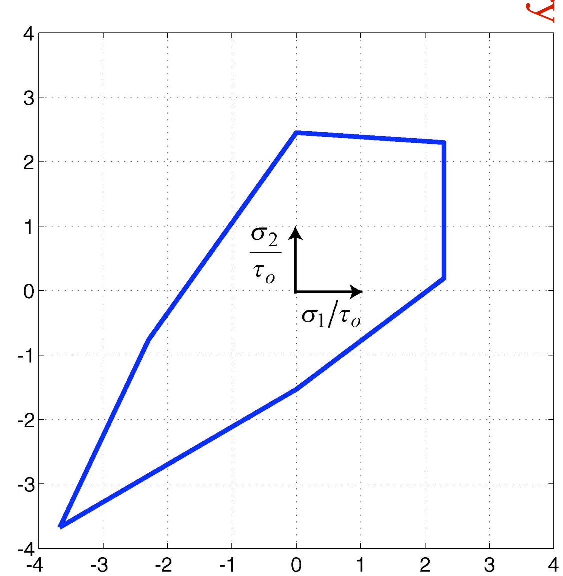
kinematics:

flow rule:

$(n >> 1)$

a non-associated flow theory

BCC yield surface (a=0.6) – restricted model



Two-dimensional projection of the yield surface. Euler angles for this crystal orientation are

$$\eta, \beta, \phi = (0.785, 2.53, 0)$$

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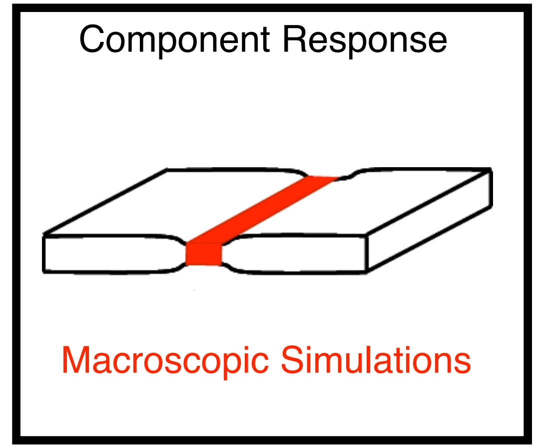
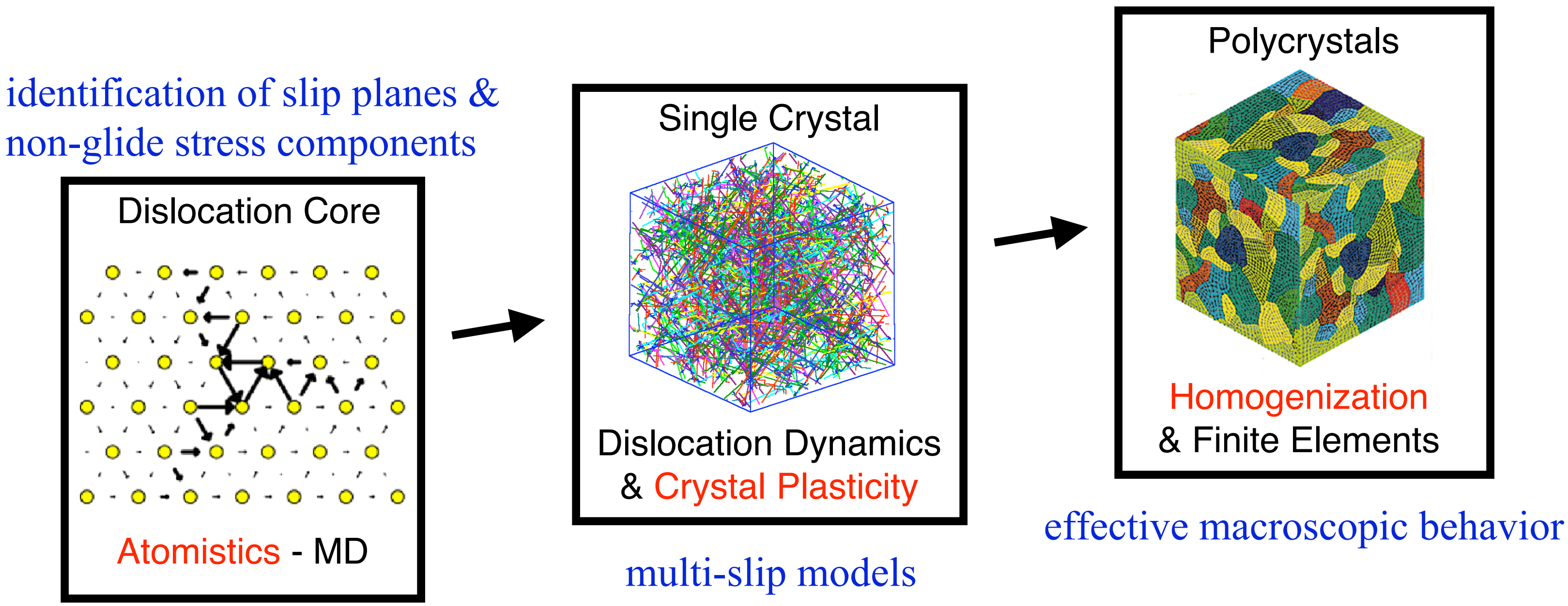
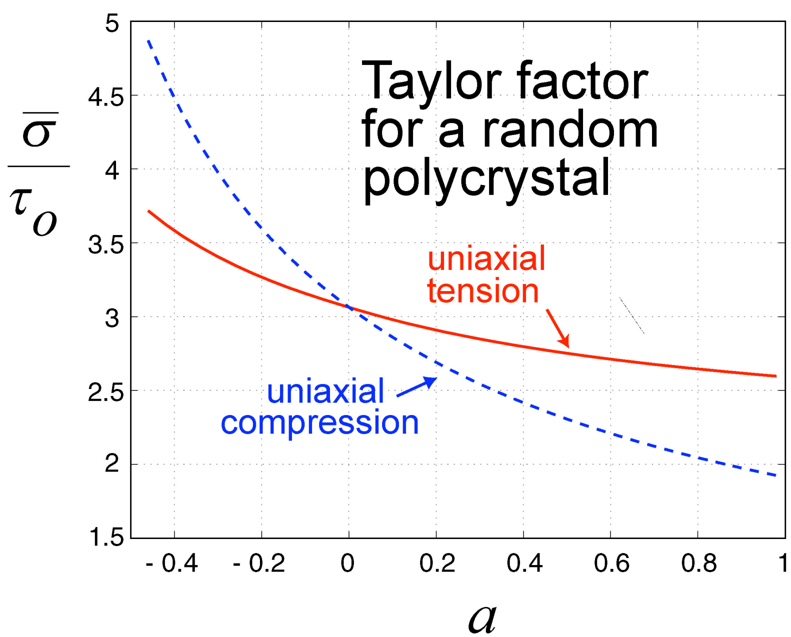
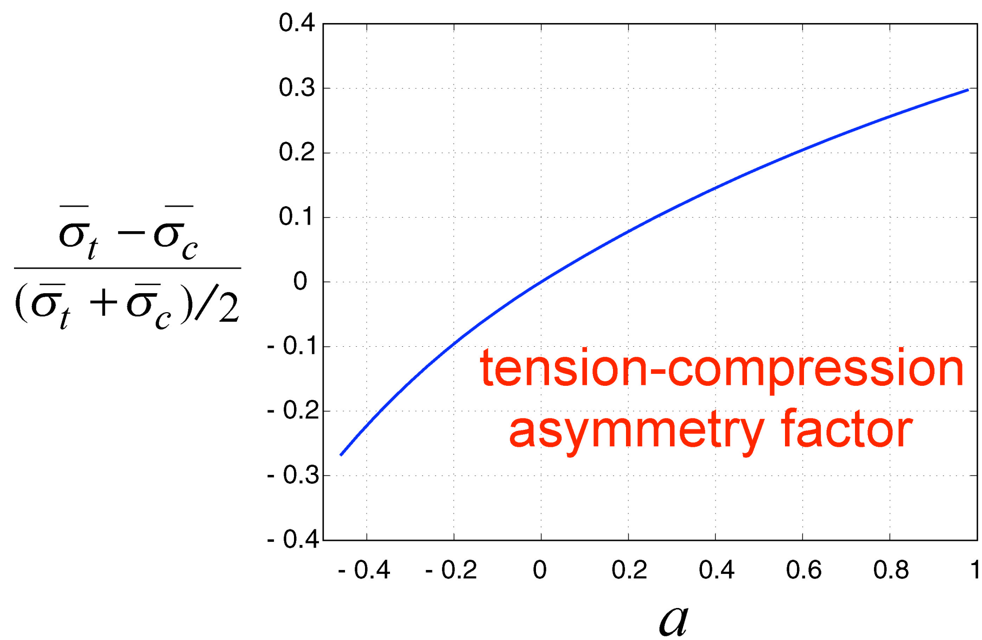




Random BCC Polycrystal with Non-Glide Stresses

Consider a polycrystal of randomly oriented BCC grains each satisfying the yield criteria: . Neglecting elastic strains and assuming the strain in each crystal is the same as the macroscopic strain (Taylor hypothesis), a quadratic programming problem is used to solve for the minimum of 5 slips in each crystal, which gives an upper bound to the limit yield surface. For Schmid behavior (a=0) the classical Taylor factor is 3.07 times the slip-system yield stress in tension and compression.

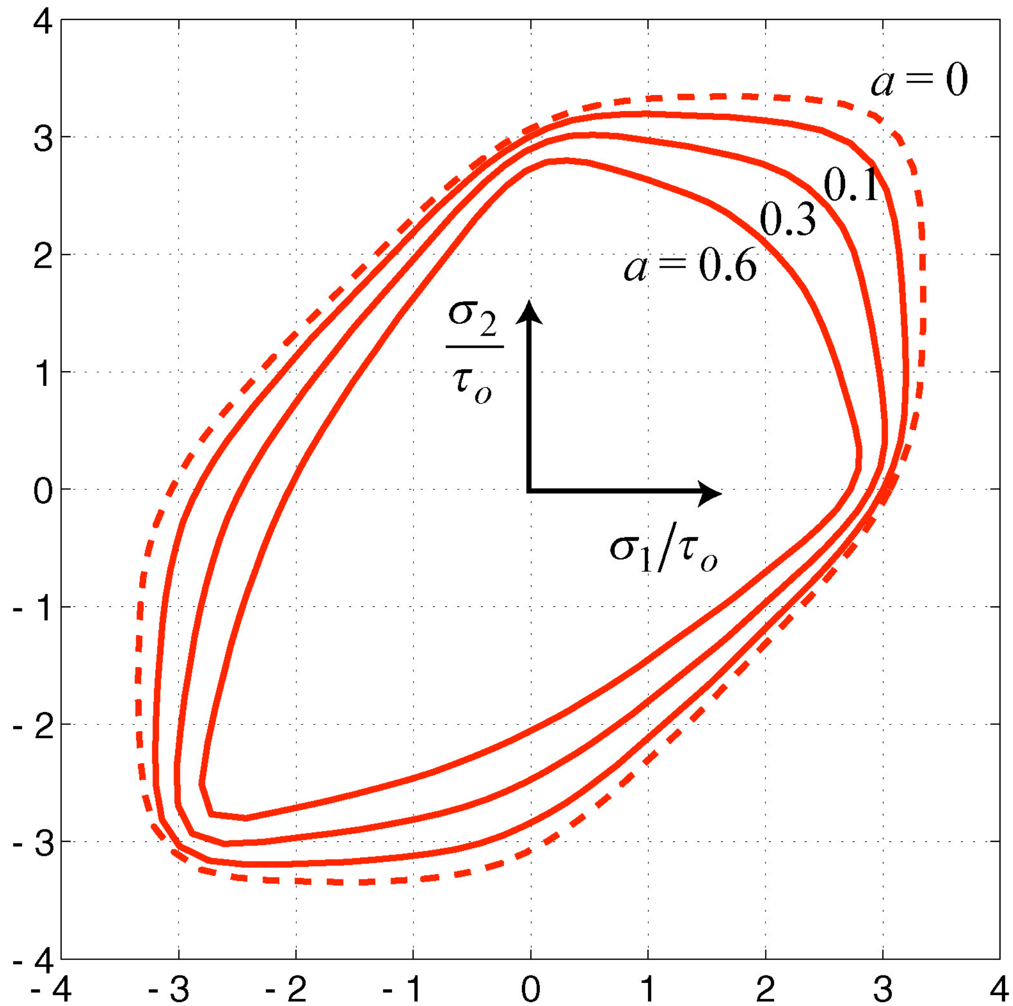




2D Yield Surfaces for Random BCC Polycrystals

based upon single crystal yield criteria that include the effects of non-glide stresses:

where a and τ_o are material parameters



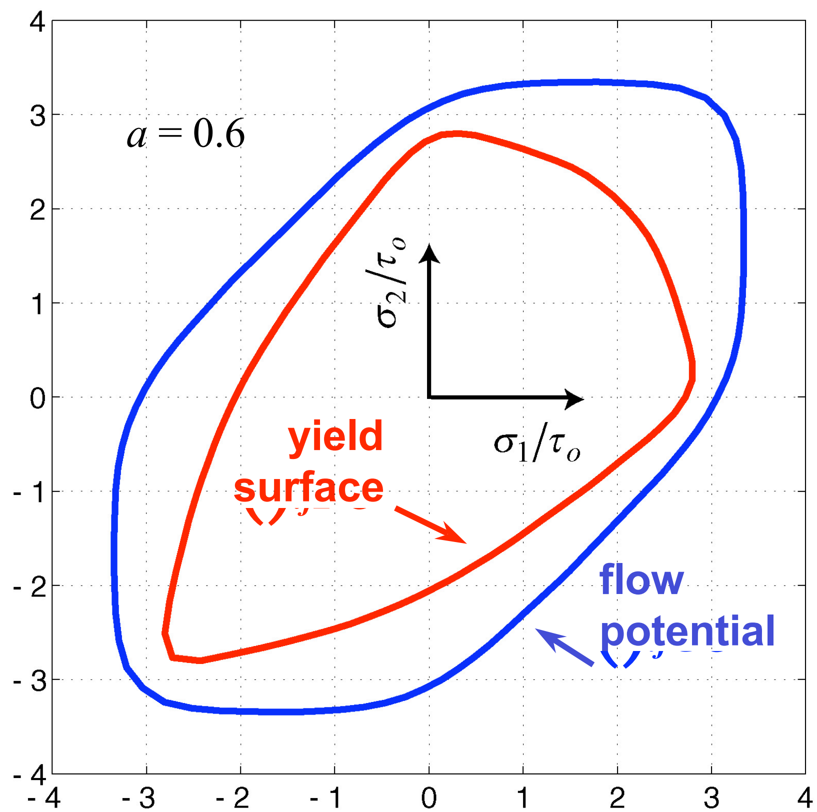
Non-Associated Flow Behavior

macroscopic (engineering) theory

F=*G* for classical associated flow behavior

plastic strain-rate

These *isotropic* surfaces shown are predicted from a Taylor model of a random BCC polycrystal with single crystal yield criteria fitted to atomistic calculation of the stress-state dependence of the Peierls barrier in molybdenum.



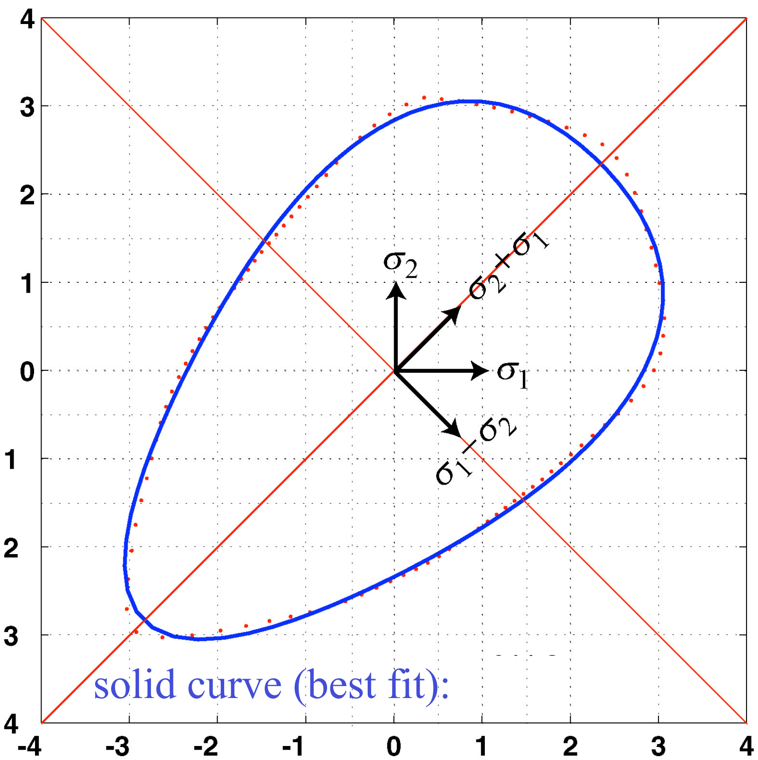
Macroscopic Yield Functions for Random BCC Polycrystals

Yield stress in tension

Yield stress in compression

note: reduces to

the von Mises surface

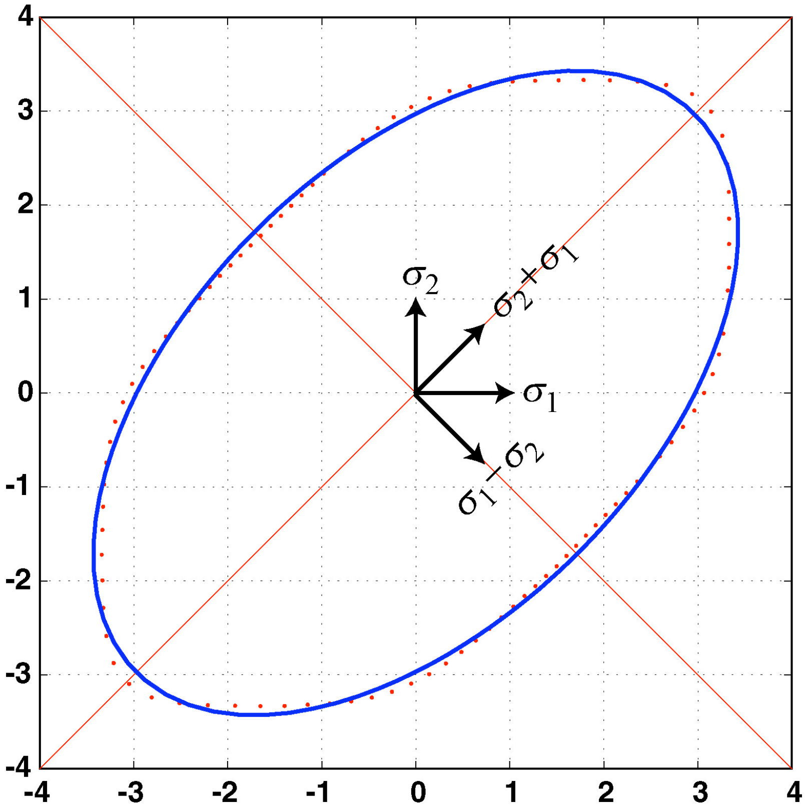


points plotted are from Taylor calculation for BCC polycrystal with *the effects of non-glide stresses both parallel to and perpendicular to the Burgers vector*

Macroscopic Flow Potentials for Random BCC Polycrystals

G is the flow potential:

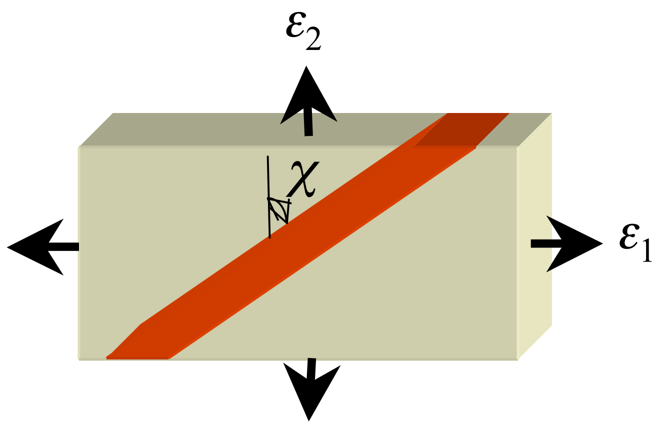
hardening law:

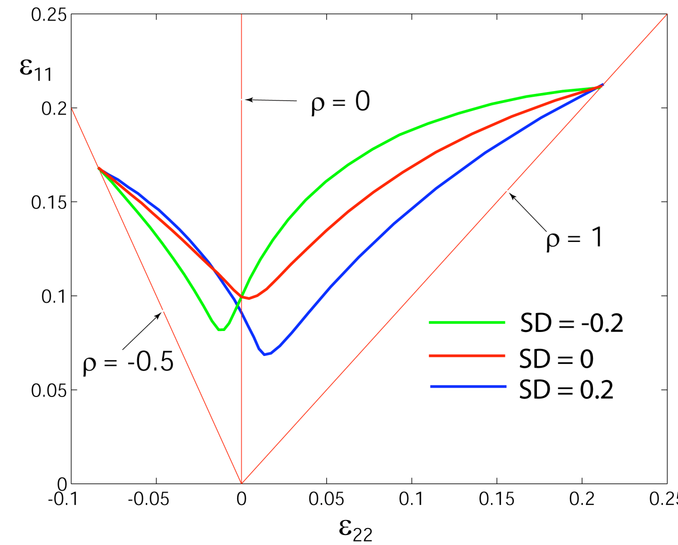


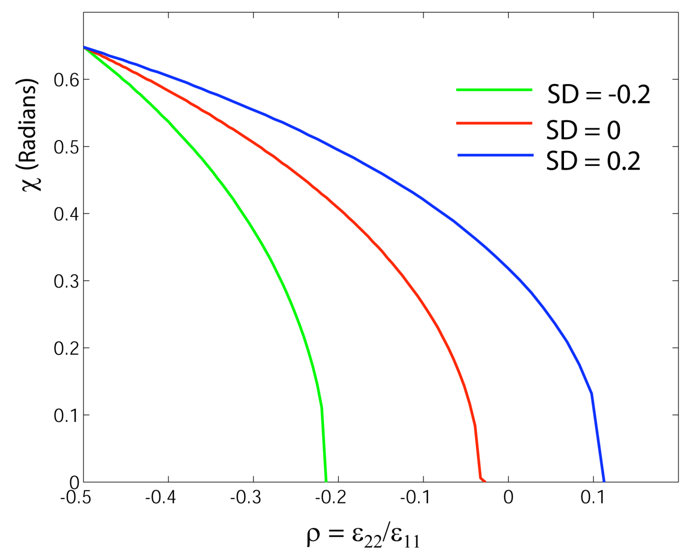
solid curve (best fit):

points plotted are from Taylor calculation for BCC polycrystal

Effects of Non-Associated Flow on Bifurcations from Homogeneous Plane Stress Loading States





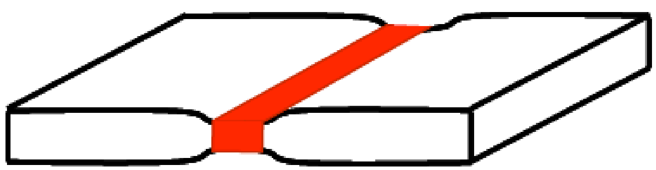


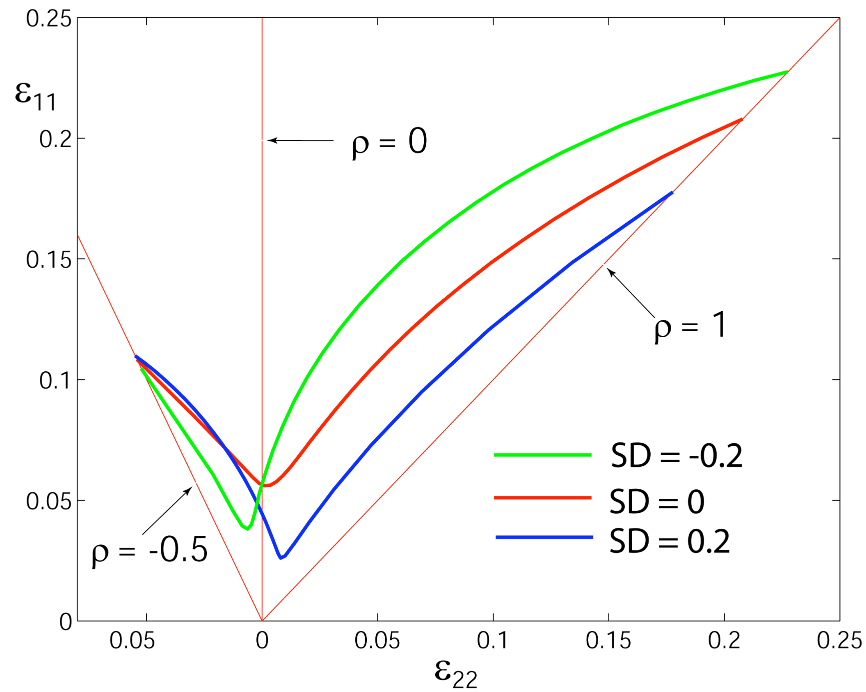
If **ΔD** represents the jump in strain rate across the band (shown in red) and **C** the incremental modulus. The bifurcation condition is given by

$$\Delta \mathbf{D} : \mathbf{C} : \Delta \mathbf{D} = 0$$

Effects of Non-Associated Flow on Forming Limits

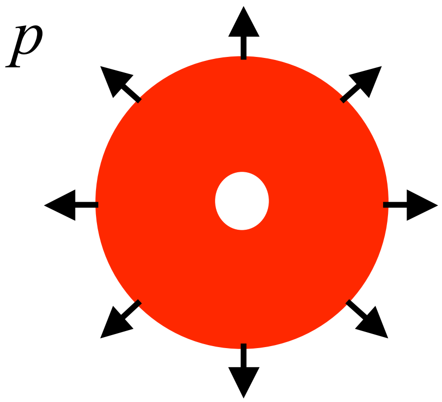
Sheet necking under biaxial straining



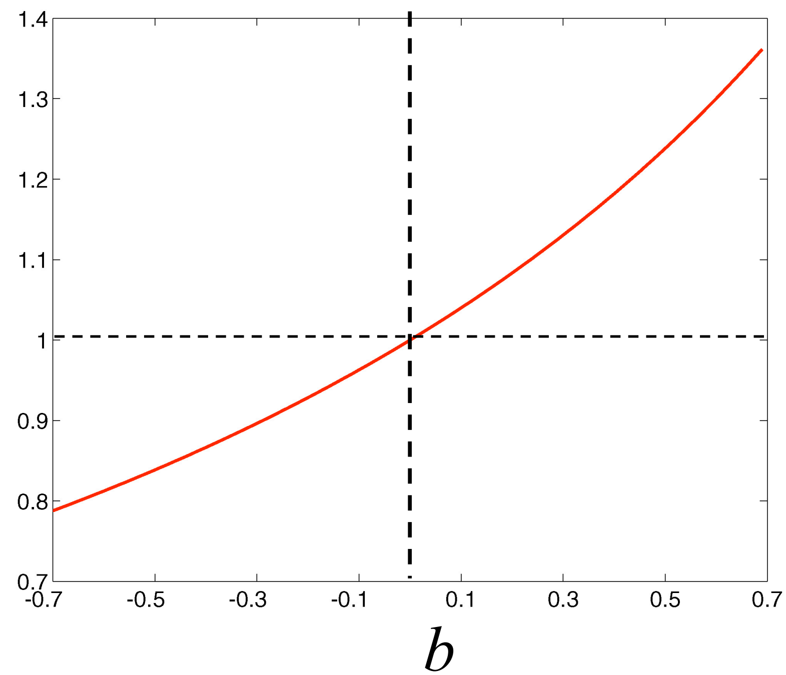


MK analysis of **sheet necking** using deformation theory for strain hardening coefficients of $N = 0.1$.

Effects of Non-Associated Flow on Cavitation Instabilities



critical pressure at
unstable cavity growth



CONCLUSIONS

- **From the multiscale simulations beginning with the input from atomistics we observe that the non-glide stresses have similar order-of-magnitude effects at single and polycrystal levels and generally on macroscopic response.**
- **Since these effects have their origin in dislocation core transformations, they arise generally at high stress levels, particularly at high strain-rates and/or low temperatures.**
- **There are comparable order-of-magnitude effects on *strain localization* in the form of bifurcations, sheet necking, and on cavitation instabilities to name a few.**
- **In the language of continuum plasticity, at each scale a significant effect of *non-associated flow behavior* is present.**