Friction, Fracture, and Earthquake Physics

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Atomic-Level Measures of Strength, Deformation and Reactivity

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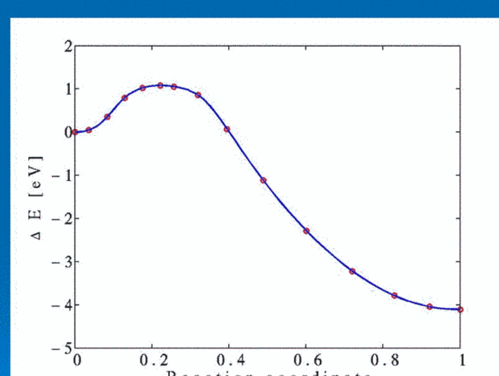
probing *large-strain deformation* through atomistic simulation

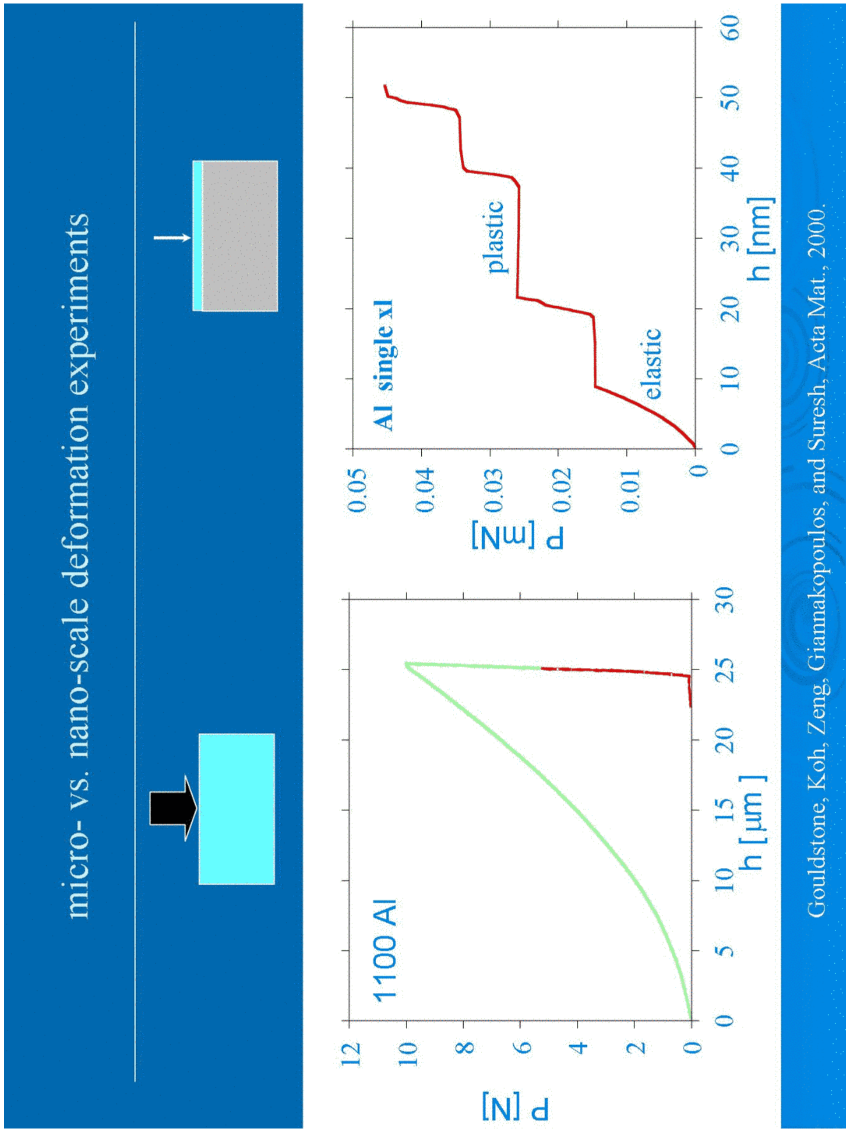
charge density redistribution at saddle points in stress-strain curves

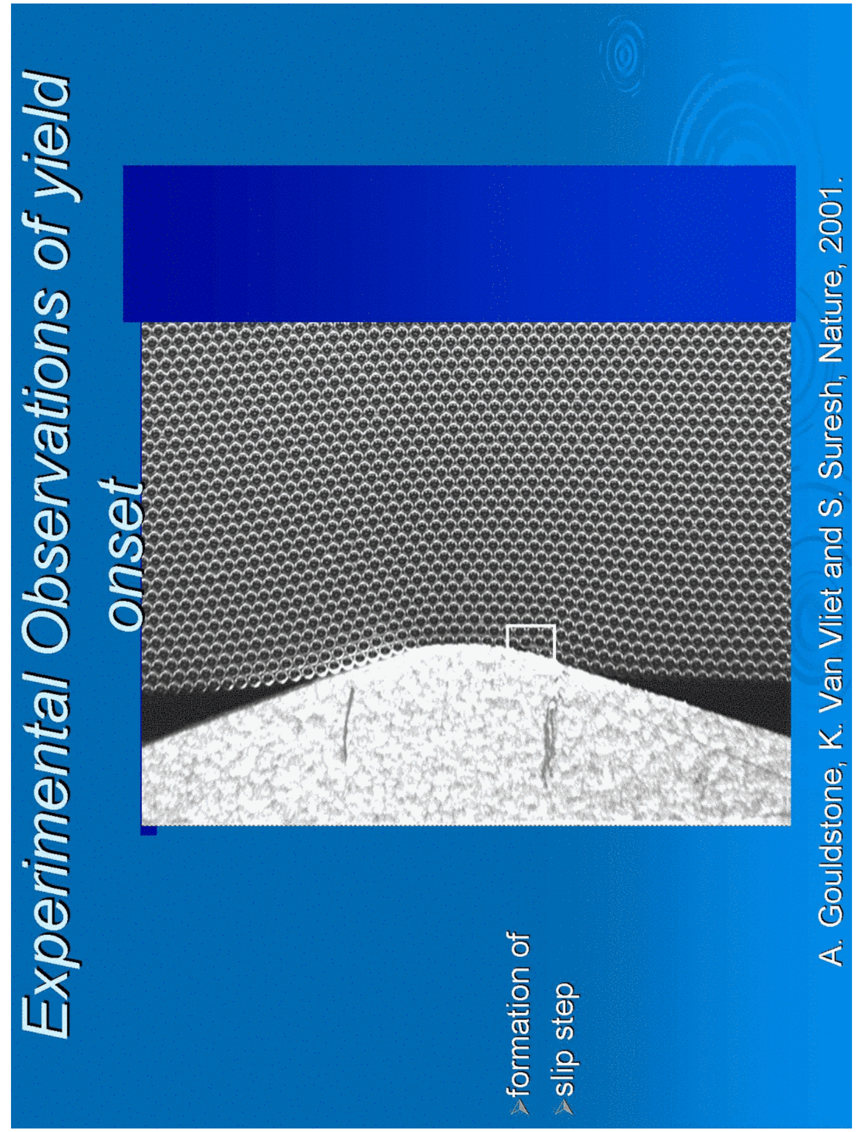
reaction pathway (MEP) to locate saddle point and local atomic configurations

unit processes: shear instability (dislocation and twinning), crack extension

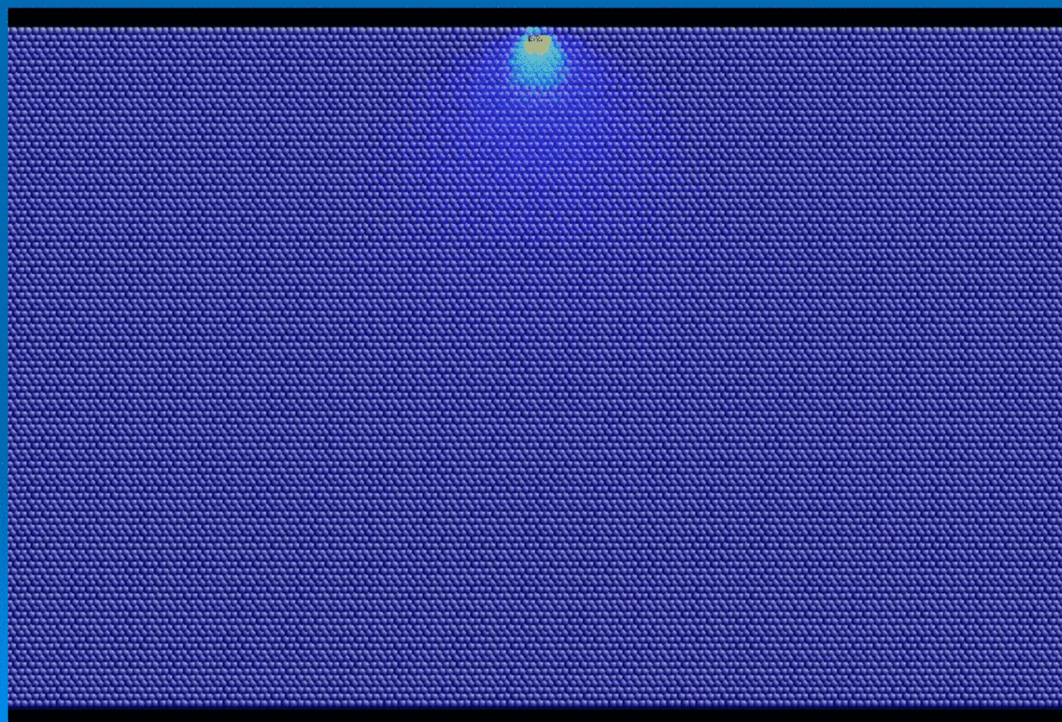


MEP activation barrier
atomic configurations


micro- vs. nano-scale deformation experiments
1100 Al
P [N]
h [μm]
Al single xl
plastic
elastic
P [mN]
h [nm]
Gouldstone, Koh, Zeng, Giannakopoulos, and Suresh, Acta Mat., 2000.


Experimental Observations of yield onset
formation of
slip step
A. Gouldstone, K. Van Vliet and S. Suresh, Nature, 2001.

Nanoindentation in 2D (MD): von Mises Stress Invariant Distribution



Stability criteria for defect nucleation in a perfect lattice under inhomogeneous deformation

A general continuum formulation by R. Hill (1962) invoking ‘acceleration discontinuity’

A similarly general derivation of condition for shear localization by J. R. Rice (1976)

We can show --

$$\Delta F = \frac{1}{2}\int_{V(x)} D_{ijkl} u_{ij}(x) u_{kl}(x) dV$$

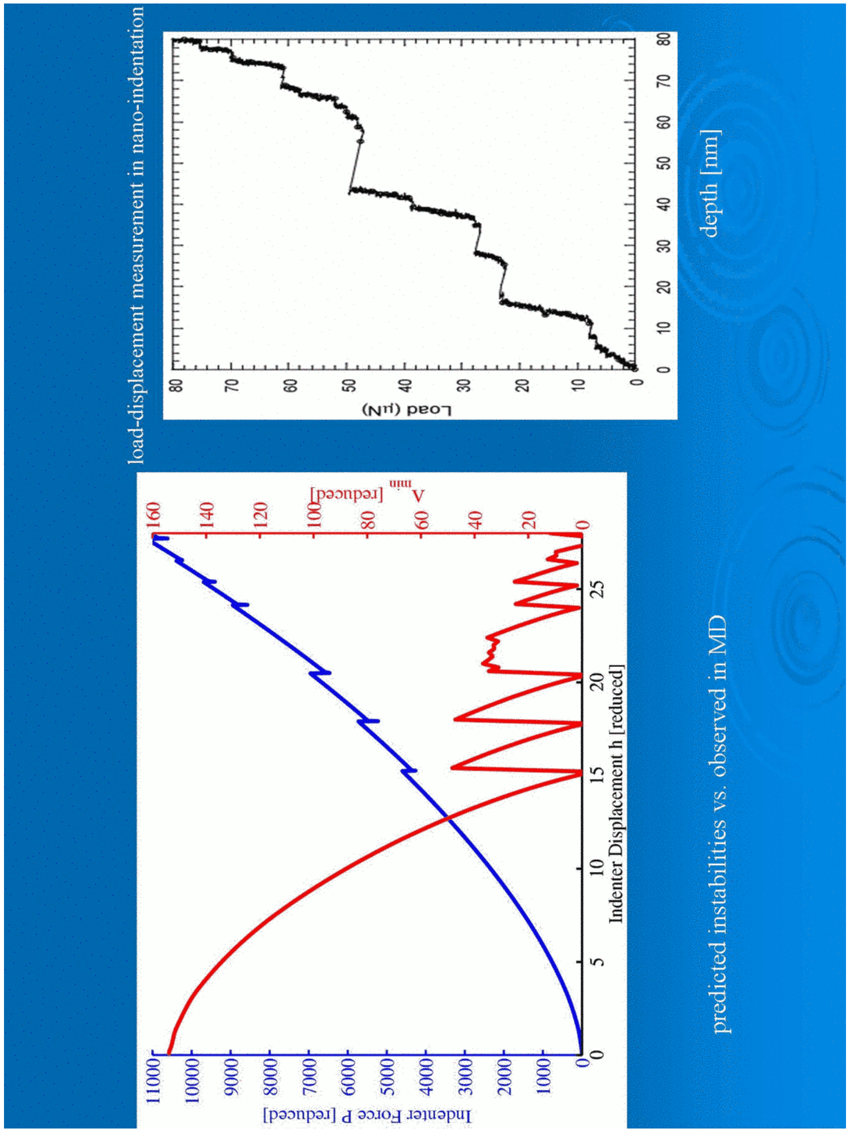
$$D_{ijkl} = C_{ijkl} + \tau_{jl}\delta_{ik} \qquad u_{ij} = \partial u_i(x)/\partial x_j$$

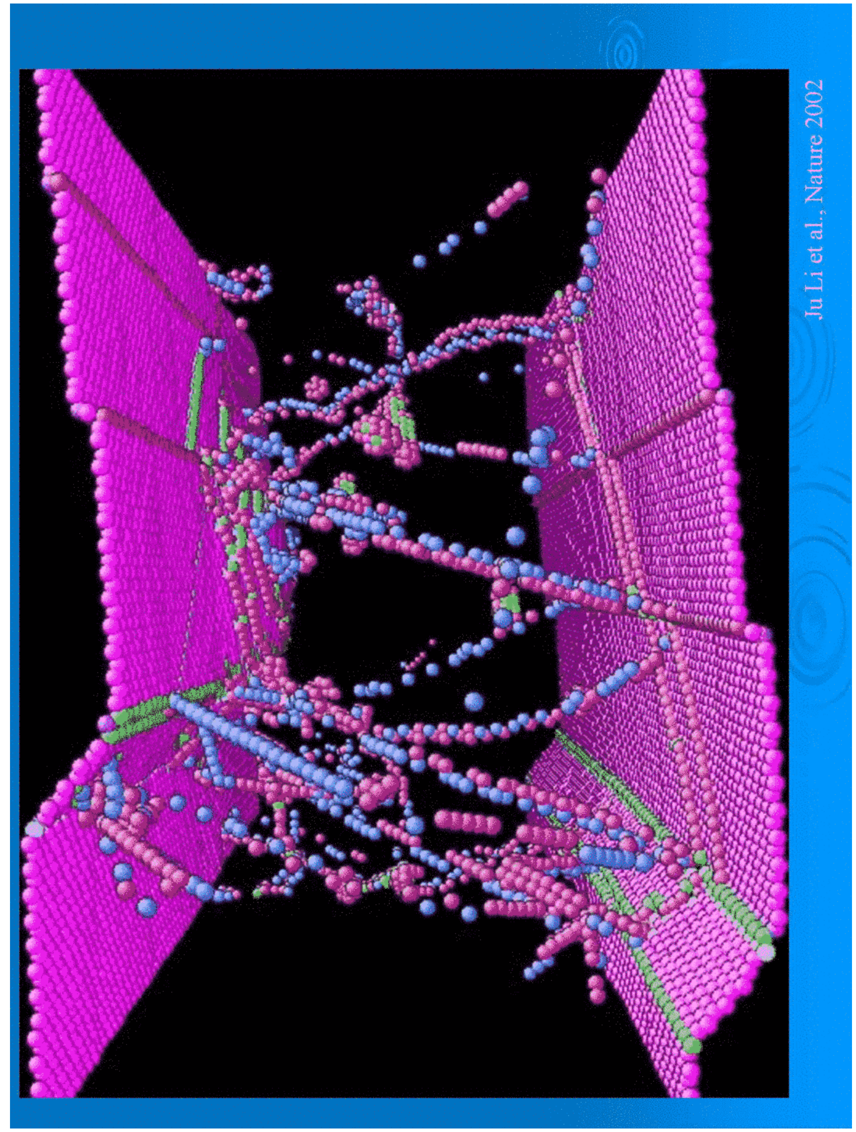
$$u_i(x) = w_i e^{ikx}$$

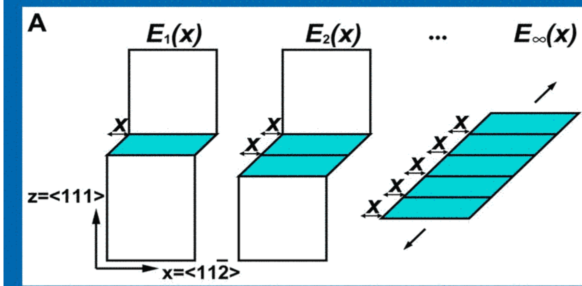
$\Lambda(w,k) = (C_{ijkl} w_i w_k + \tau_{jl}) k_j k_l = 0$ is the condition for defect nucleation

This criterion is *local* because we determine C and τ using atomistic expressions

Li et al. Nature 2002, Van Vliet et al. Phys Rev 2003, Ting et al. J Mech Phys Solids 2003


load-displacement measurement in nano-indentation
Load (μN)
depth [nm]
Indenter Force P [reduced]
A_{min} [reduced]
Indenter Displacement h [reduced]
predicted instabilities vs. observed in MD


Ju Li et al., Nature 2002



Multiplane Generalized Stacking Fault Energy

$$\gamma_n(x) \equiv \frac{E_n(x)}{nS_0}, \qquad n = 1,2,3,\ldots,\infty$$

$\gamma_1(x)$: GSF surface

$\gamma_1(b_p) = \gamma_{SF}$: intrinsic stacking fault

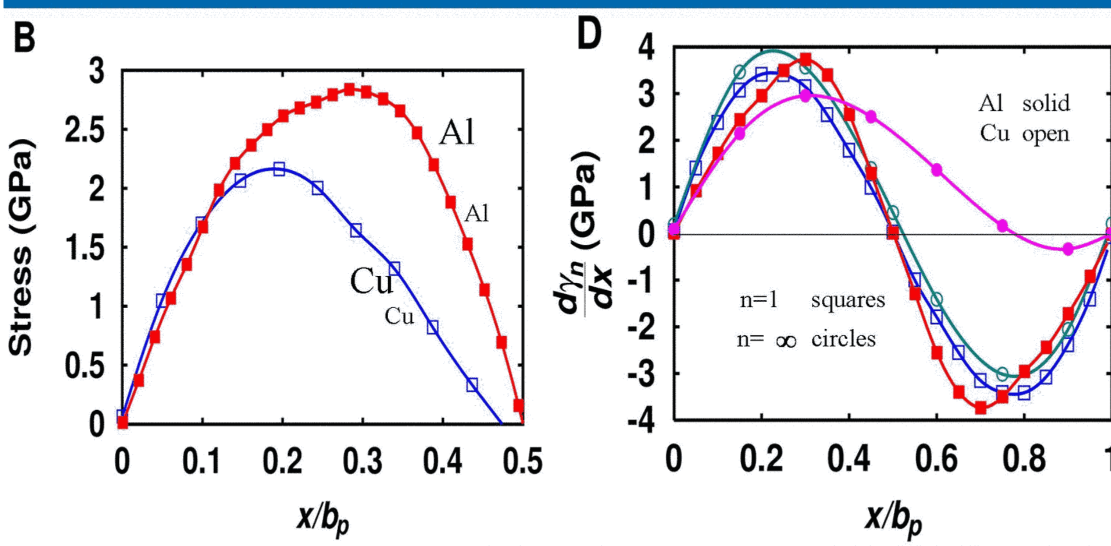
$\frac{d\gamma_1(x<b_p)}{dx} = 0 \rightarrow \gamma_{US}$: unstable stacking energy

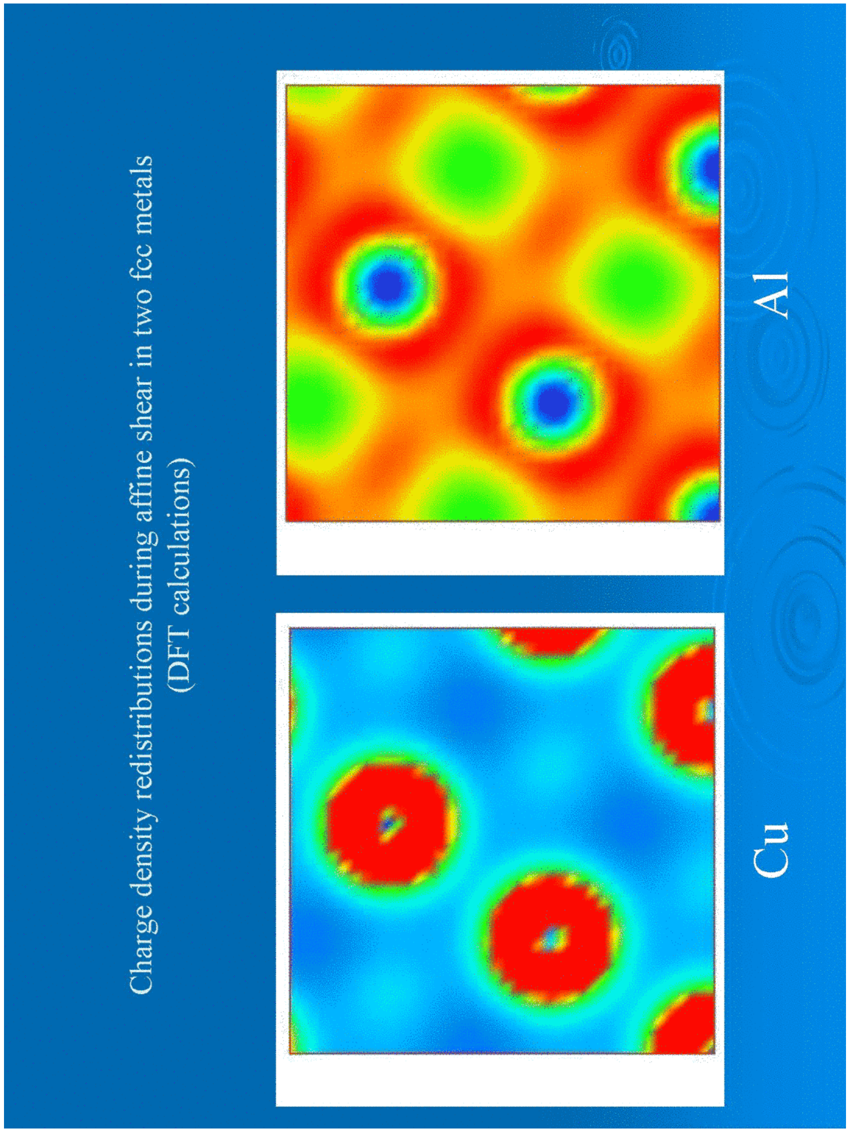
Table 1. Benchmark results, comparison of present calculations (Calc), experiments (Expt), and previous calculations (Oth calc). Dashes indicate that results are not available.

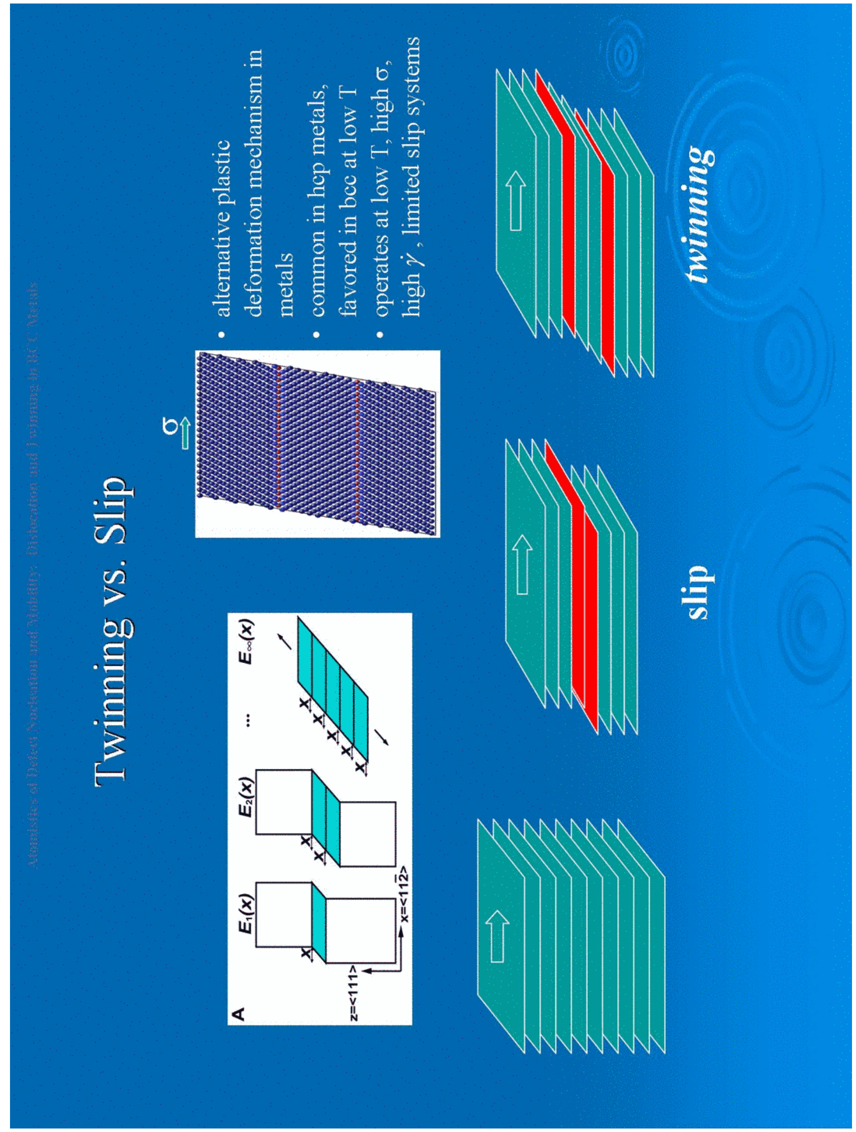
Variable	Al			Cu		
	Calc*	Expt	Oth calc	Calc*	Expt	Oth calc
a_0 (Å)	4.04	4.03†	4.04‡	3.64	3.62†	3.64§
G_r' (GPa)	25.4	27.4‖	19–25¶	31.0	33.3‖	26–34¶
G_u' (GPa)	25.4	27.6‖	24–30¶	40.9	44.4‖	36–44¶
γ_{sf} (mJ/m^2)	158	166#	143**, 164††	39	45#	(49)‡‡
γ_{us} (mJ/m^2)	175	—	183**, 224††	158	—	(210)‡‡

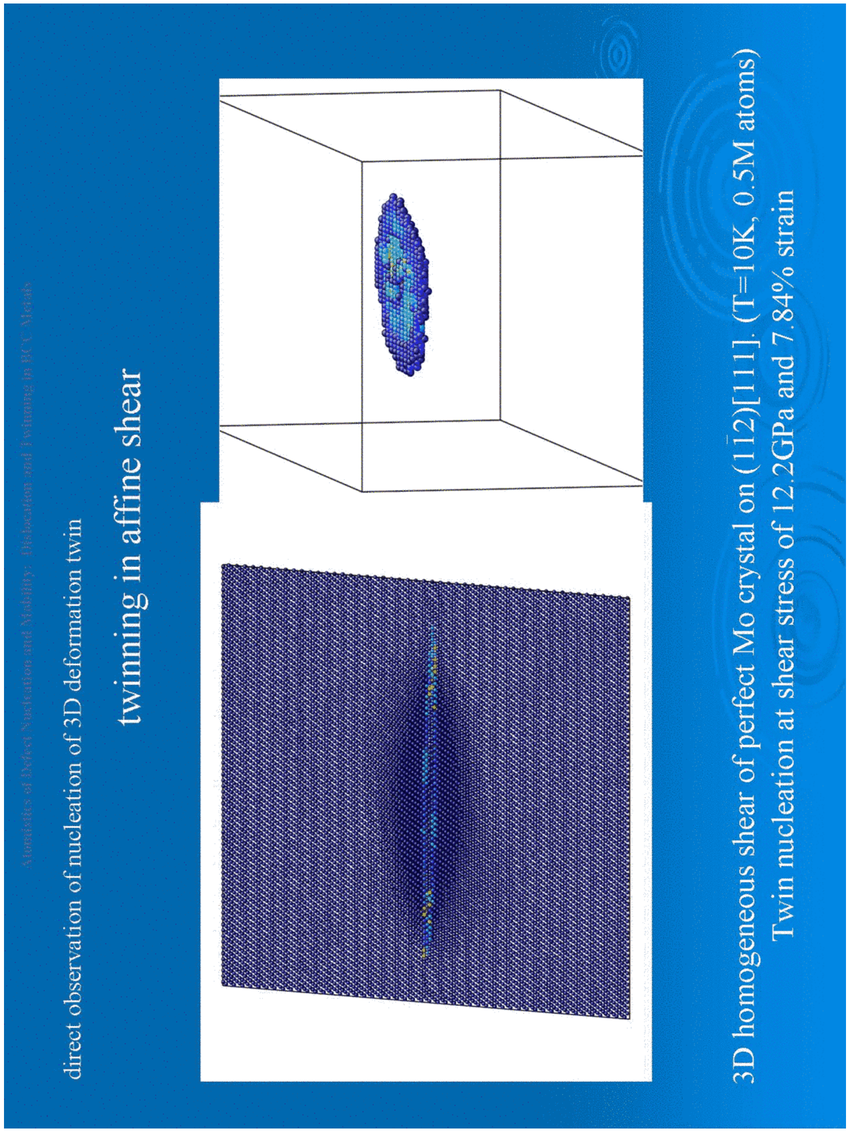
*VASP, US-GGA, 18 × 25 × 11 Monkhorst-Pack $\vec{k}$ points. †(25) Al at temperature T = 0 K, Cu at T = 298 K. ‡(26) GGA. §(27) Full-potential linearized augmented plane wave method (WIEN97 program), GGA. ‖(28) calculated from elastic constants at T = 0 K. ¶(4) LDA. #(29). **(30) LDA. ††(31) LDA. ‡‡(5) LDA, unrelaxed.

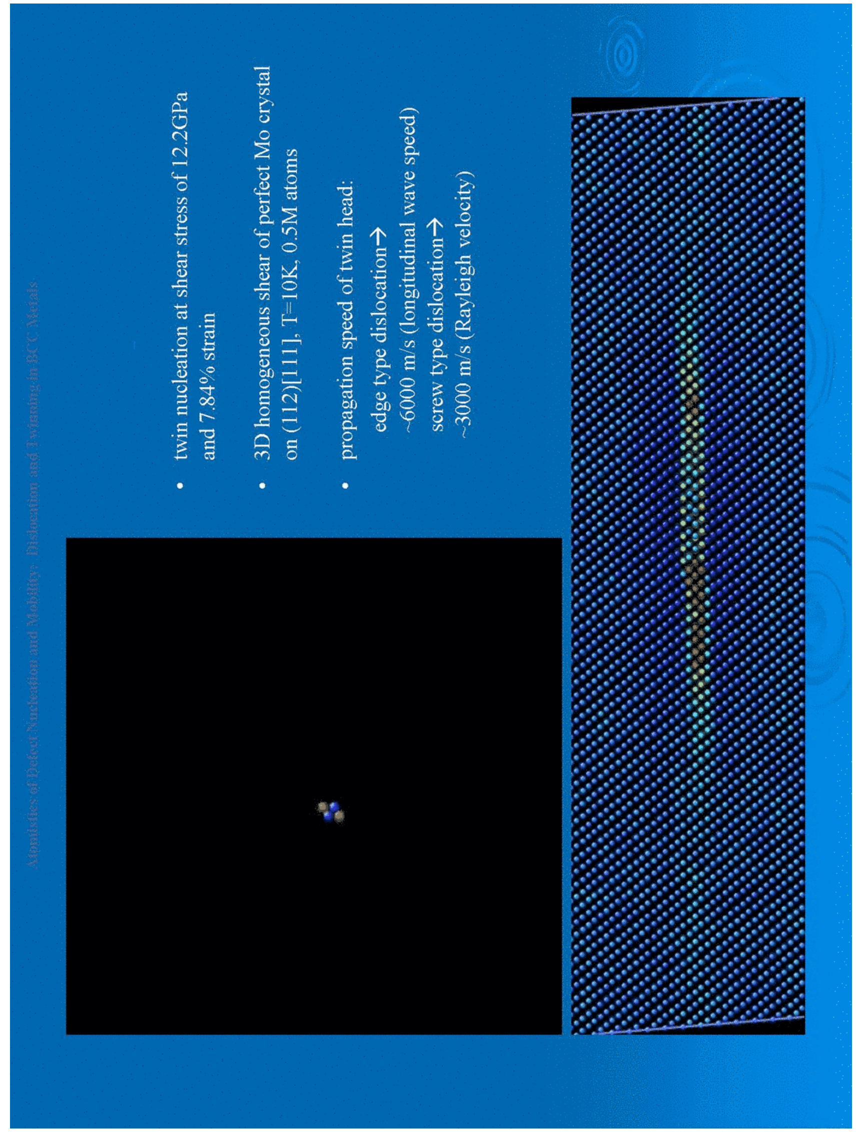
Pure Shear Stress-Displacement Curve

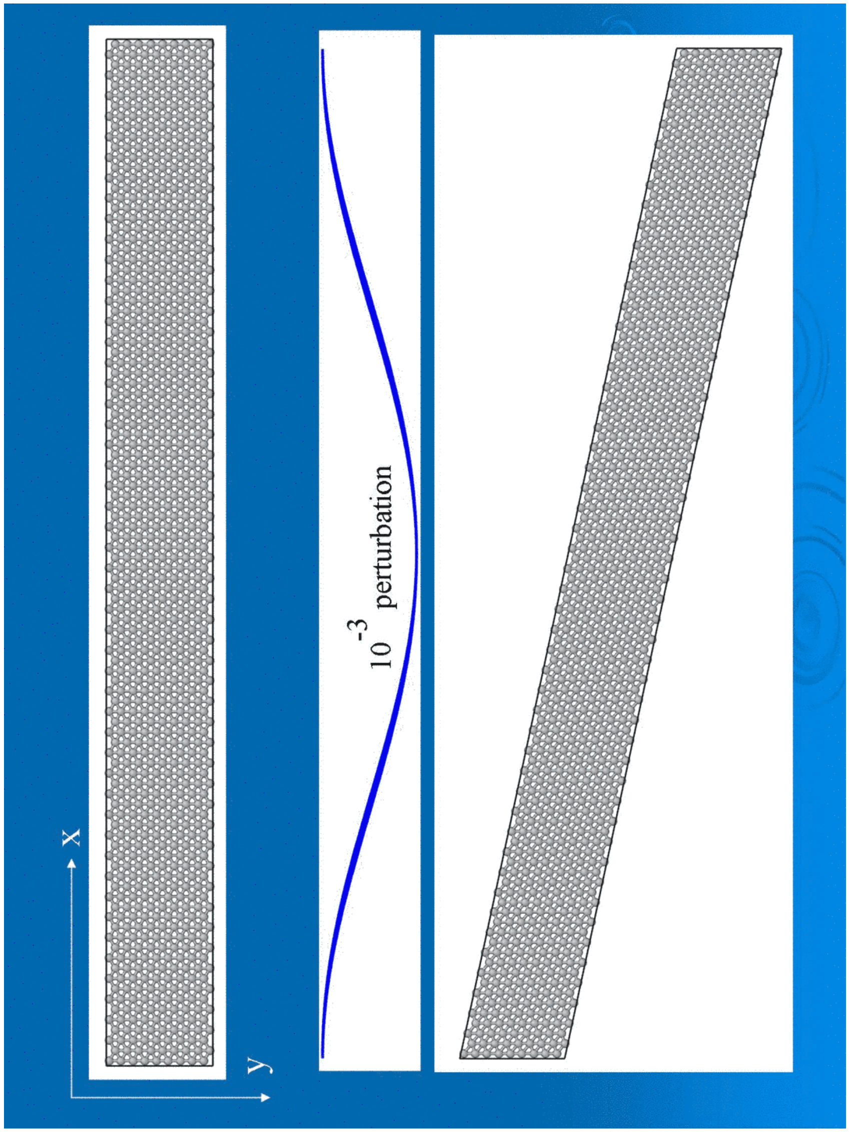


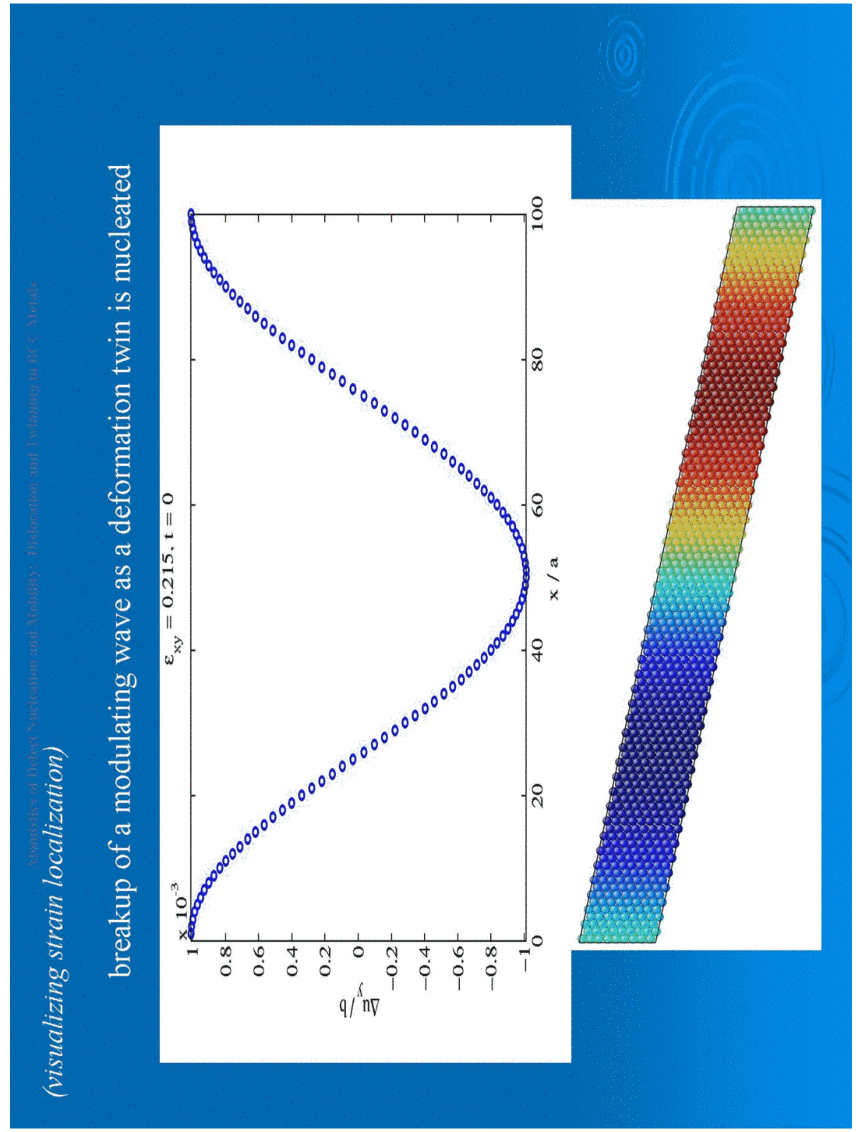

Charge density redistributions during affine shear in two fcc metals
(DFT calculations)
Cu
Al

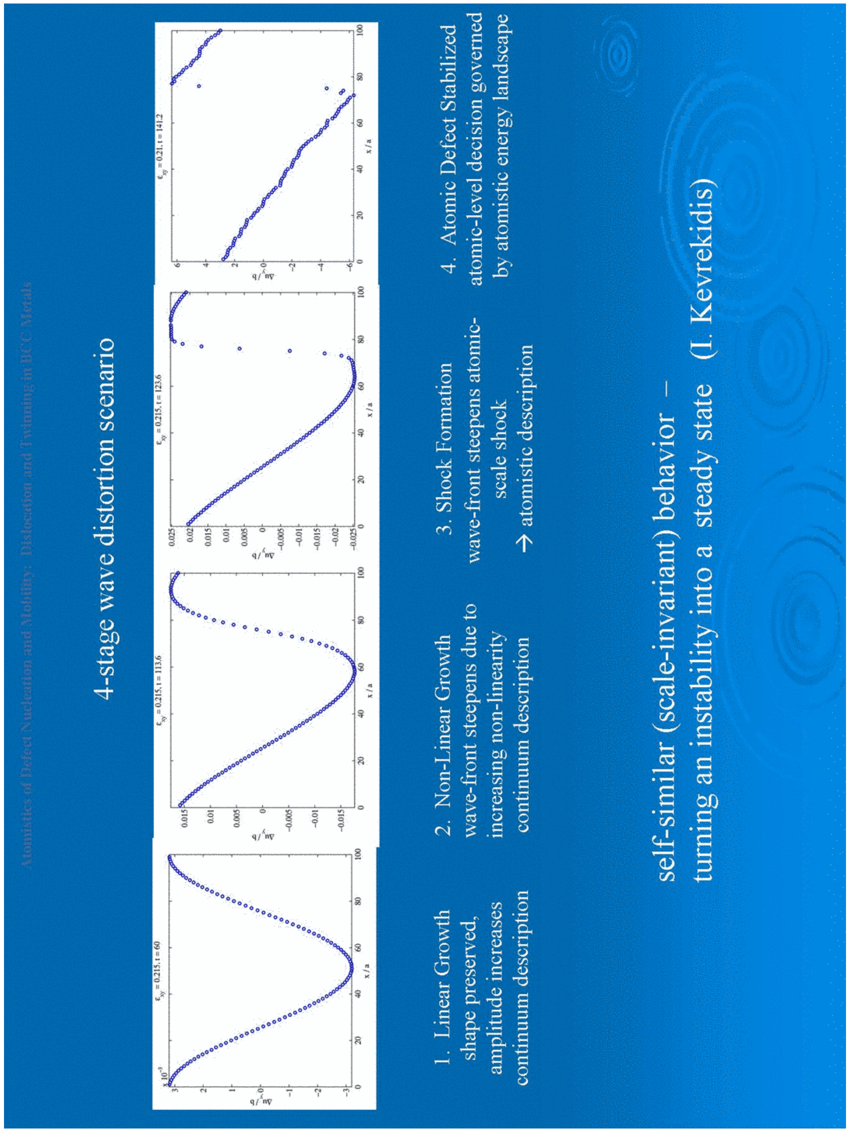

Twinning vs. Slip
A
$E_1(x)$
$E_2(x)$
$E_\infty(x)$
z=<111>
x=<11$\bar{2}$>
σ
• alternative plastic deformation mechanism in metals
• common in hcp metals, favored in bcc at low T
• operates at low T, high σ, high γ, limited slip systems
slip
twinning

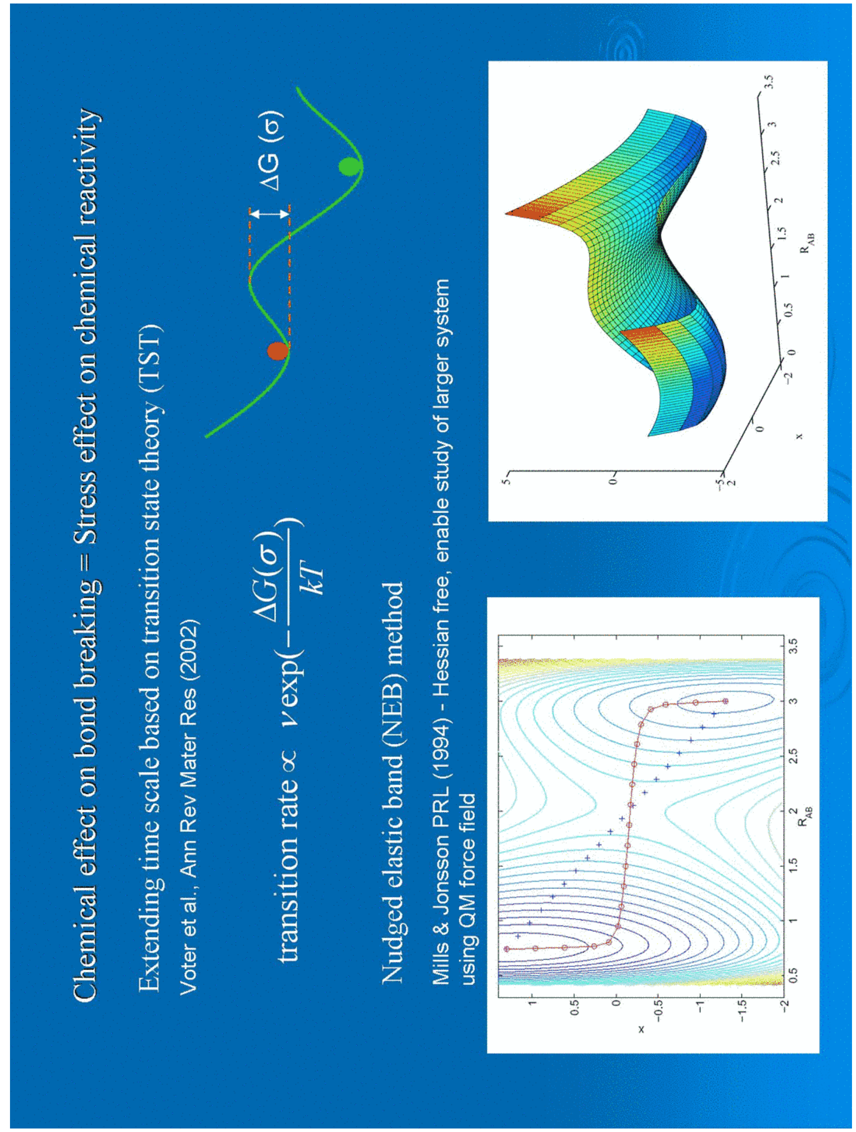

Atomistics of Defect Nucleation and Mobility: Dislocation and Twinning in BCC Metals
direct observation of nucleation of 3D deformation twin
twinning in affine shear
3D homogeneous shear of perfect Mo crystal on $(1\bar{1}2)[111]$. (T=10K, 0.5M atoms)
Twin nucleation at shear stress of 12.2GPa and 7.84% strain

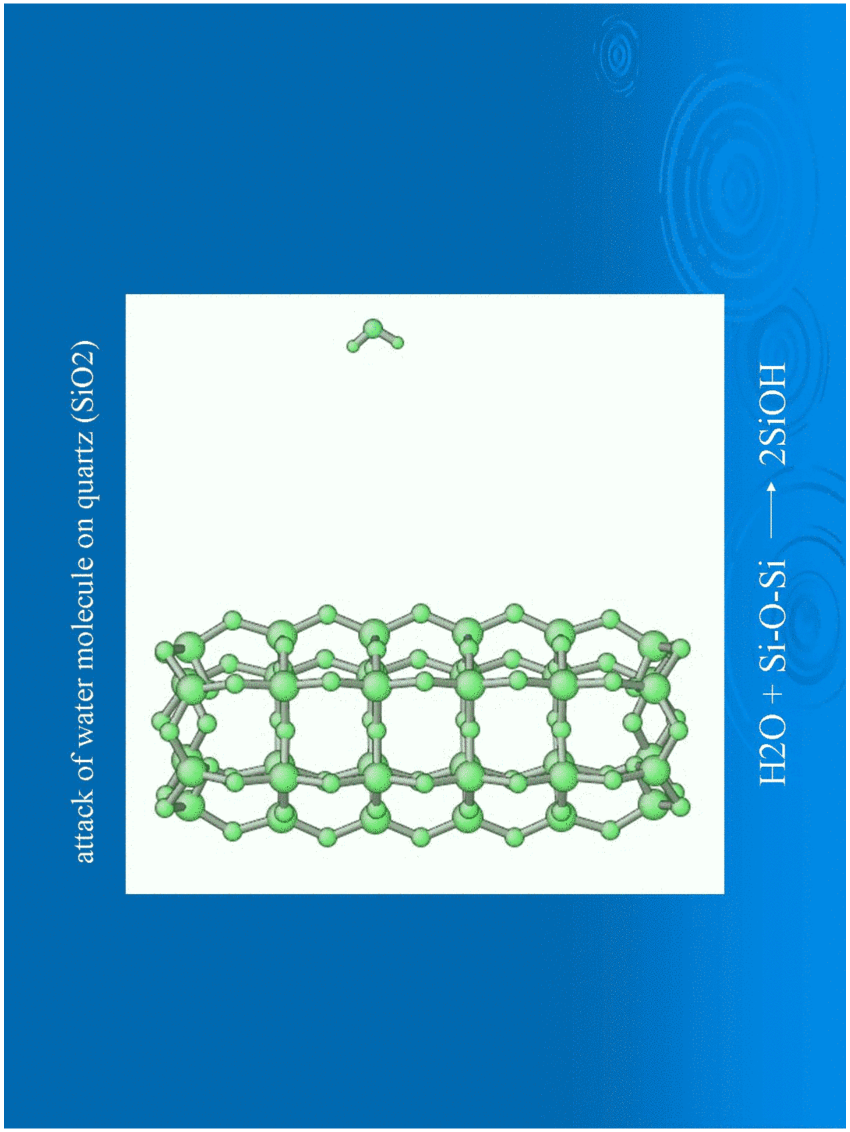

Atomistics of Defect Nucleation and Mobility: Dislocation and Twinning in BCC Metals
• twin nucleation at shear stress of 12.2GPa and 7.84% strain
• 3D homogeneous shear of perfect Mo crystal on (112)[111], T=10K, 0.5M atoms
• propagation speed of twin head:
edge type dislocation→
~6000 m/s (longitudinal wave speed)
screw type dislocation→
~3000 m/s (Rayleigh velocity)

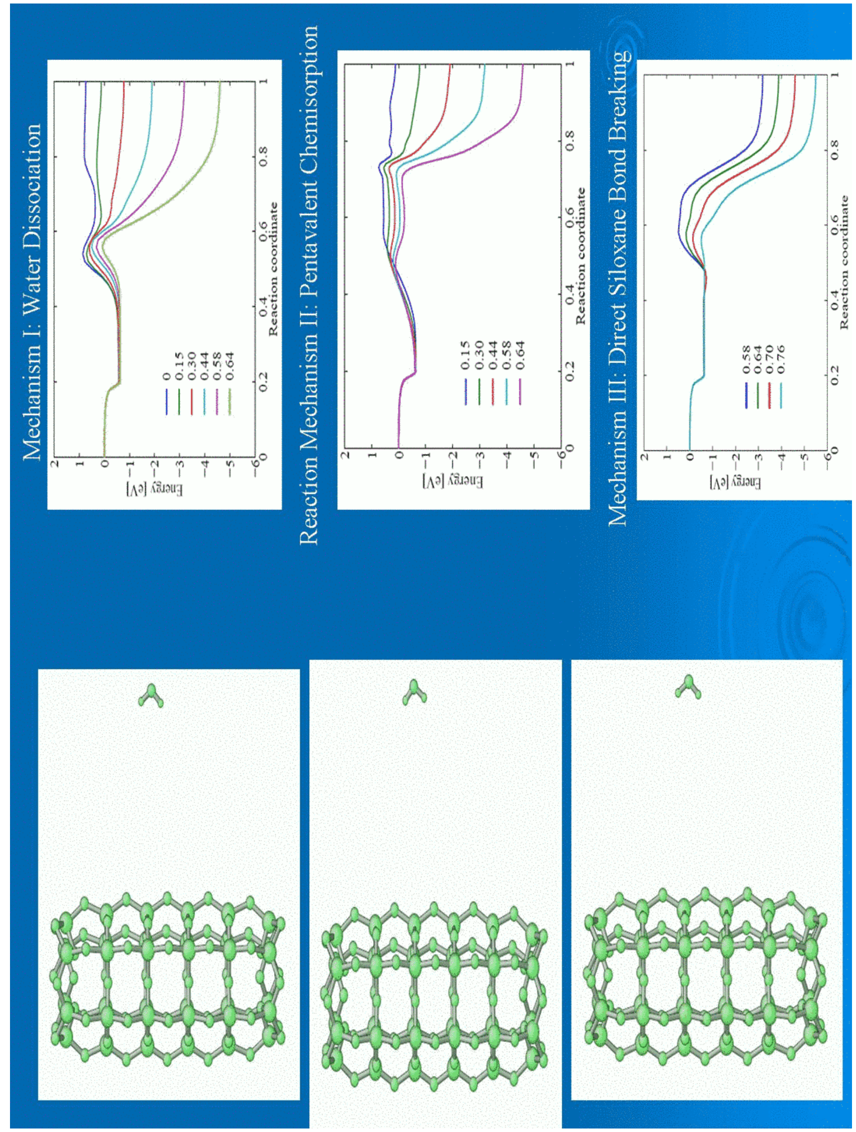

x
y
10^-3 perturbation


(visualizing strain localization)
breakup of a modulating wave as a deformation twin is nucleated
ε_xy = 0.215, t = 0
x 10^-3
Δu_y / b
x / a

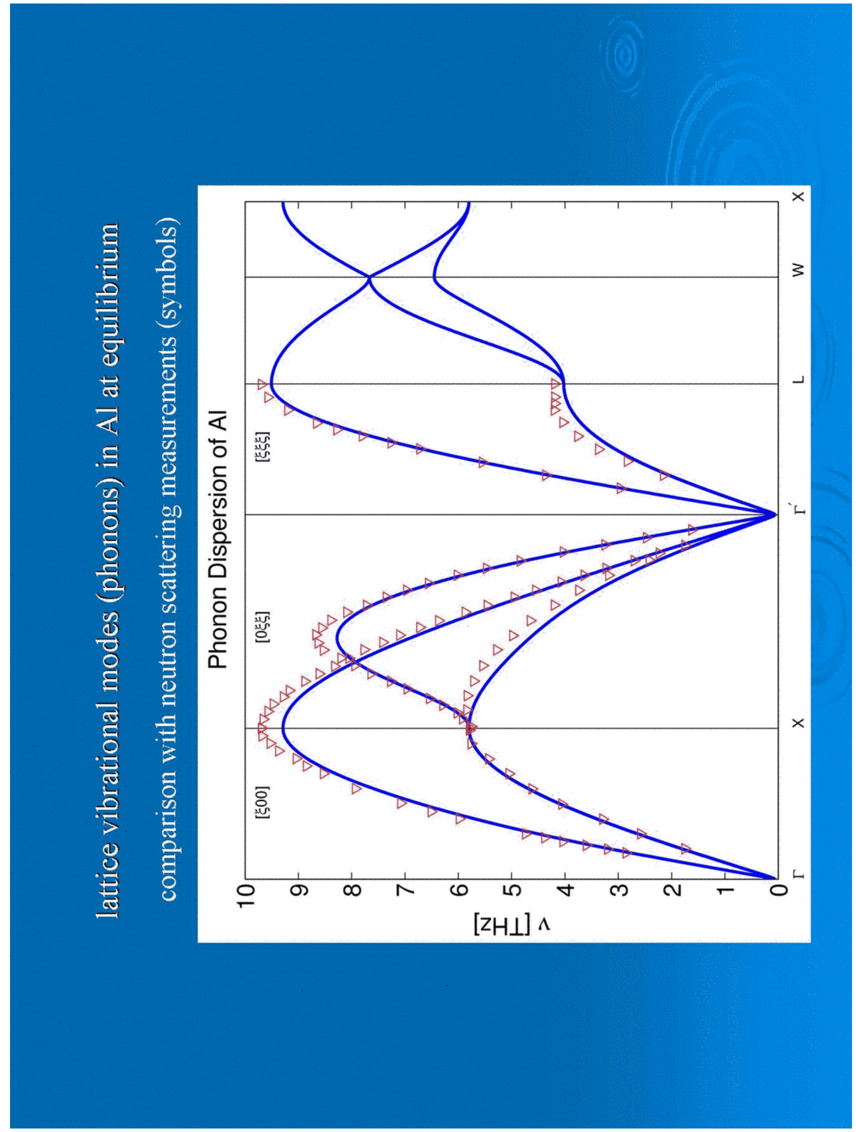

Atomistics of Defect Nucleation and Mobility: Dislocation and Twinning in BCC Metals
4-stage wave distortion scenario
1. Linear Growth
shape preserved,
amplitude increases
continuum description
2. Non-Linear Growth
wave-front steepens due to
increasing non-linearity
continuum description
3. Shock Formation
wave-front steepens atomic-
scale shock
→ atomistic description
4. Atomic Defect Stabilized
atomic-level decision governed
by atomistic energy landscape
self-similar (scale-invariant) behavior –
turning an instability into a steady state (I. Kevrekidis)


Chemical effect on bond breaking = Stress effect on chemical reactivity
Extending time scale based on transition state theory (TST)
Voter et al., Ann Rev Mater Res (2002)
ΔG (σ)
transition rate $\propto \nu \exp(-\frac{\Delta G(\sigma)}{kT})$
Nudged elastic band (NEB) method
Mills & Jonsson PRL (1994) - Hessian free, enable study of larger system
using QM force field

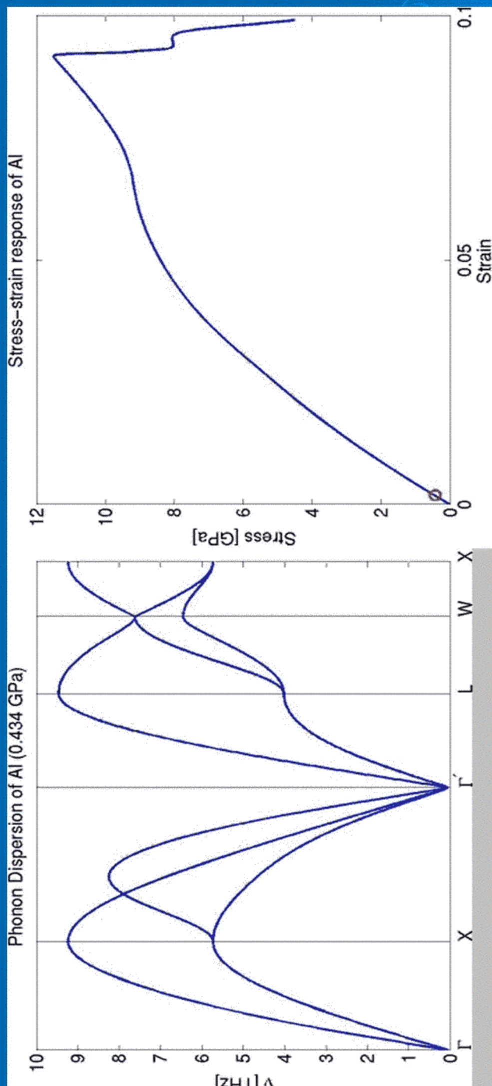

attack of water molecule on quartz (SiO2)
H2O + Si-O-Si ⟶ 2SiOH


Mechanism I: Water Dissociation
Reaction Mechanism II: Pentavalent Chemisorption
Mechanism III: Direct Siloxane Bond Breaking
Energy [eV]
Reaction coordinate


Some reasons for atomistics …
Shear localization
Bond strain ~ Bond reactivity (mechanics + chemistry)
Soft-mode scenario of structural instability


lattice vibrational modes (phonons) in Al at equilibrium
comparison with neutron scattering measurements (symbols)
Phonon Dispersion of Al
ν [THz]
0
1
2
3
4
5
6
7
8
9
10
Γ
X
Γ´
L
W
X
[00ξ]
[ξξ0]
[ξξξ]

phonon softening in a highly-strained lattice --
correspondence between soft modes and critical deformation behavior



phonon dispersion calculations (finite stress)

Direct MD Simulation at 10K

Collaborators:

Ju Li, Ting Zhu, Jinpeng Chang, Shigenobu Ogata,
Krystyn Van Vliet, Subra Suresh

support: **NSF, AFOSR, Honda, DARPA, LLNL**