Multi-algorithm Methods for Multiscale Simulations
January 14 - 17, 2004, Hilton Gardens Inn, Livermore, CA

(Atomistic Measures of Materials Strength and Reactivity)
Shear Localization in Solids: Simulation and Analysis

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Results to motivate algorithms
(including analysis and visualization)

Critical behavior (instability)

Common grounds –
strain field (solid)
flow field (liquid)

Chemical reactivity of stressed bonds

3 case studies in shear deformation --

a central issue is the sudden localization of shear strain in homogeneous deformation

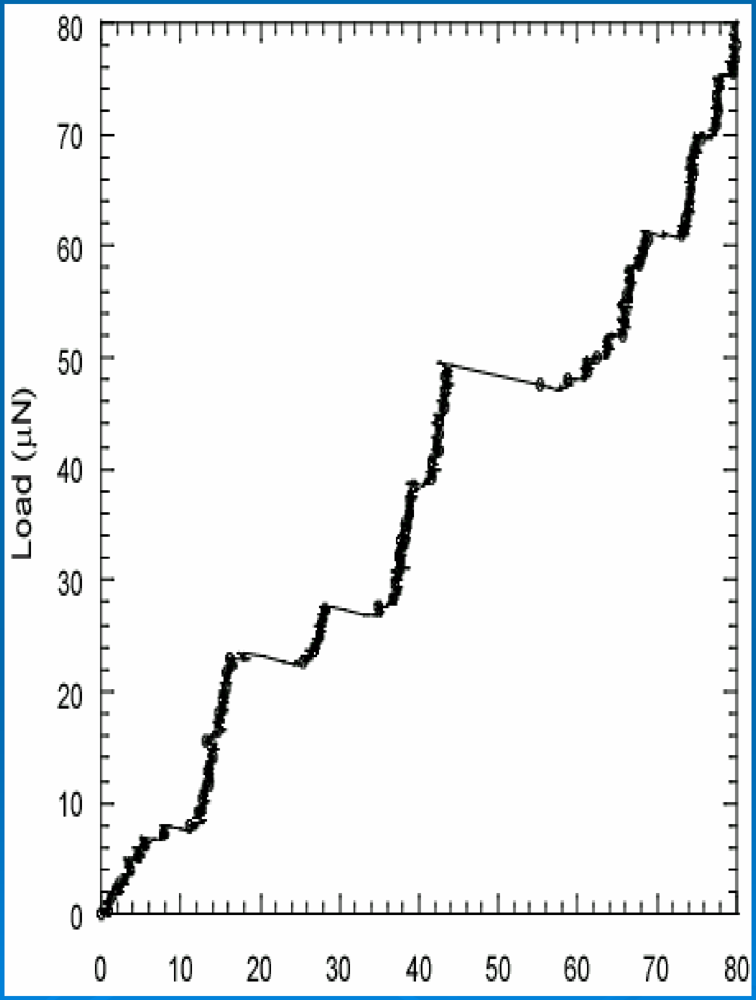
Dislocation nucleation in nano-indentation

Ideal shear strength of metals (Al and Cu)

Homogeneous nucleation of deformation twinning

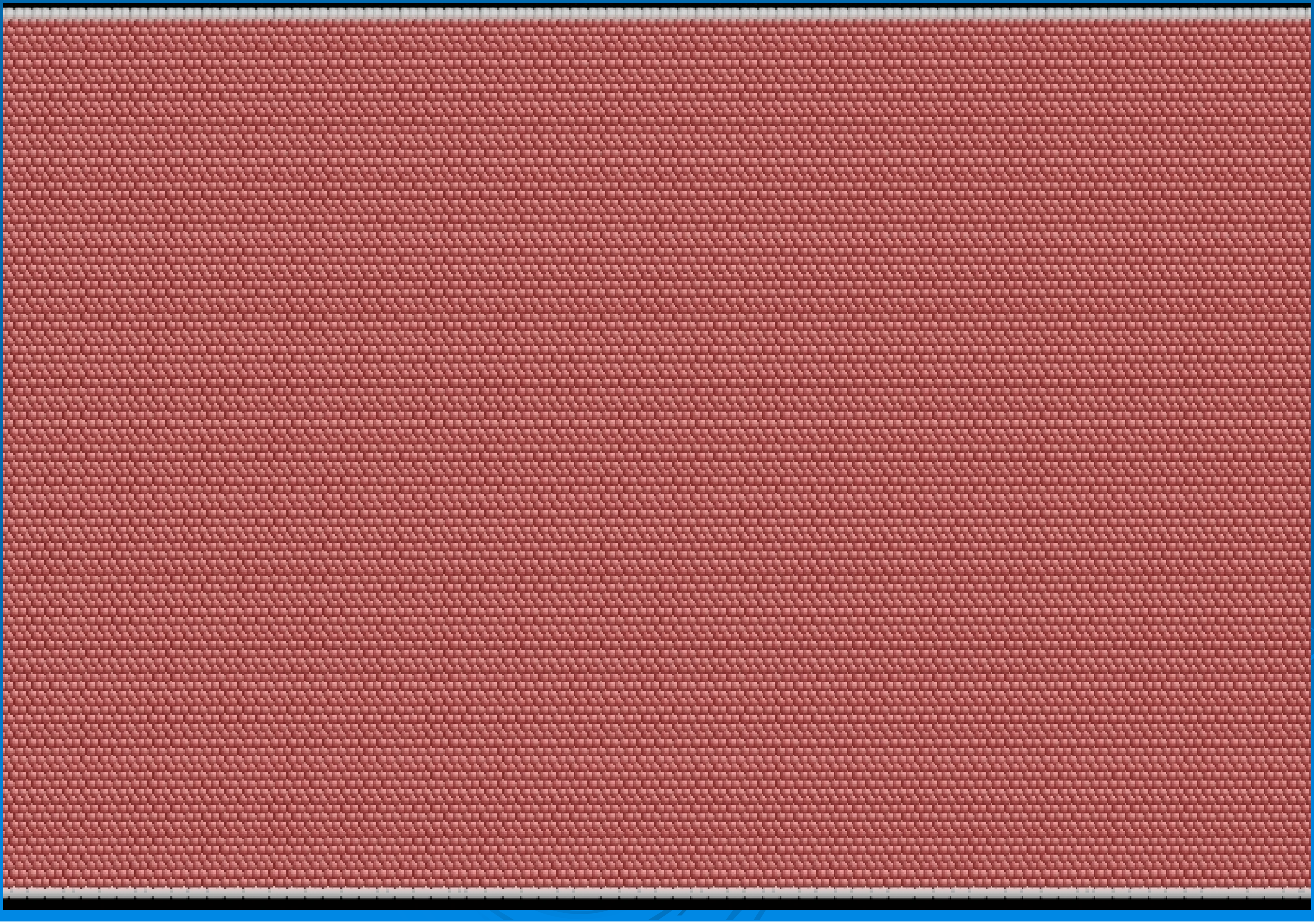
Water reaction with a silica nanorod

A typical load-displacement measurement in nano-indentation



depth [nm]

Nanoindentation in 2D (MD)
coordination number encoding



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 --

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

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

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

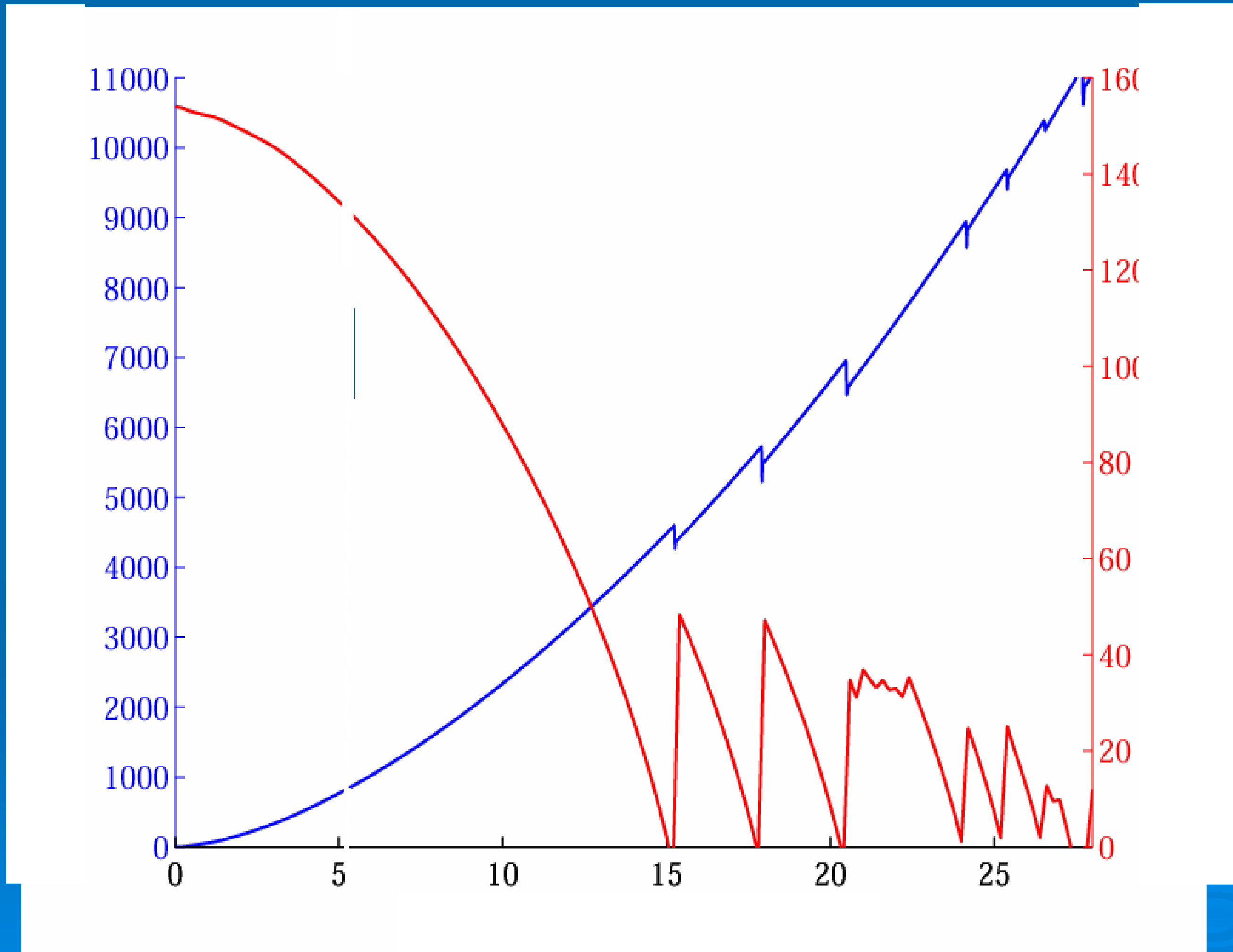
$\Lambda(w,k) = (C_{ijkl} w_i w_k + \tau_{jl}) k_j k_l = 0$ is the condition for defect nucleation

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

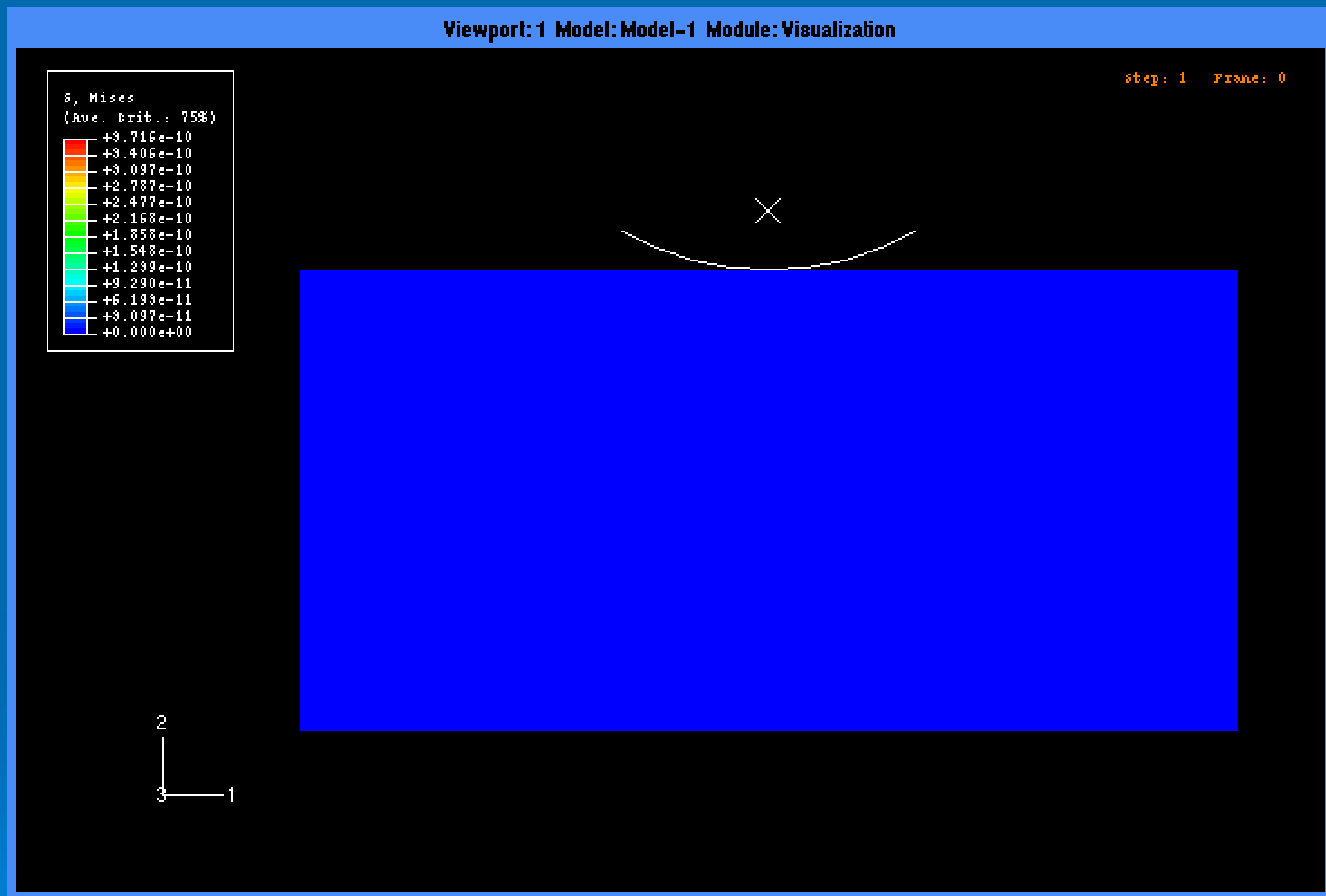
J. Li et al. Nature 2002, K. Van Vliet et al. Phys Rev 2002, Z. Ting et al. J Mech Phys Solids 2004

Load vs. indentation depth (displacement controlled)

Comparison of MD indentation response with stability criterion predication

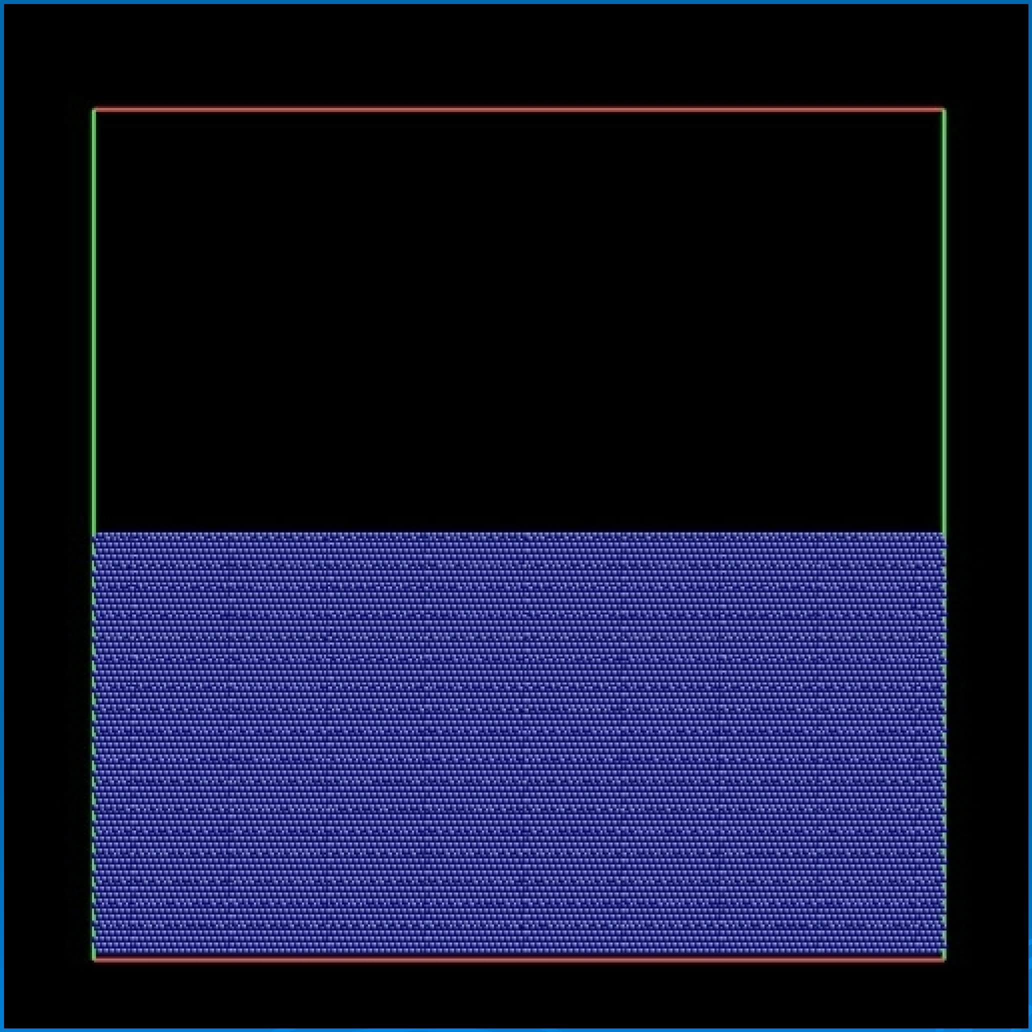


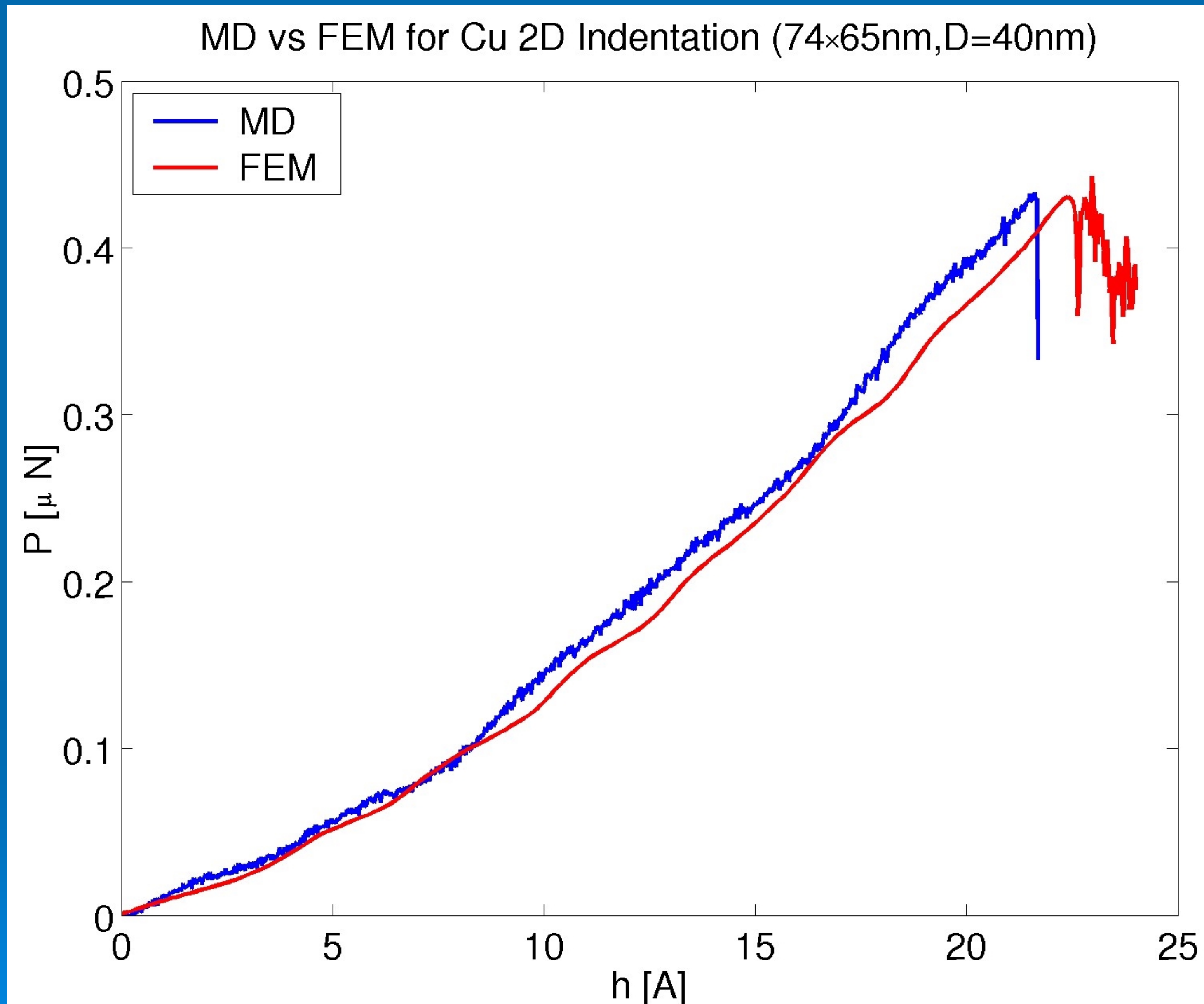
IPFEM – Cu (2D)

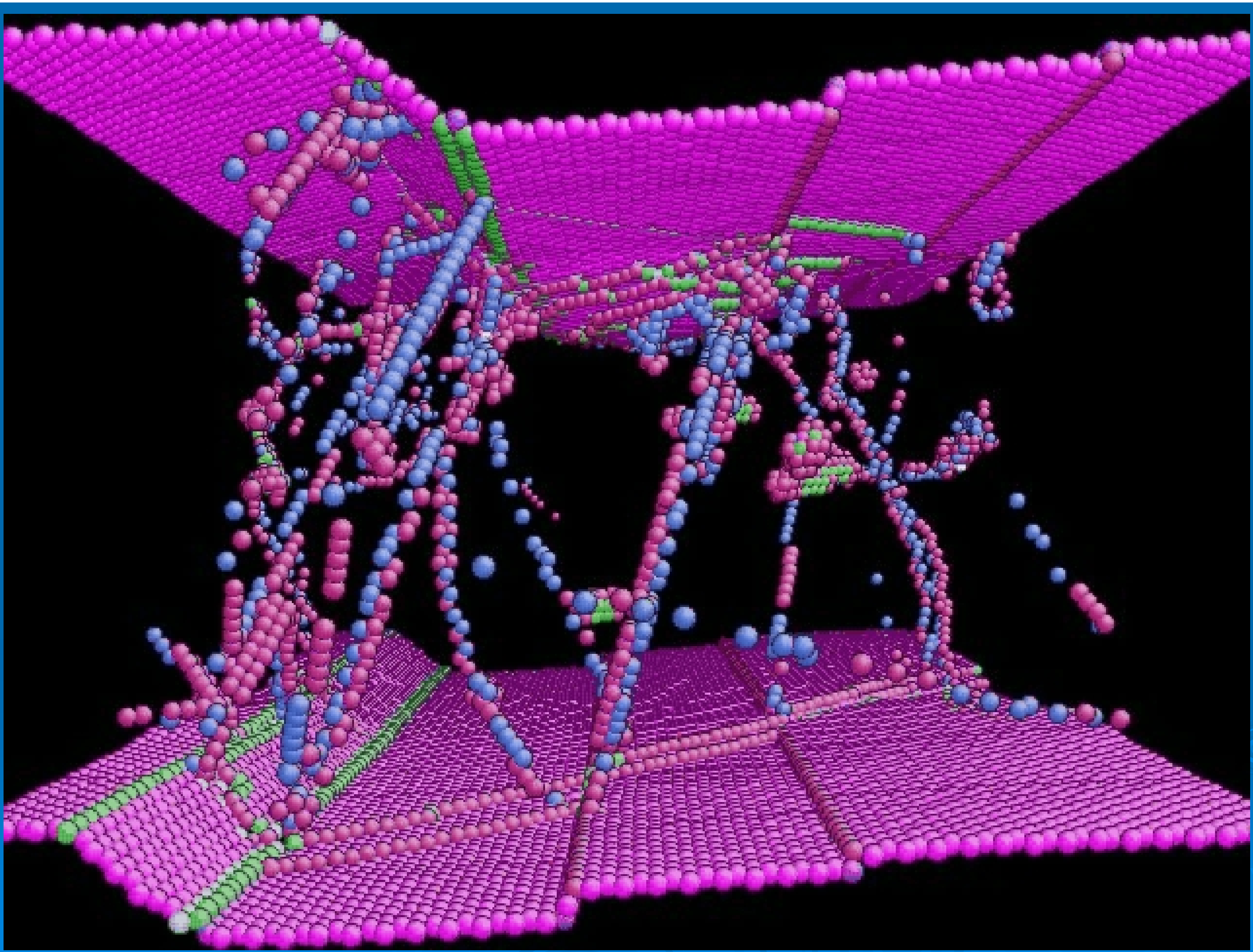


Viewport: 1 Model: Model-1 Module: Visualization
S, Mises
(Ave. Crit.: 75%)
+3.716e-10
+3.406e-10
+3.097e-10
+2.787e-10
+2.477e-10
+2.168e-10
+1.858e-10
+1.548e-10
+1.239e-10
+9.290e-11
+6.193e-11
+3.097e-11
+0.000e+00
Step: 1 Frame: 0
2
3
1

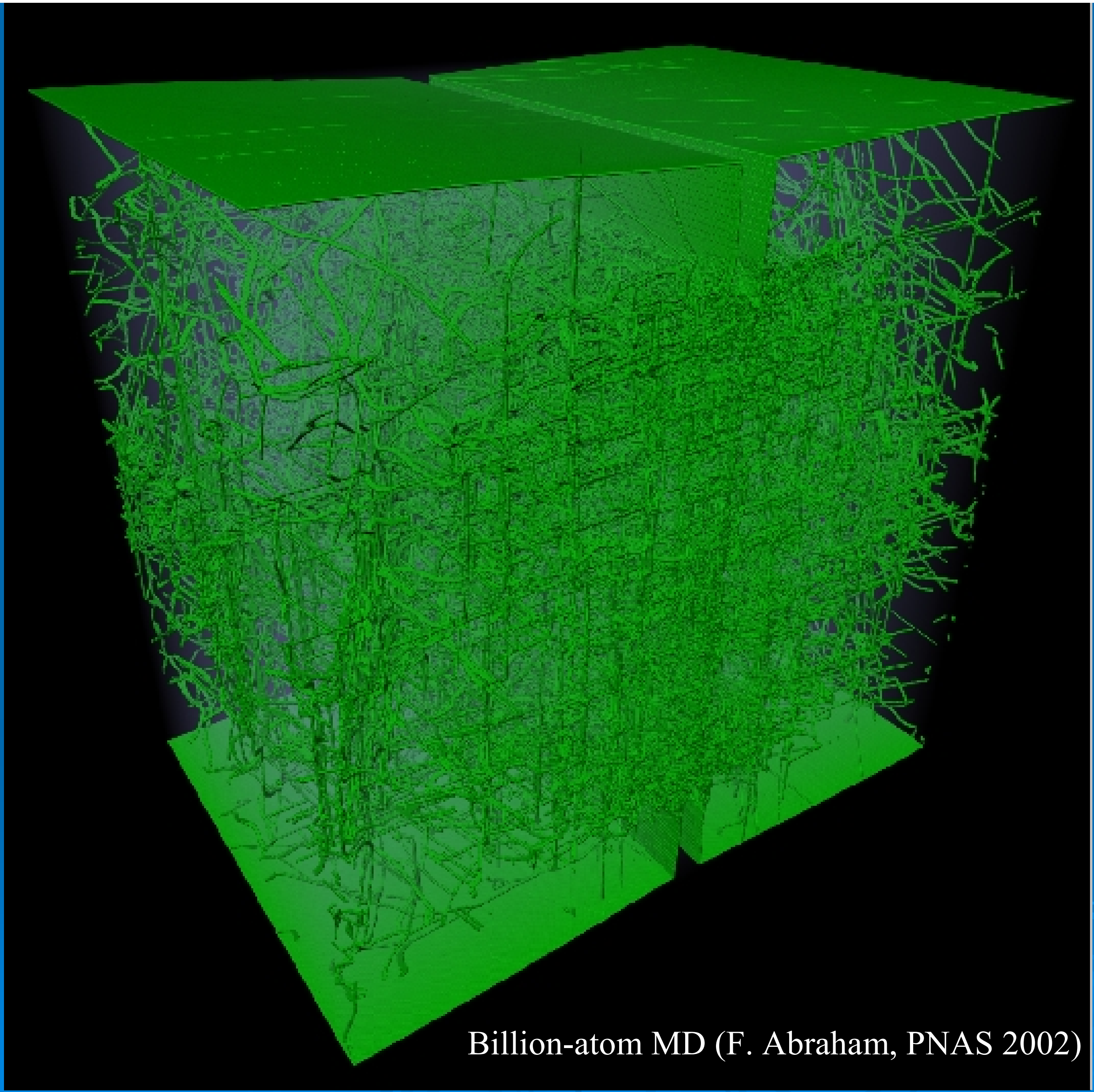
MD Cu (2D) – Mises stress




MD vs FEM for Cu 2D Indentation (74×65nm,D=40nm)
MD
FEM
P [μ N]
0
0.1
0.2
0.3
0.4
0.5
0
5
10
15
20
25
h [A]



Ju Li et al., Nature 2002



Billion-atom MD (F. Abraham, PNAS 2002)

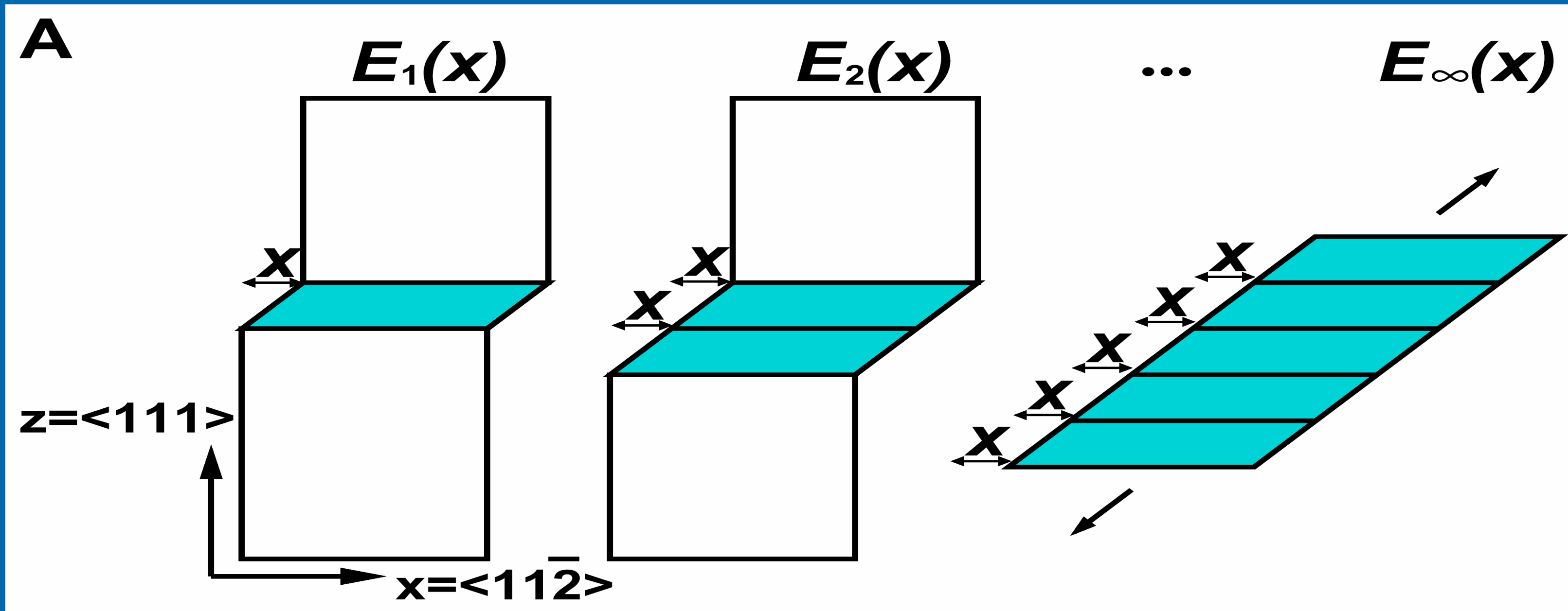
Ideal Pure Shear Strength of Aluminum and Copper

Although Al has a smaller modulus in {111}<112> shear than Cu, its ideal shear strength is greater because of a more extended deformation range

This can be demonstrated by electronic structure calculations, and the results explained in terms of the bonding characteristics of these two metals

Ogata et al., Science **298**, 807 (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 ♑📫

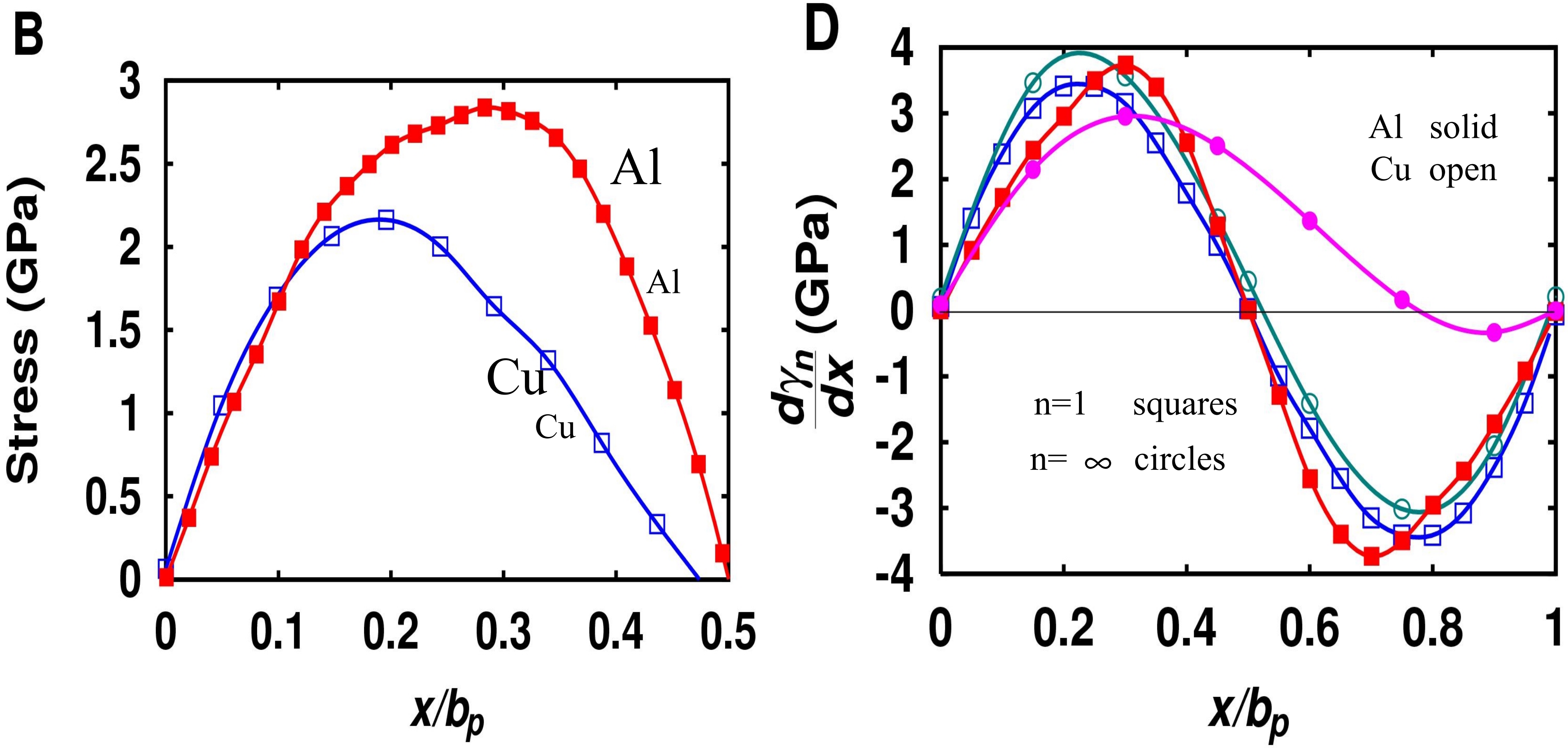
surface

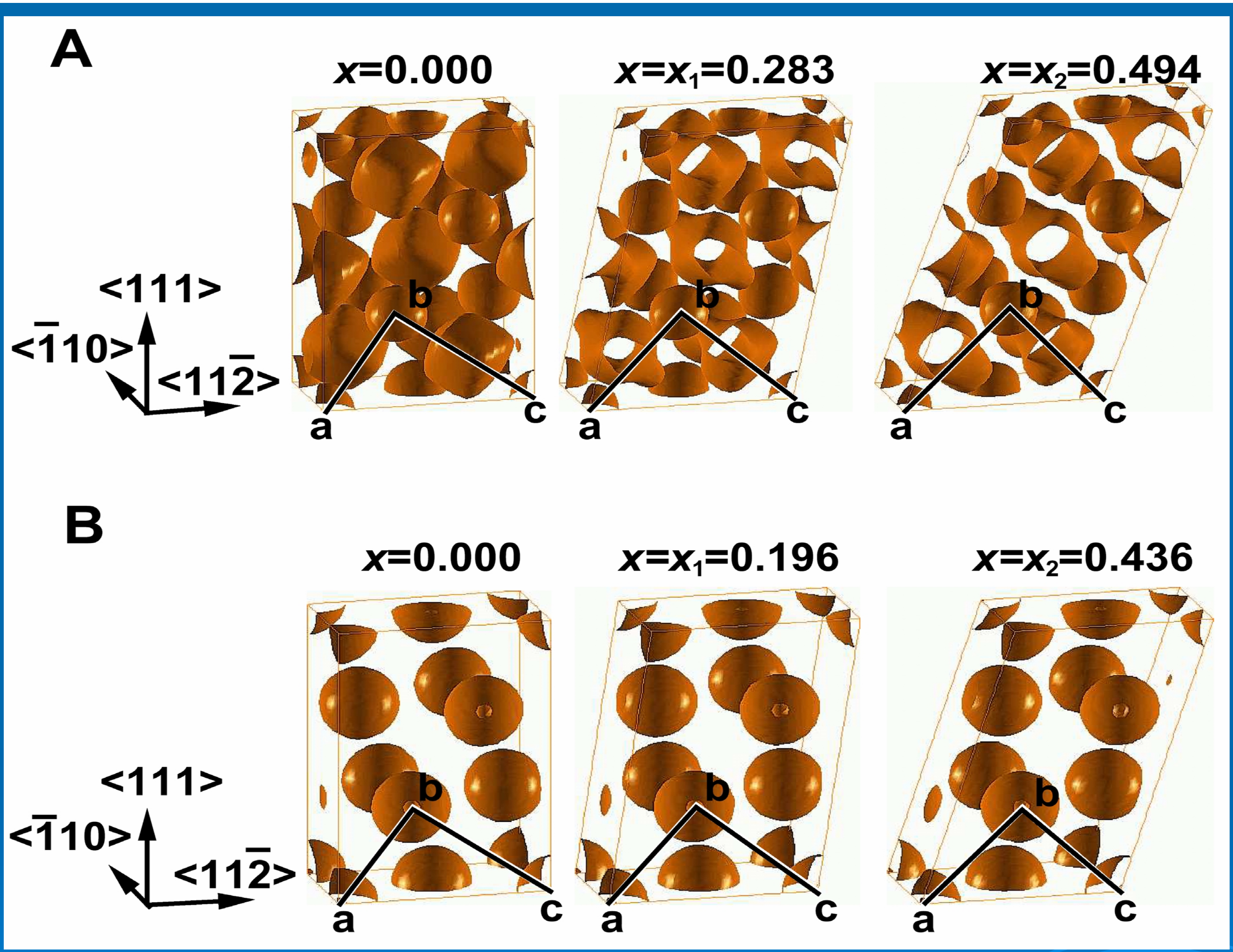
$\gamma_1(b_p) = \gamma_{SF}$: intrinsic stacking fault energy

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

Rice-Thomson criterion: ratio of g_{US} to g_S (surface energy) controls material ductility

Pure Shear Stress-Displacement Curve



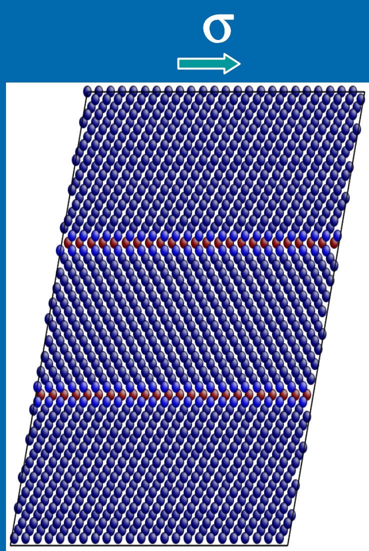


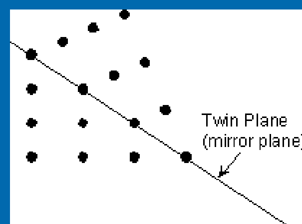
Al: hinged-rod, directional bonding, frustration

Cu: sphere-in-glue, bond can distort and redistribute within volume

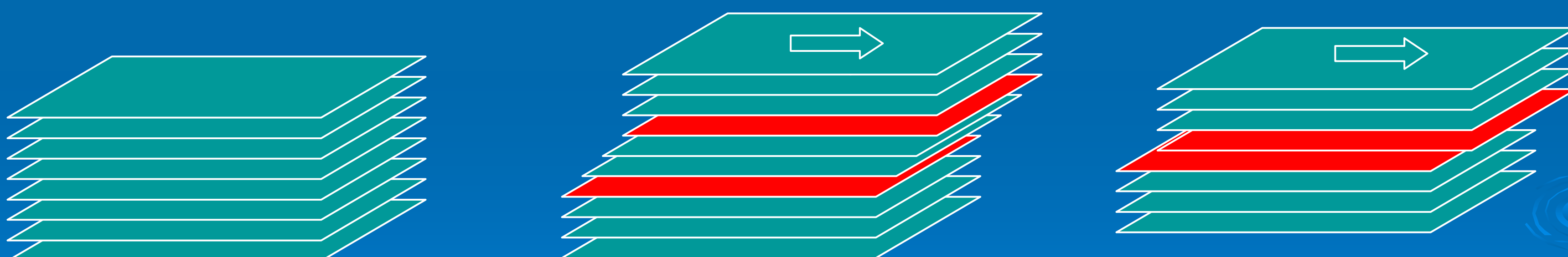
Direct observation of 3D twinning

Twinning vs. Slip





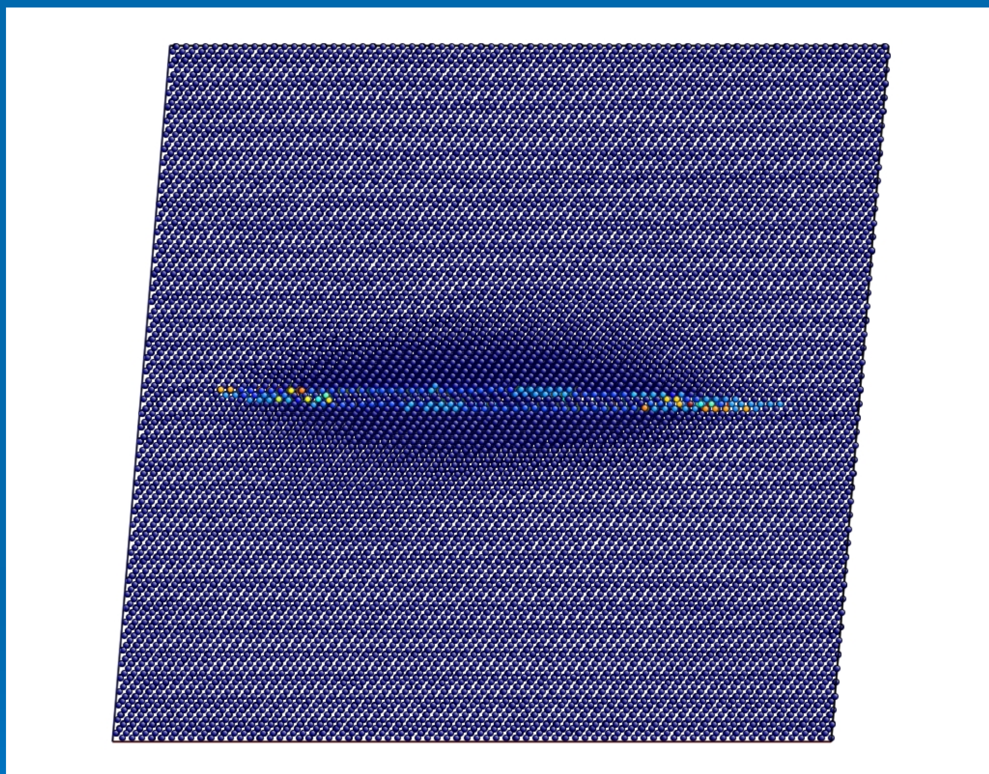
- Alternative plastic deformation mechanism in metals (vs. dislocation-based slip)
- Regular, symmetrical lattice reorientation
- Common in hcp metals, favored in bcc at low T
- Operates at low T, high σ, high $\dot{\gamma}$, limited slip systems
- Deformation twin (hcp,bcc) vs. annealing twin (fcc)

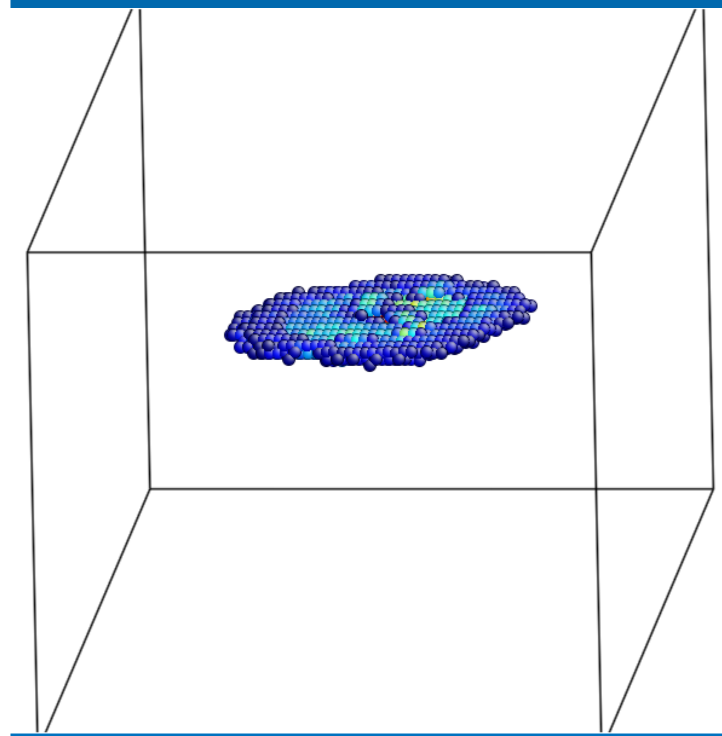


	Twinning vs.	***Slip:***
atomic displacemnet:	fractional atomic spacing	Burgers vector
lattice orientation:	change	unchanged

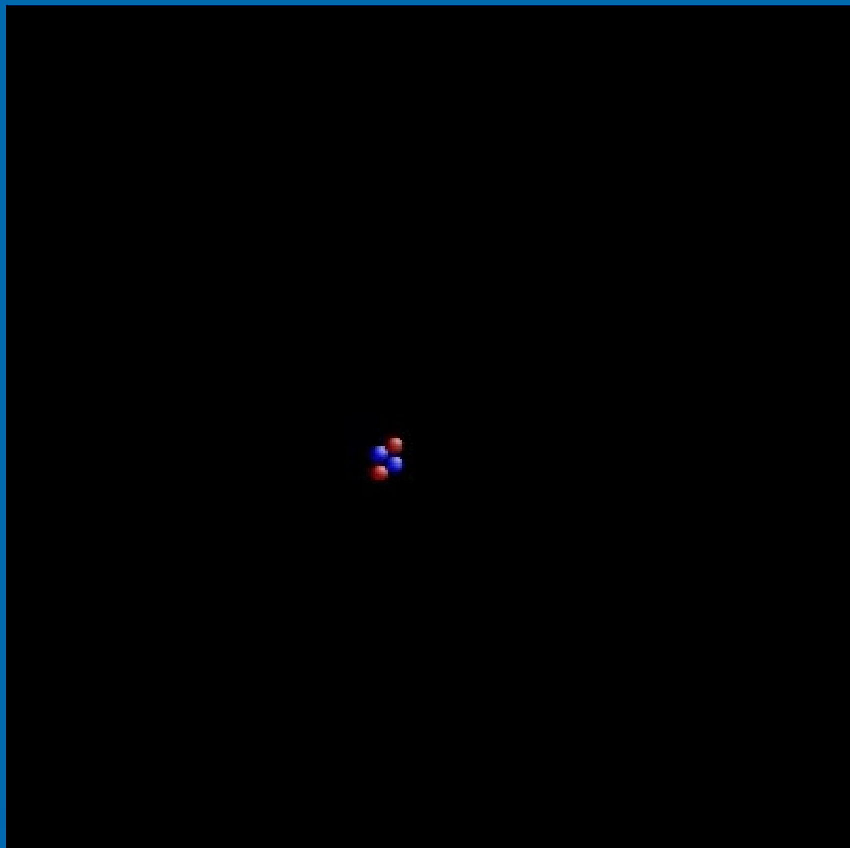
Direct observation of 3D twinning

Twinning in 3D Shear

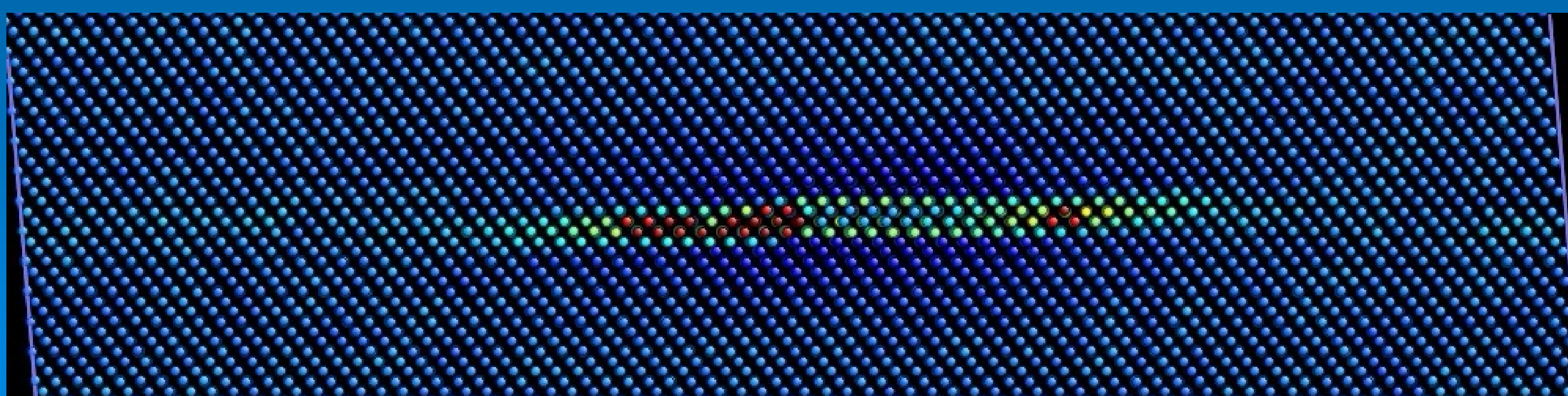




3D homogeneous shear of perfect Mo crystal on $(11\bar{2})[111]$. (T=10K, 0.5M atoms)
Twin nucleation at shear stress of 12.2GPa and 7.84% strain



- Twin nucleation at shear stress of 12.2GPa and 7.84% strain
- Propagation speed of twin head:
- 3D homogeneous shear of perfect Mo crystal on (112)[111]. (T=10K, 0.5M atoms)
  Edge type dislocation→
  ~6000 m/s (longitudinal wave speed)
  Screw type dislocation→
  ~3000 m/s (Rayleigh velocity)

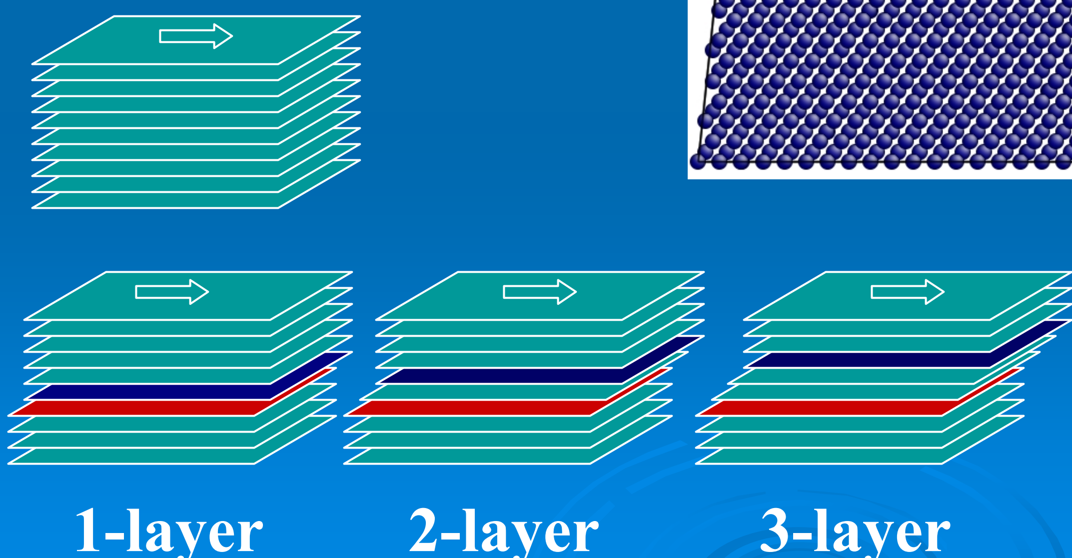


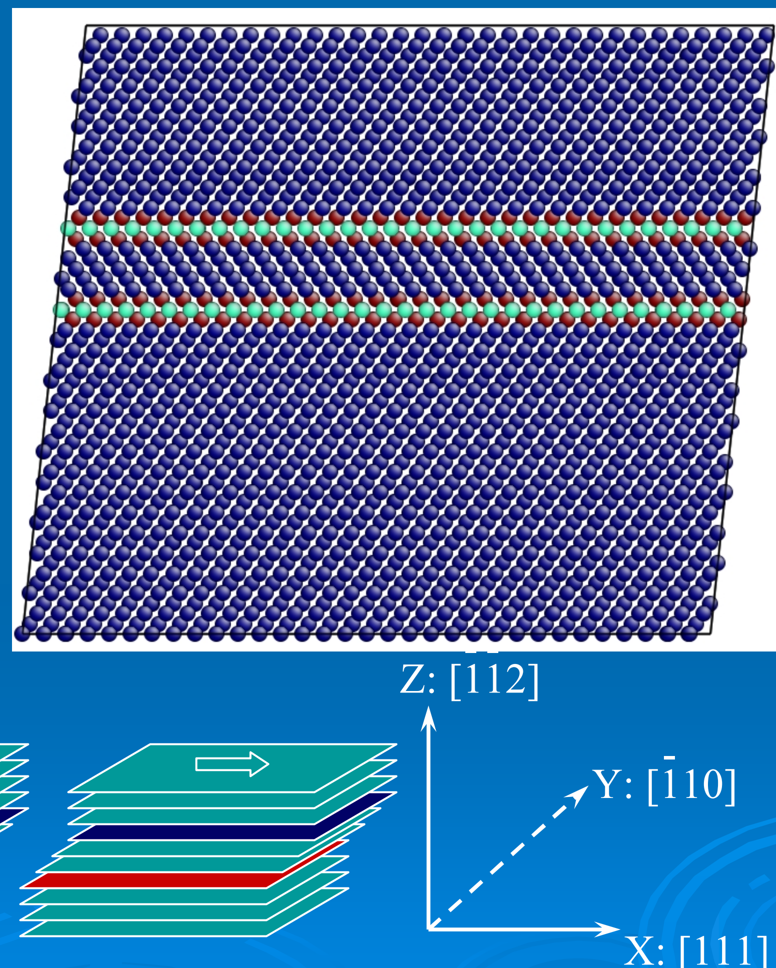
1-D Chain analysis

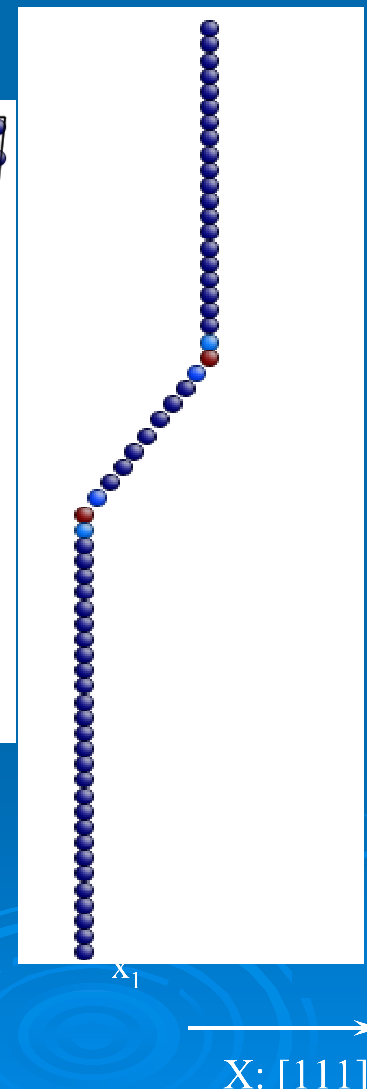
1-D Chain Model

$$\Delta x_i = x_i - x_{i-1}$$

$$E_{1D-Chain} = \gamma(\Delta x_1, \Delta x_2, \ldots, \Delta x_i, \ldots)$$





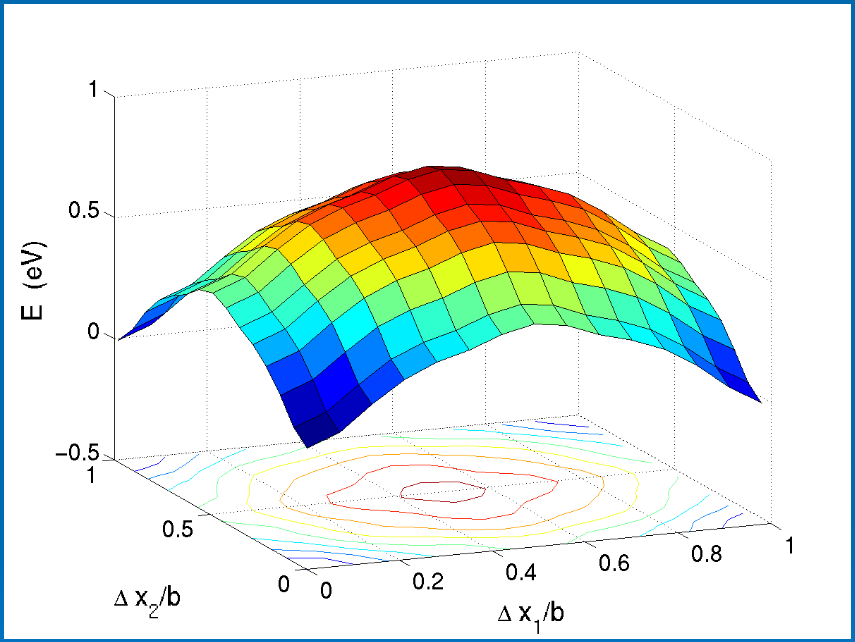


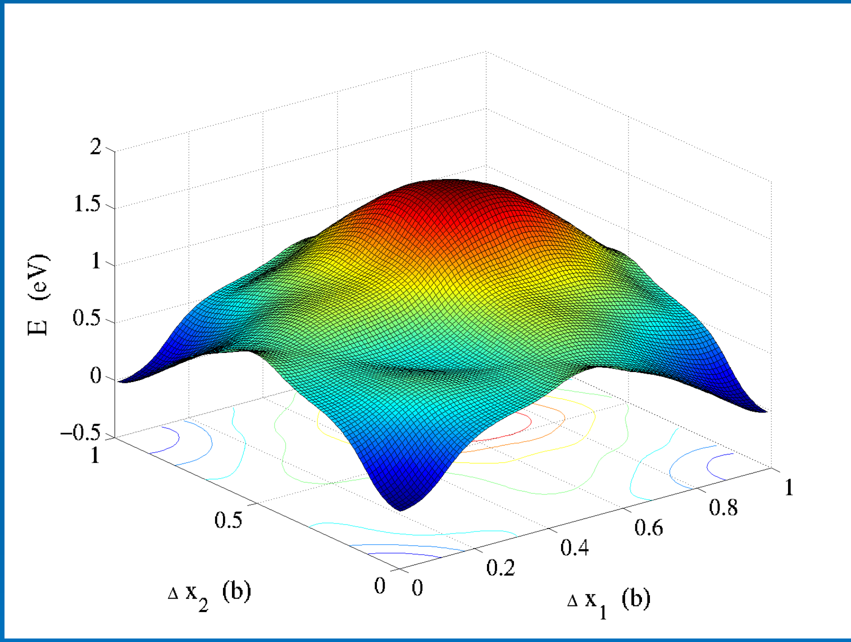
J. Chang, PhD Thesis, MIT, 2004

1-D Chain analysis

Two-Layers: Twin Embryo

$E(0..0, \Delta x_1, \Delta x_2\ 0..0)$



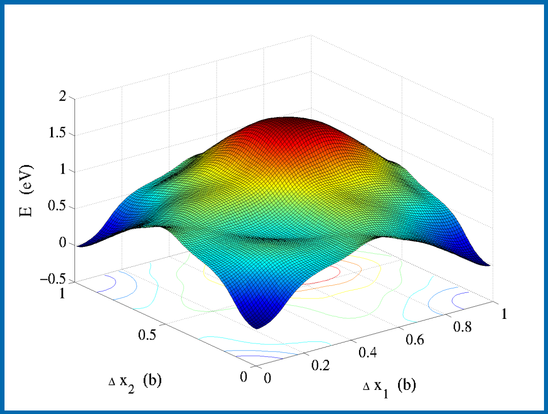


On (110)[111]:
Energy minima only at integer lattice spacings

On (112)[111]:
Energy minimum at (b/3, b/3): 2-layer twin

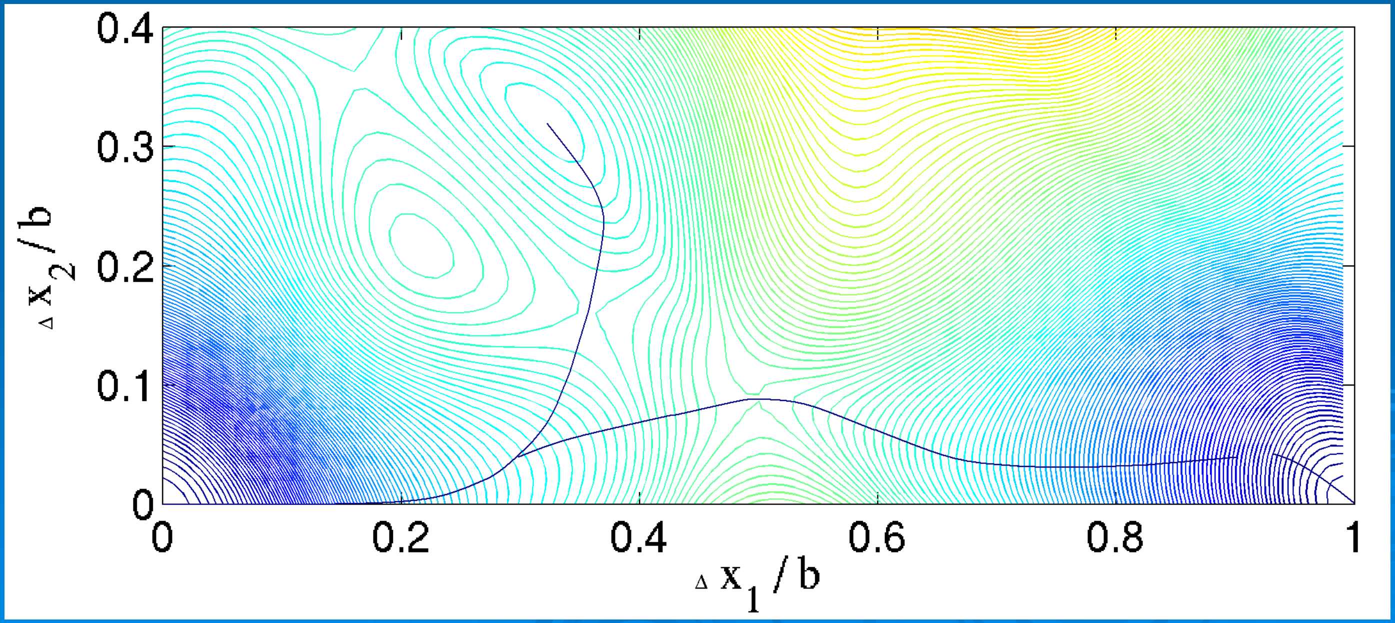
1-D Chain analysis

Energy Contour & Min-E Path

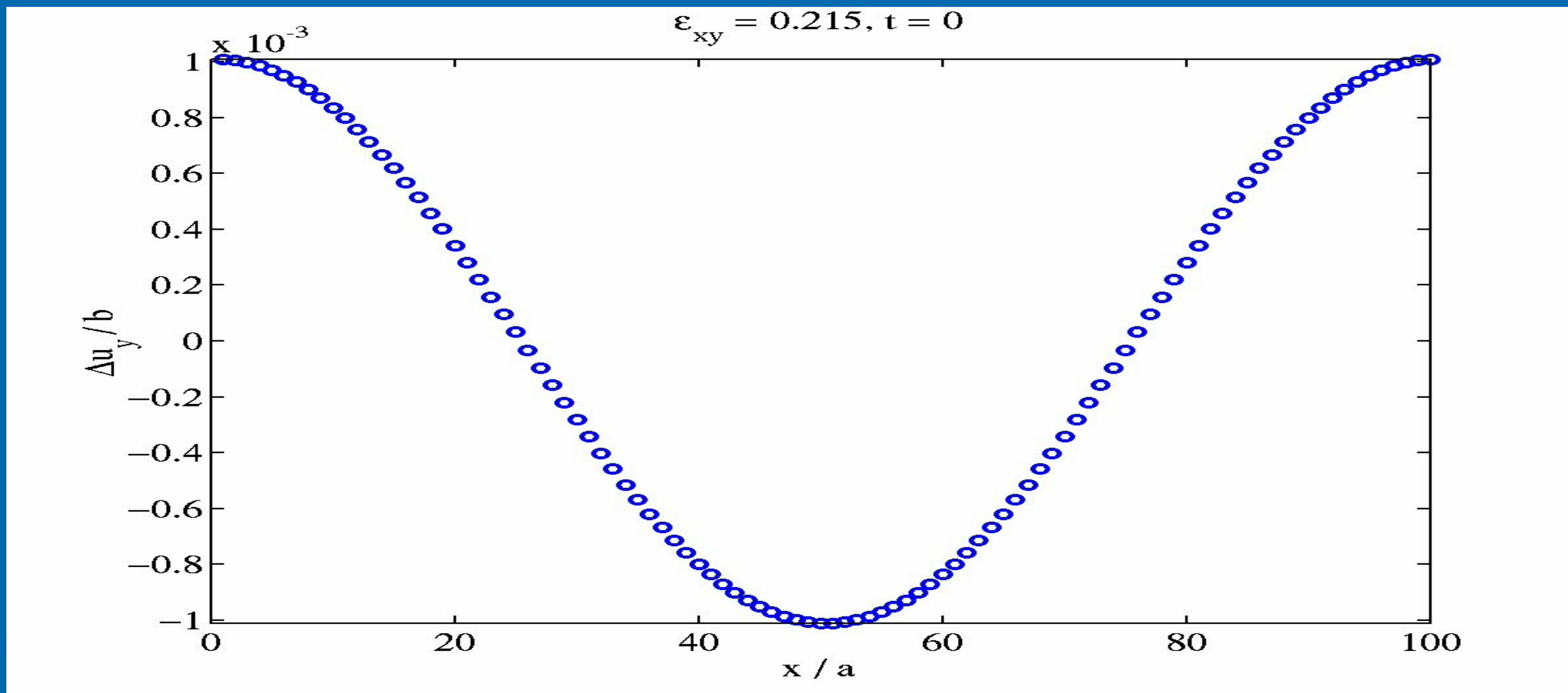


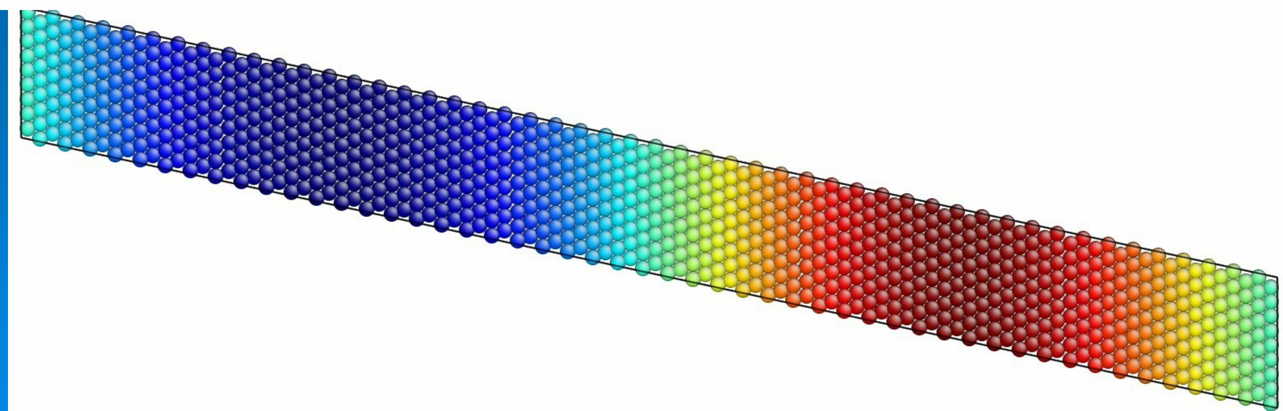
- Path bifurcation at ~(b/3,0)
- Energy barrier for twinning
  γ_{twin}=0.17 eV/A
- Energy barrier for slip
  γ_{us}=0.19 eV/A

Twinning Criterion: $\gamma_{twin} < \gamma_{us}$



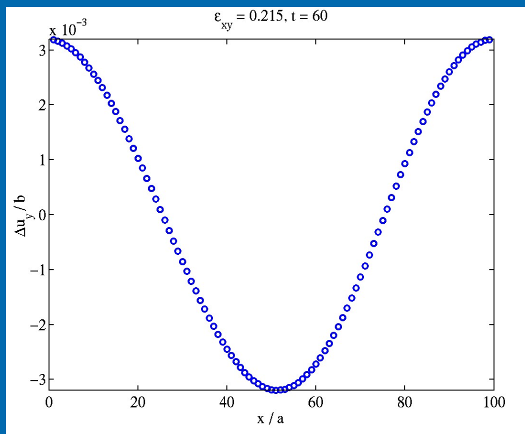
How does a continuum wave evolve into an atomic defect?





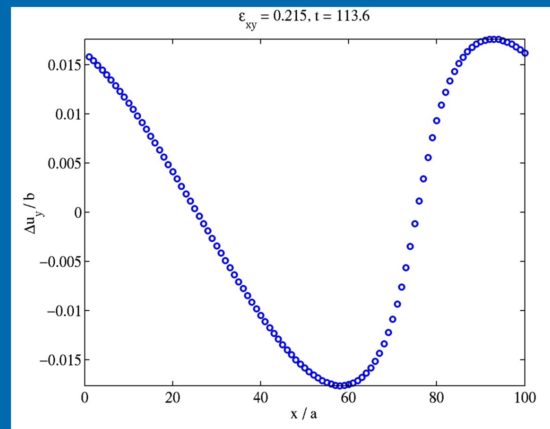
Strain localization

4-Stage Wave Steepening Scenario



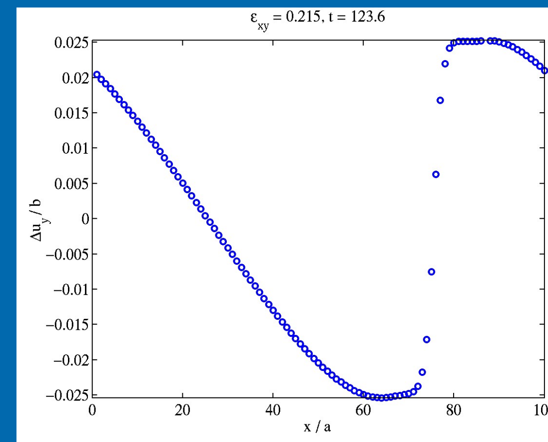
1. Linear Growth

shape preserved
amplitude icreases
continuum description



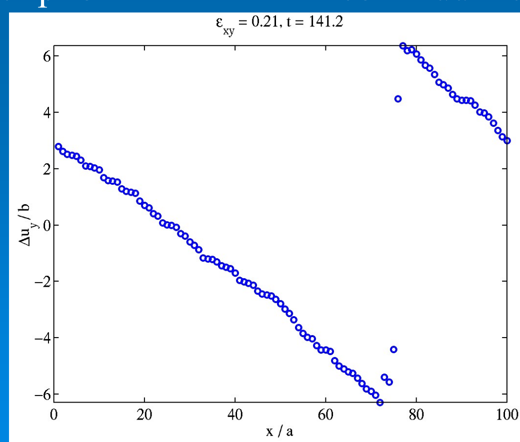
2. Non-Linear Growth

wave-front steepens due to
increasing non-linearity
continuum description



3. Shear Shock Formation

wave-front steepens to form an
atomically sharp shock
→ atomistic description



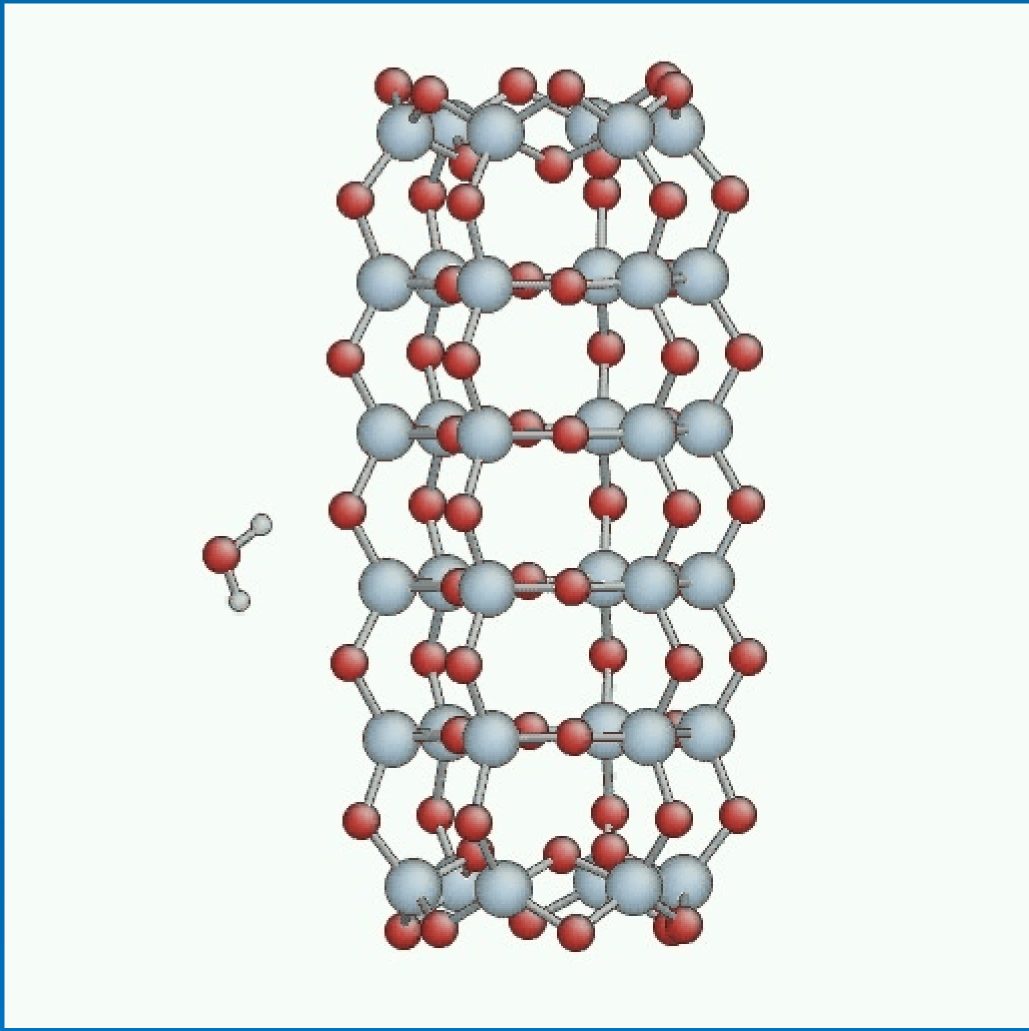
4. Formation of Atomic Defect

Atomic-level decision:
formation of dislocation, twin, …
determined by atomistic energy landscape

J. Chang, PhD Thesis, MIT, 2004

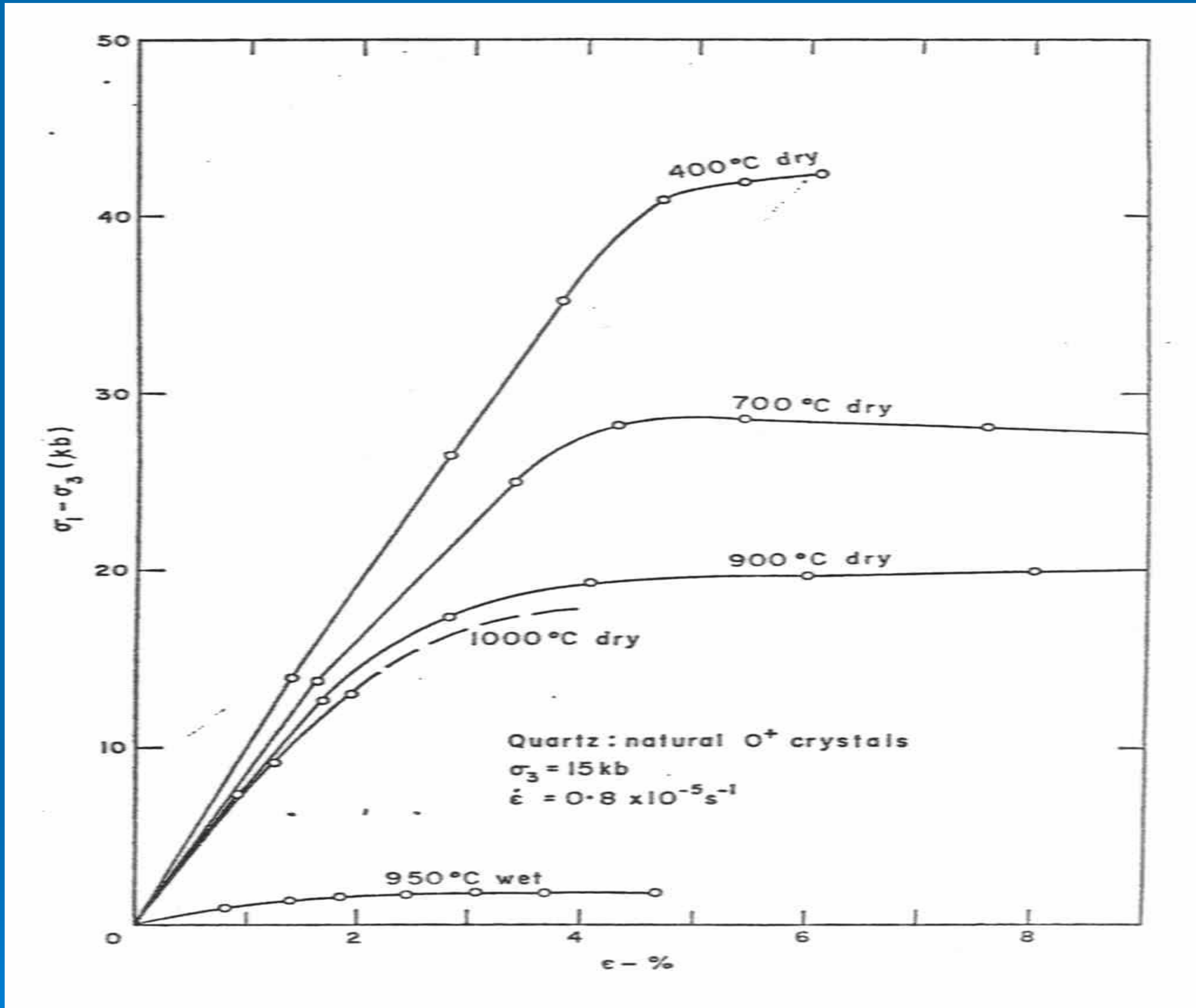
deformation and reaction of a silica nanorod --

inspired by the phenomenon of ‘Hydrolytic Weakening’



hydrolysis of an Si-O-Si bond to form silanol --

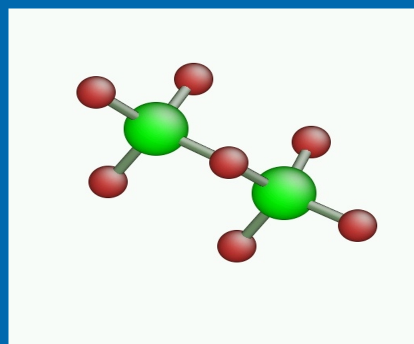
$$H_2O + Si - O - Si \rightarrow 2SiOH$$

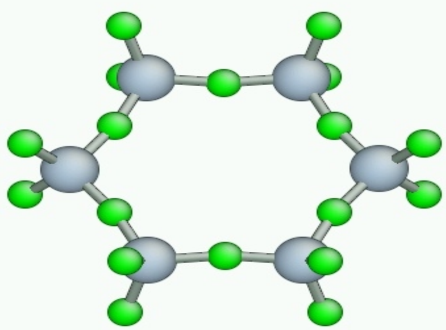


D. Griggs, Geophys. J. R. Astr. Soc 14, 19 (1967)

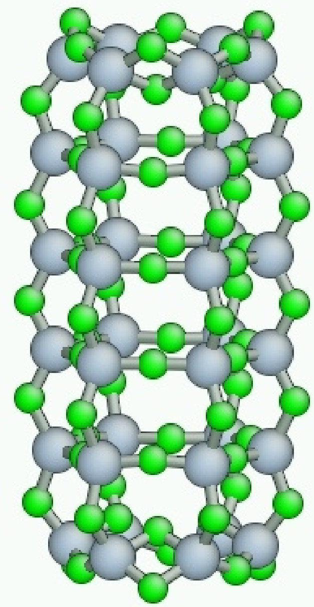
Quartz Nanorod

Structural unit: SiO_4 tetrahedron

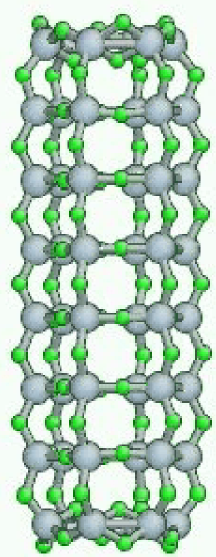




Si_6O_{18} beryl

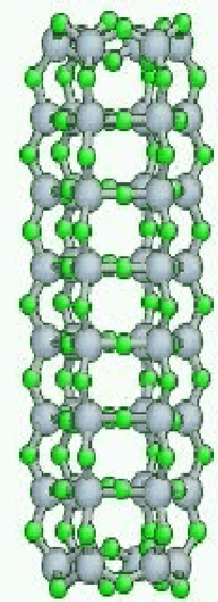


Nanorod (108 atoms)



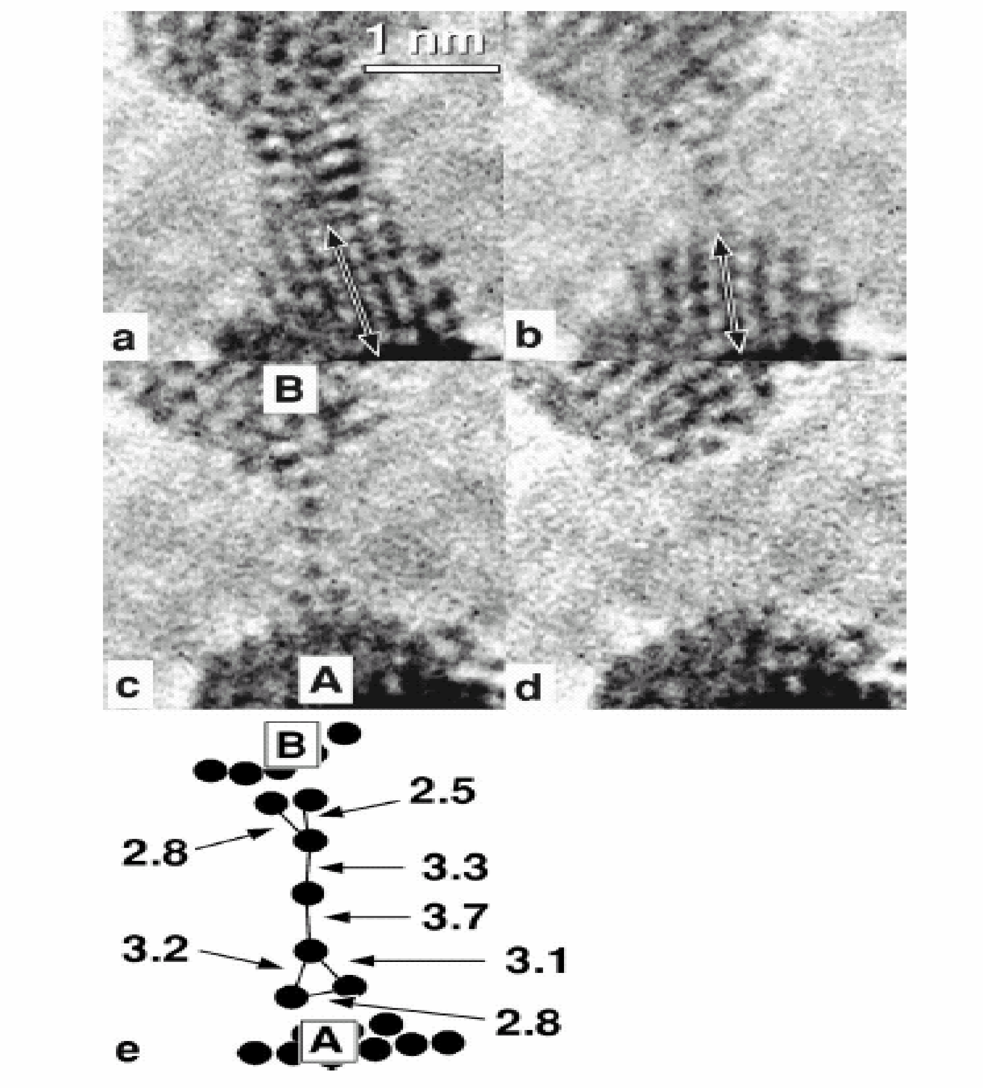
Tensile failure at $1^{o}K$

nanorod_1K.avi

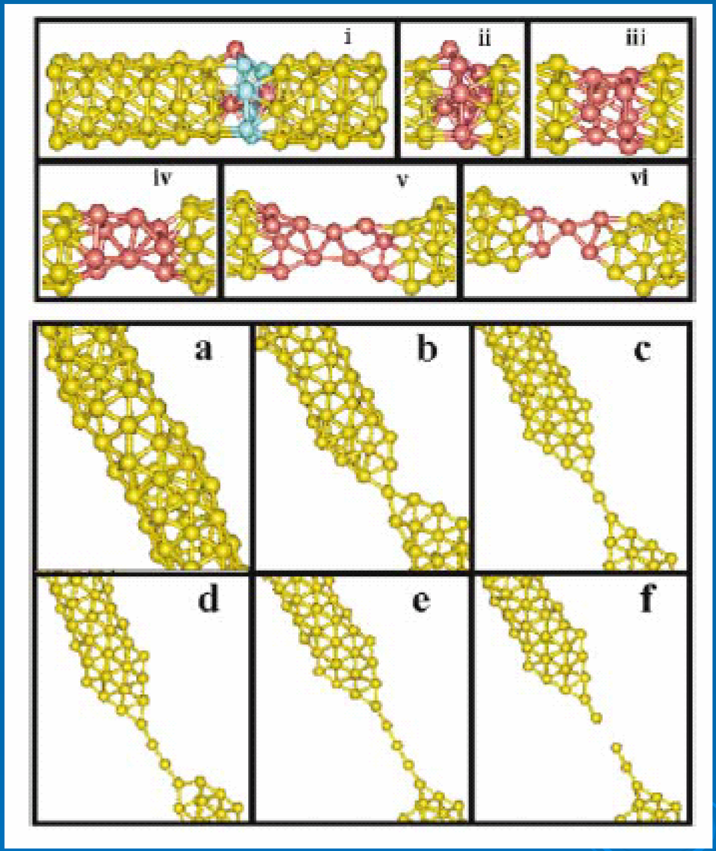


Tensile failure at $100^{o}K$

nanorod_100K.avi

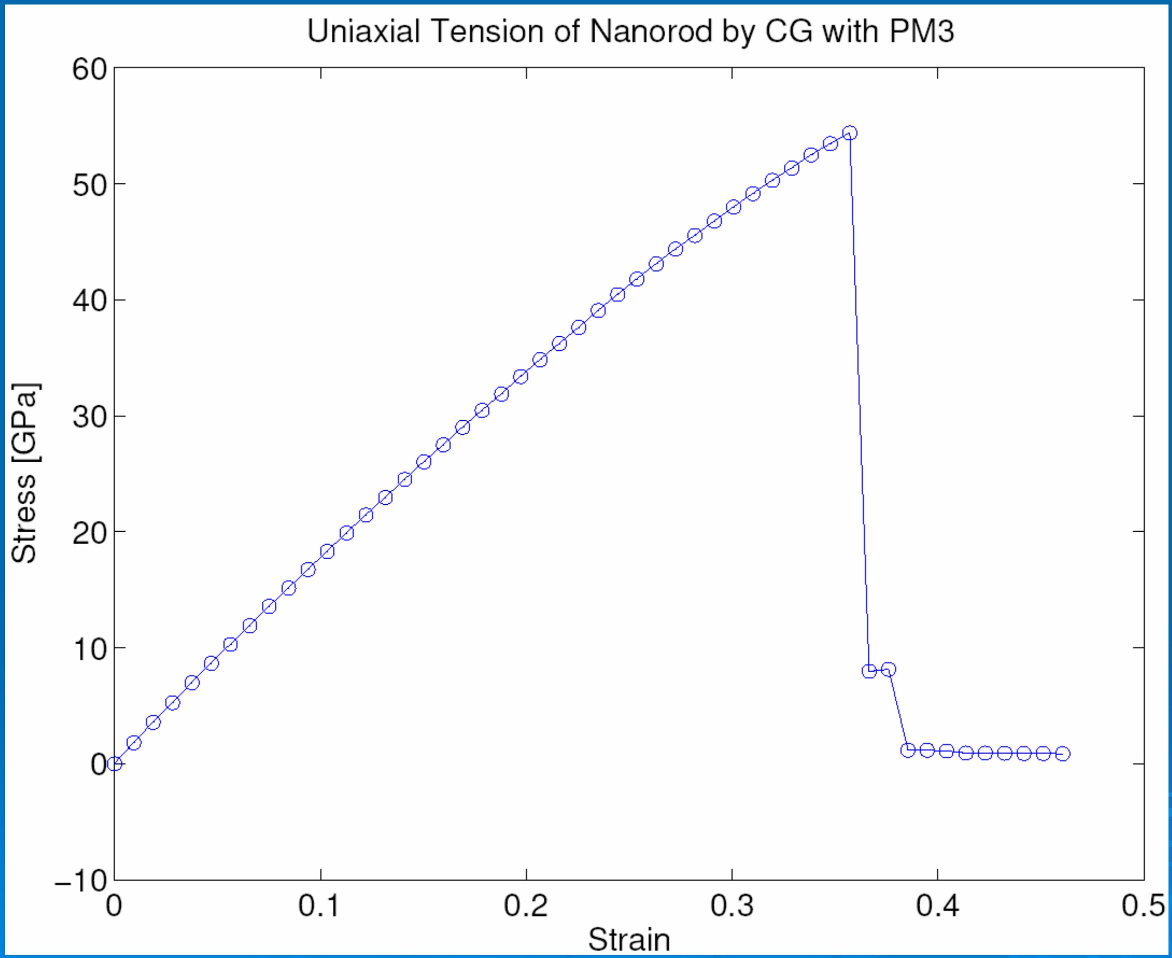


Real-time imaging gold nanojunctions
Rodrigues and Ugarte, PRB (2001)



TB-MD simulations
Da Silva et al., PRL (2001)

Rupture of nanorod under uniaxial tension

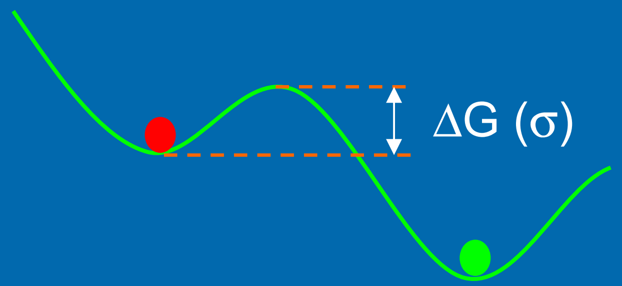


Chemical effect on bond breaking = Stress effect on chemical reactivity

Extending time scale based on transition state theory (TST)

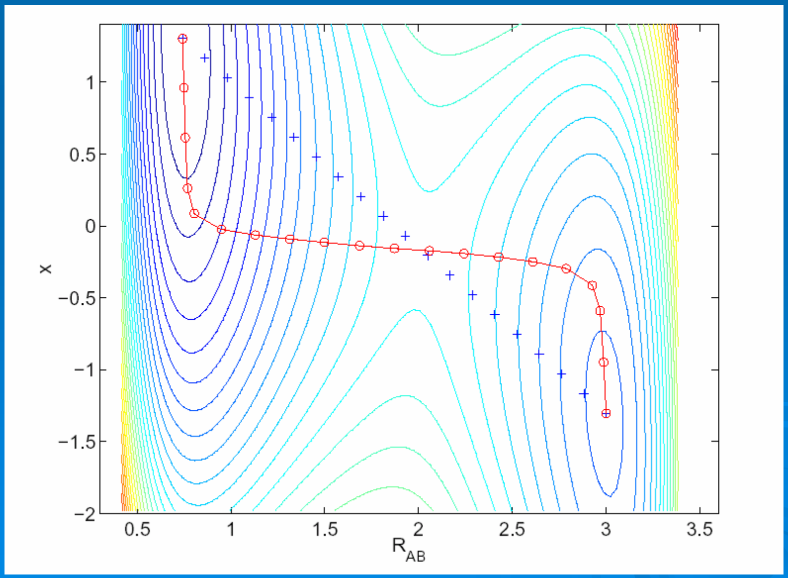
Voter et al., Ann Rev Mater Res (2002)

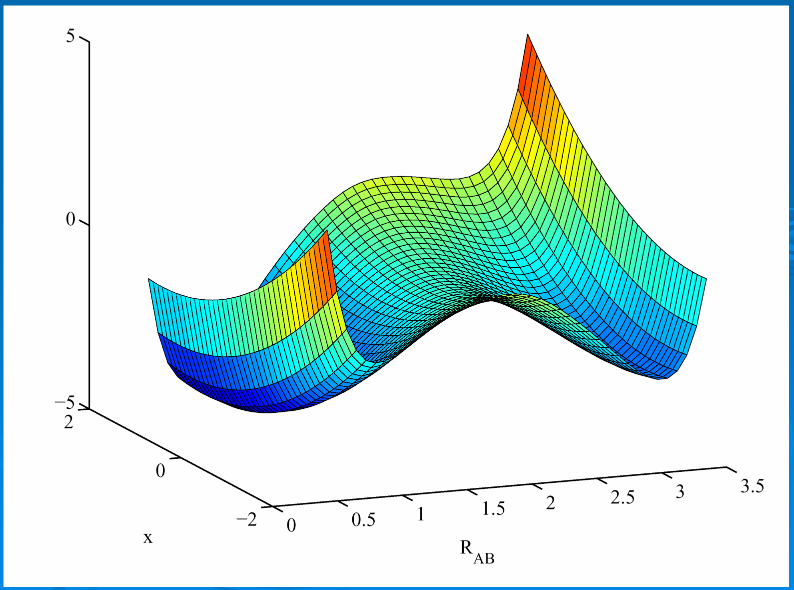
$$\text{transition rate} \propto \nu \exp\left(-\frac{\Delta G(\sigma)}{kT}\right)$$

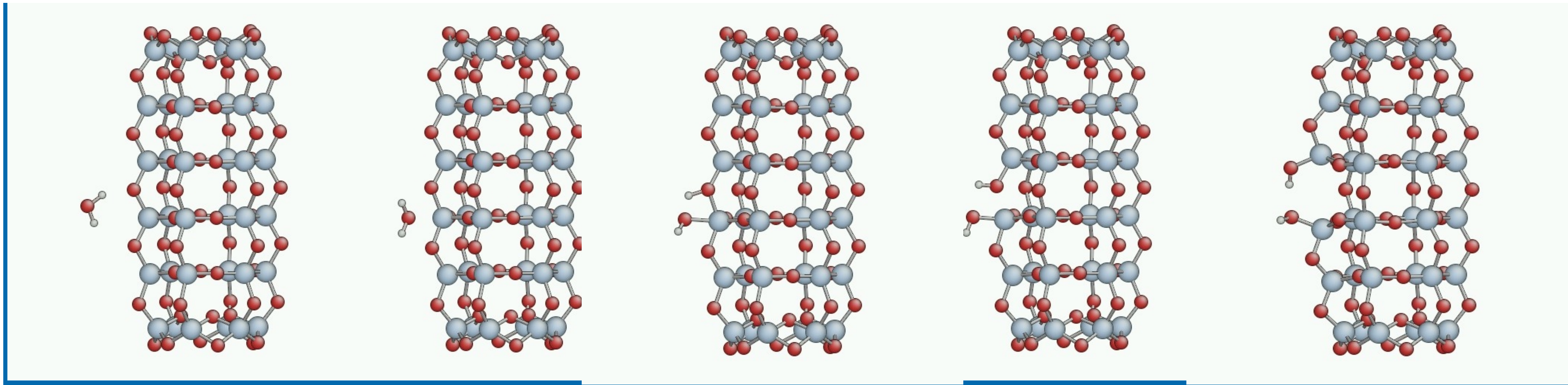


Nudged elastic band (NEB) method

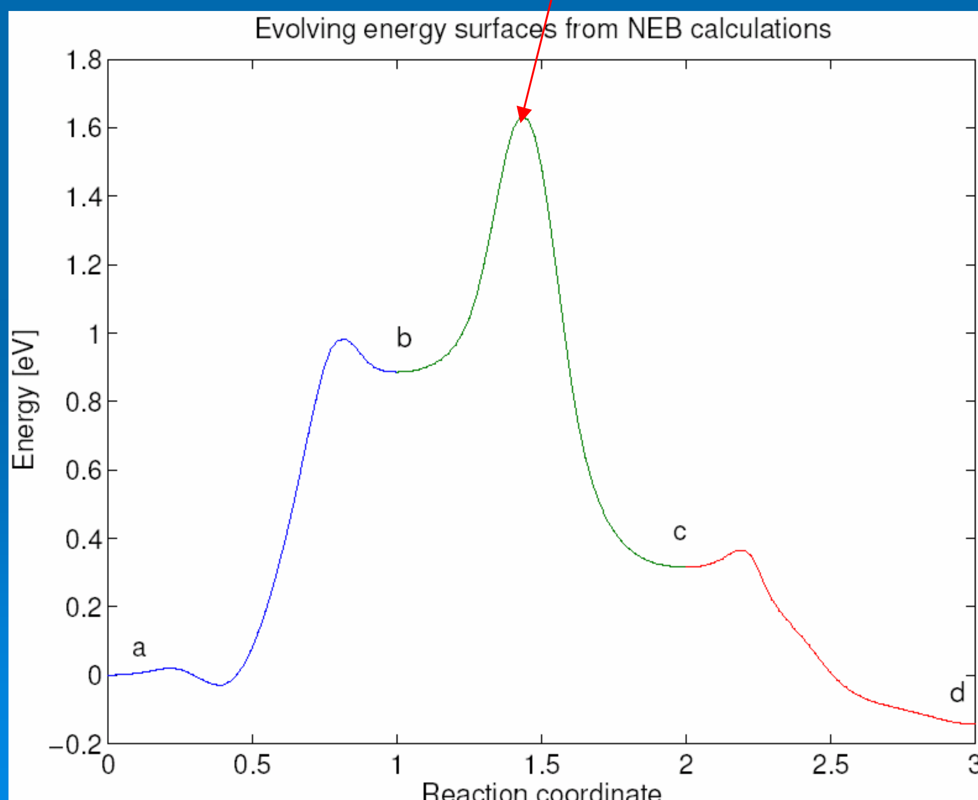
Mills & Jonsson PRL (1994) - Hessian free, enable study of larger system using QM force field



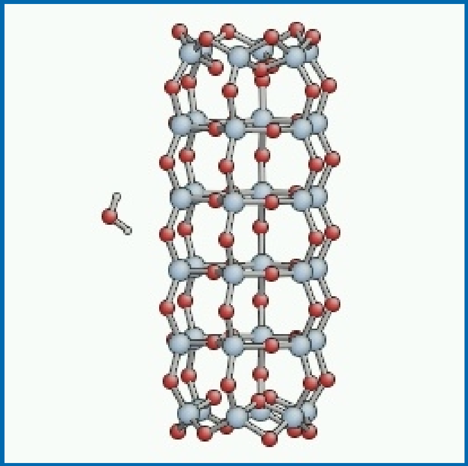




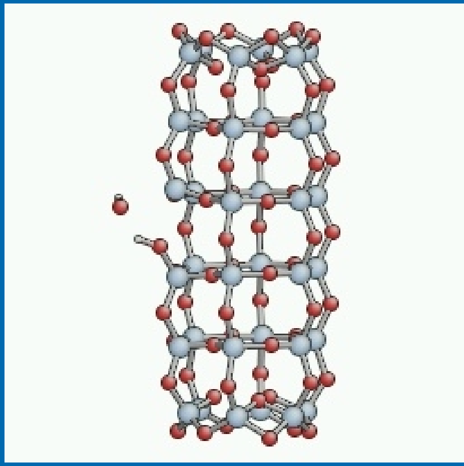
a b Saddle point configuration c d



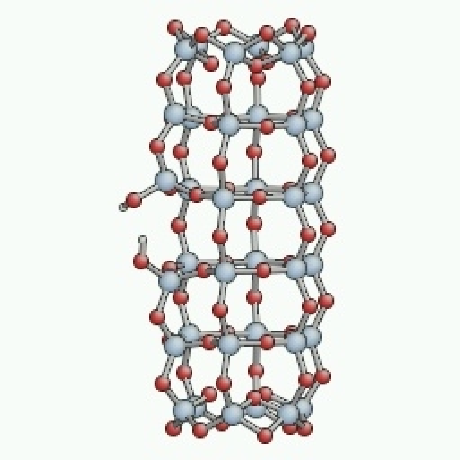
Stress=16.7GPa



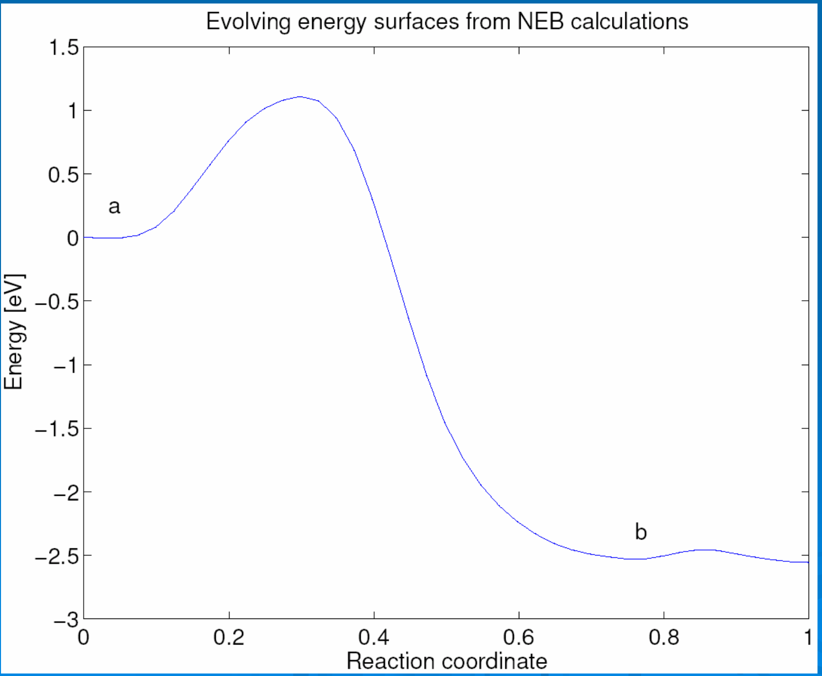
(a)



Saddle point configuration



(b)



Stress=33.76GPa

At the atomistic level, mechanical deformation, transport, and reaction are all governed by the interaction of ions and electrons (in saddle-point configurations).

Just as mesoscale continues to be a challenge to multiscale modeling, the challenge here lies at the interface --

hard/soft materials

bulk/nanostructures

chemistry/biology/nanoscience