From nano to macro: Introduction to atomistic modeling techniques

Lecture series, CEE, Fall 2005, IAP, Spring 2006

Atomistic modeling of metals and application to the mechanics of ultra thin copper films deposited on substrates

Lecture 2

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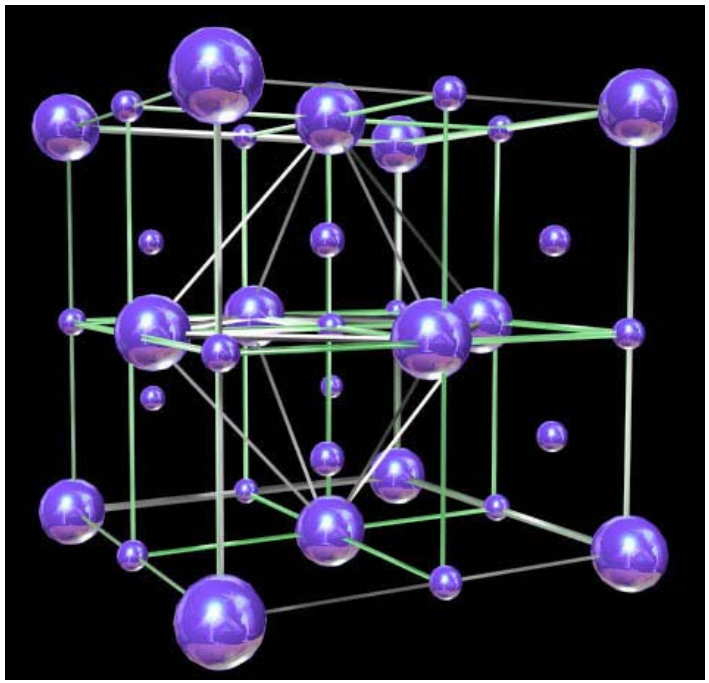
Outline and content (Lecture 2)

- Review: Atomistic modeling techniques
- Modeling of metals using pair potentials and multi-body potentials (pair potentials like Morse, LJ, etc., and EAM/MEAM potentials)
- Numerical implementation for modeling the behavior of metals
- Brief review of dislocation mechanics (dislocation interactions, nano-confinement)
- Application: Understanding the mechanical properties of ultra thin copper films deposited on substrates
- Conclusion and outlook

Review: Atomistic modeling techniques

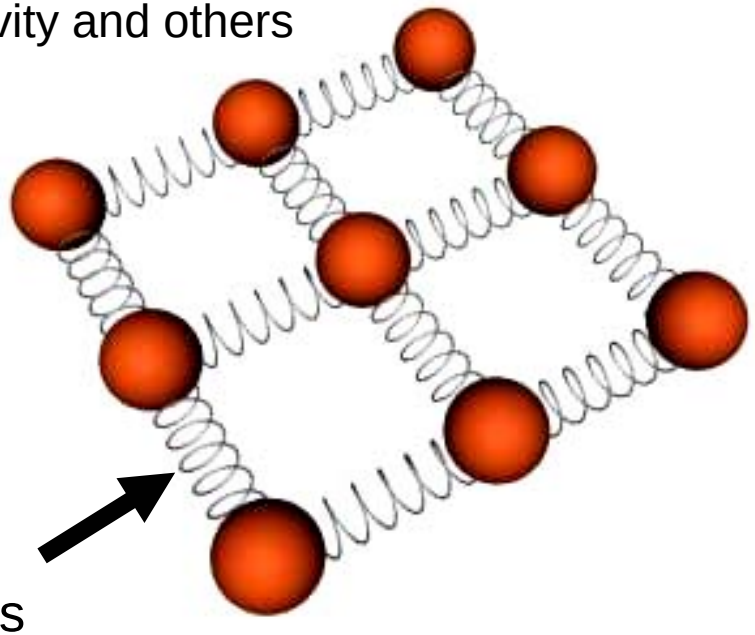
The problem to solve

- In atomistic simulations, the goal is to understand and model the motion of each atom in the material
- The collective behavior of the atoms allows to understand how the material undergoes deformation (metals: dislocations), phase changes or other phenomena, providing links between the atomic scale to meso/macro phenomena



http://www.freespiritproductions.com/pdatom.jpg

Vibration, change of location, connectivity and others



"Spring" connects atoms…

http://www.sr.bham.ac.uk/xmm/images/structures/spherespring_300_248.jpg

Classical molecular dynamics (MD)

- Classical MD calculates the time dependent behavior of a molecular system by integrating their equations of motion (*F*=force vector, *a*=acceleration vector)

$$F = ma$$

- The word “classical” means that the core motion of the constituent particles obeys the laws of classical mechanics
- Molecular dynamics simulations generate information at the microscopic level, which are: Atomic positions, velocities, forces
- The conversion of this microscopic information to macroscopic observables such as pressure, stress tensor, strain tensor, energy, heat capacities, etc., requires theories and strategies developed in the realm of statistical mechanics
- Statistical mechanics is fundamental to the study of many different atomistic systems

Important: The Ergodic hypothesis states

$$\langle A \rangle_{ensemble} = \langle A \rangle_{time}$$

Ensemble average = Time average (atomistic data usually not valid instantaneously in time and space)

Integrating the equations of motion

- Verlet algorithm
- Leap-frog algorithm
- Beeman's algorithm

Update of positions

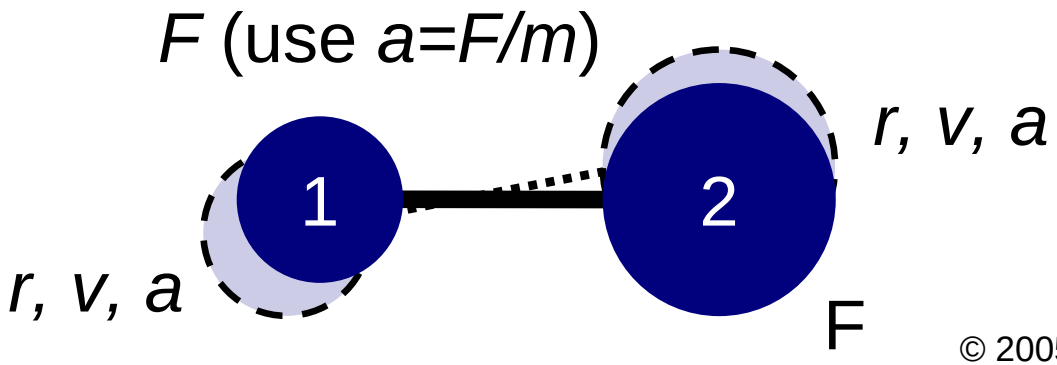
$$r(t+\delta t) = r(t) + v(t)\delta t + \frac{1}{2}a(t)\delta t^2$$

- Velocity Verlet (popular)

Update of velocities

$$v(t+\delta t) = v(t) + \frac{1}{2}\left[a(t) + a(t+\delta t)\right]\delta t$$

- Algorithms to control the temperature of a system, pressure, stress, etc. exist (e.g. Nosé-Hoover, Berendson, etc.)
- NVE, NVT, NPT calculations
- Most calculations in mechanics field are NVE (nonequilibrium phenomena such as fracture)

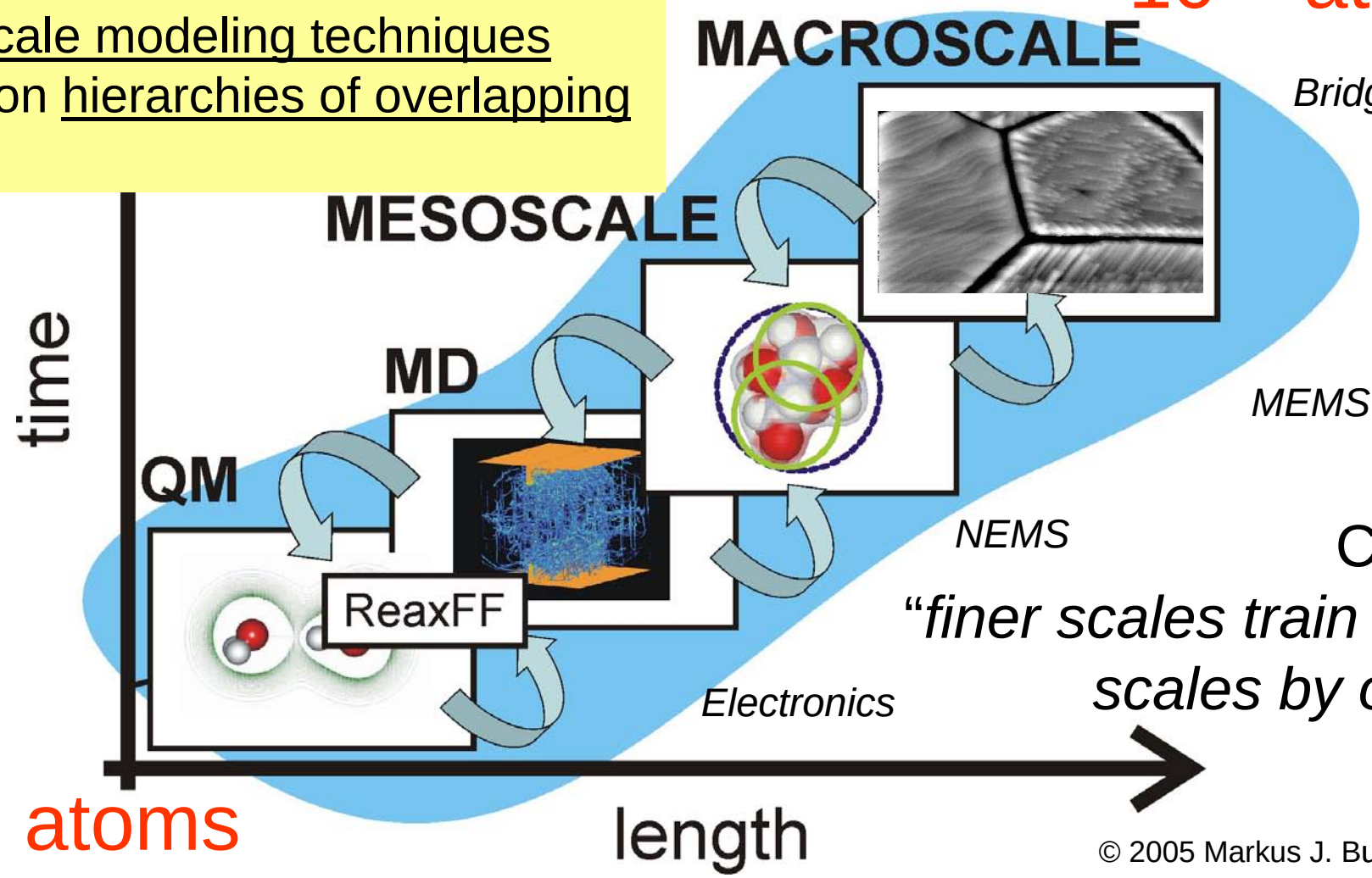


The BIG problem …

Want: Accuracy of quantum mechanics (QM) in 10^{23} atom systems…

This is impossible (today and in the foreseeable future)

Possible solution:
Multi-scale modeling techniques based on hierarchies of overlapping scales



Concept:
"*finer scales train coarser scales by overlap*"

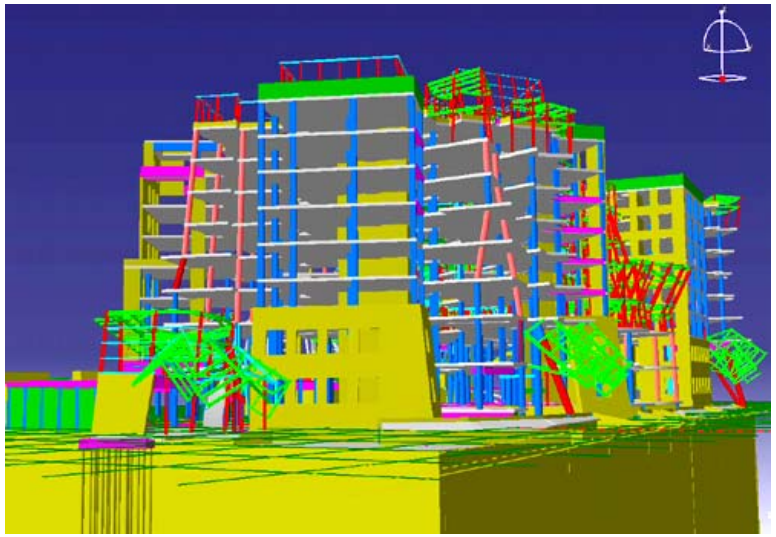
Introduction: Metals and applications

Applications of metals

- Metals are widely used in many applications, ranging from structural mechanics, surfaces, for electronic properties, magnetic properties or for optical devices
- Ages have been named after metals and their alloys (e.g. bronze age, iron age etc.), as their usage has significantly shaped technologies and the world
- Thorough understanding has big impact on engineering, technology and society

Example applications:

- Metals in ultra thin films in semiconductor applications (Cu interconnects)
- Steel frames for high-rise buildings (tensile load)



web.mit.edu/buildings/statacenter/catia02.htm

"large"

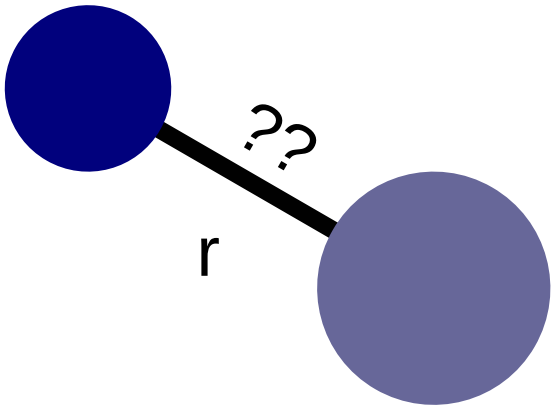
"small"

http://www.mse.berkeley.edu/groups/doyle/serdar/RESEARCH/RESEARCH.html

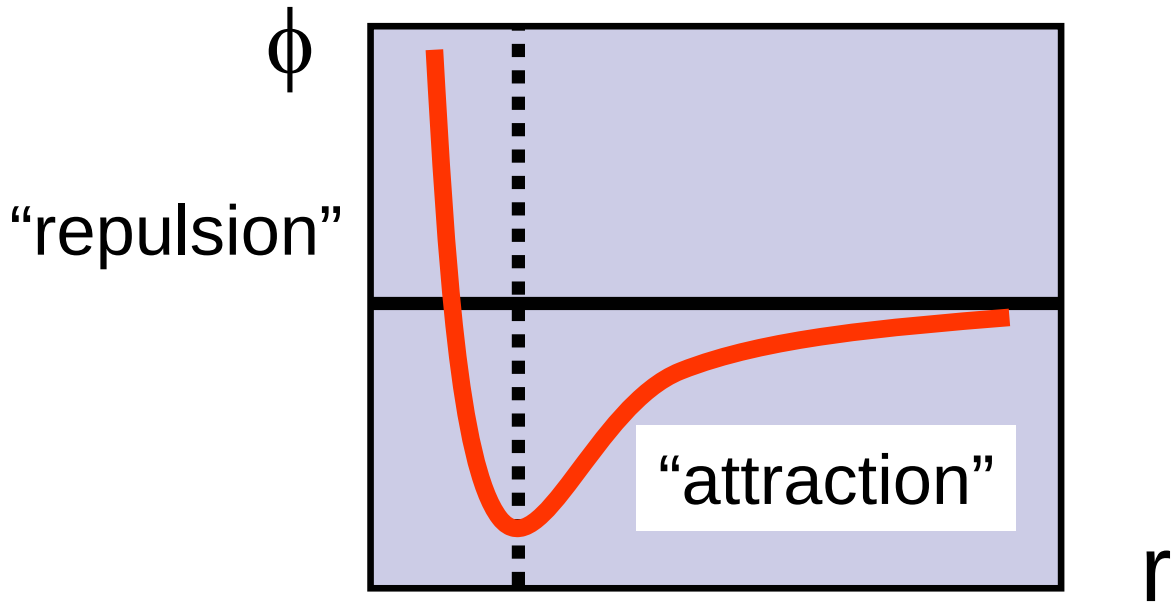
Interatomic potentials for metals

The interatomic potential

- The fundamental input into molecular simulations, in addition to structural information (position of atoms, type of atoms and their velocities/accelerations) is provided by definition of the interaction potential (equiv. terms often used by chemists is "force field")
- MD is very general due to its formulation, but hard to find a "good" potential (extensive debate still ongoing, choice depends very strongly on the application)
- Popular: Semi-empirical or empirical (fit of carefully chosen mathematical functions to reproduce the potential energy surface…)



Atomic scale (QM) or chemical property



Forces by dϕ/dr

Chemical bonding in metals
“metallic bonding”

- Bonding between atoms with low electronegativity 1,2 or 3 valence electrons, therefore there are many vacancies in valence shell.
- When electron clouds overlap, electrons can move into electron cloud of adjoining atoms.
- Each atom becomes surrounded by a number of others in a three-dimensional lattice, where valence electrons move freely from one valence shell to another.
- Delocalized valence electrons moving between nuclei generate a binding force to hold the atoms together

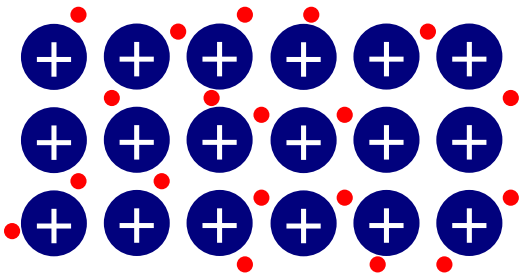
positive ions in a sea of electrons

Consequences:

- Electron gas model
- Mostly non-directional bonding, but the bond strength indeed depends on the environment of an atom, precisely the electron density imposed by other atoms

Electron (q=-1)

Ion core (q=+N)

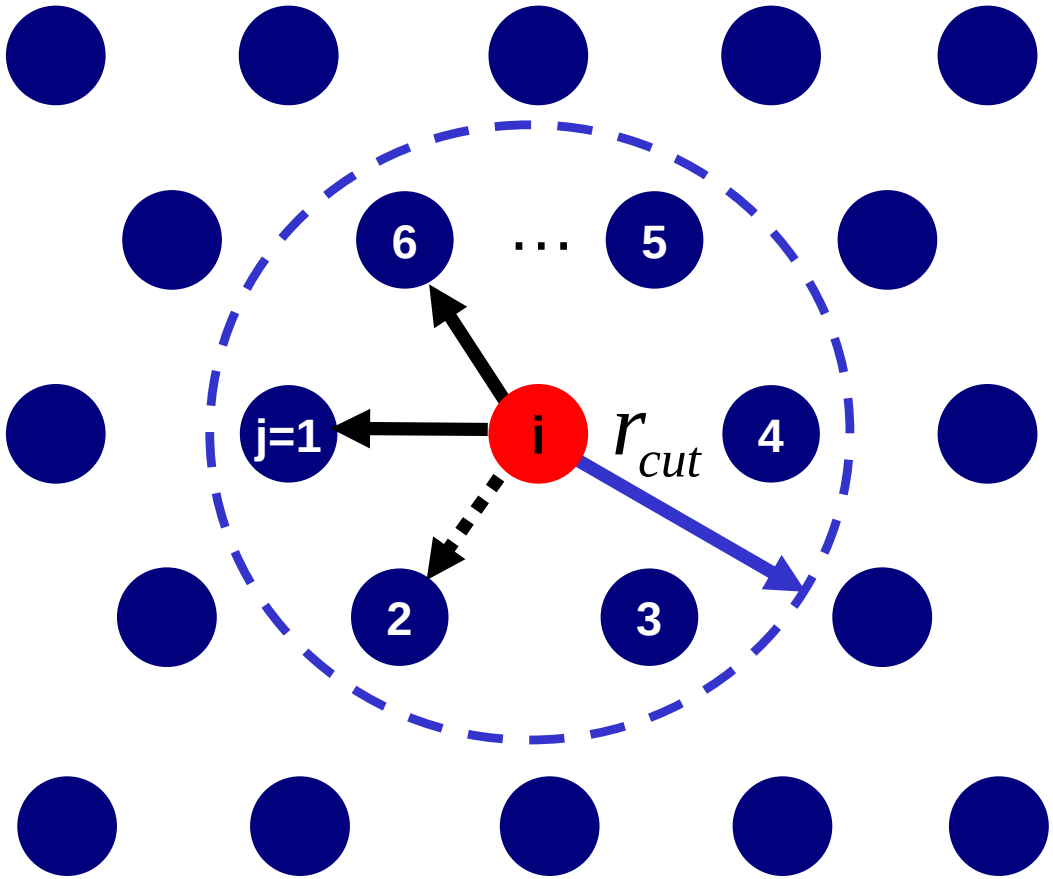


Properties of metals

Property	Physical/atomic reason
High density	Tightly packed FCC, BCC, HCP
High melting temperature	Strong forces between ion core and delocalized electrons
Good conductors of heat	Vibration transport via delocalized electrons (+phonons)
Good electrical conductors	Delocalized electrons (flow in and out)
Many metals are ductile	Glide (and climb) of dislocations
Lustrous	Reflection of light by electron gas

Modeling attempts: Pair potential

- First attempts using pair potentials



$$\phi_i = \sum_{j=1..N_{neigh}} \varphi(r_{ij})$$

Lennard-Jones 12:6

$$\varphi(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right]$$

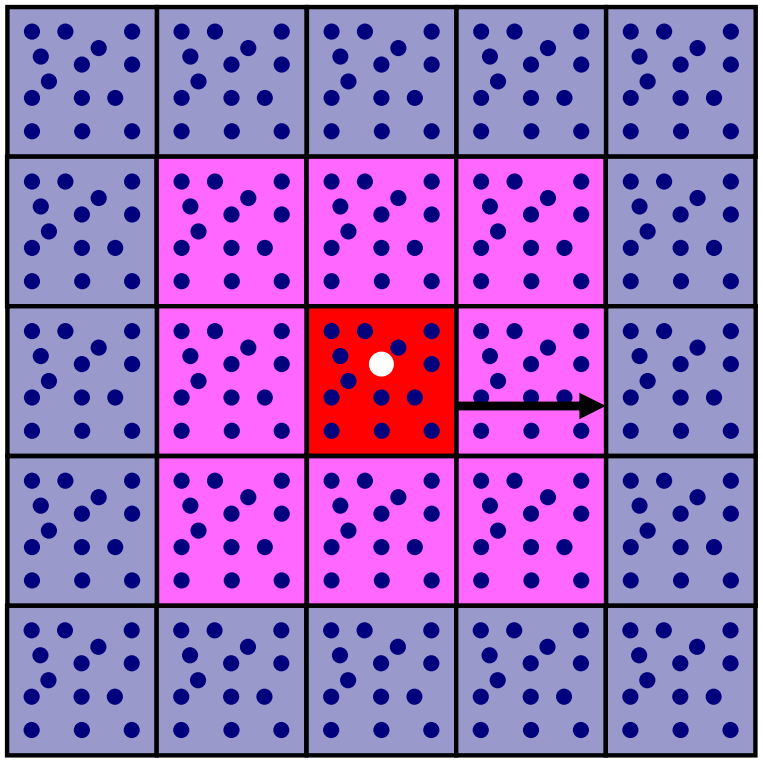
Morse

$$\varphi(r_{ij}) = D\{1 - \exp[-\beta(r_{ij} - r_0)]\}^2$$

Good for noble gas Ar
(FCC in 3D)

Numerical implementation of neighbor search: Reduction of N^2 problem to N problem

- Need nested loop to search for neighbors of atom *i:* Computational disaster
- Concept: Divide into computational cells ("bins", "containers", etc.)
- Cell radius $R>R_{cut}$ (cutoff)



- Search for neighbors within cell atom belongs to and neighboring cells (8+1 in 2D)
- Most classical MD potentials/force fields have finite range interactions
- Other approaches: Neighbor lists
- Bin re-distribution only necessary every 20..30 integration steps (parameter)

Why pair potentials fail…

- In pair potentials, the strength of each bond is dependent only on the distance between the two atoms involved:

  The positions of all the other atoms are not relevant
  (works well e.g. for Ar where no electrons are available for bonding and atoms are attracted with each other only through the weak van der Waals forces)

- However: QM tells that the strength of the bond between two atoms **is affected by the environment** (other atoms in the proximity)

- As a site becomes more crowded, the bond strength will generally decrease as a result of Pauli repulsion between electrons. The modeling of many important physical and chemical properties depends crucially on the ability of the potential to "adapt to the environment"

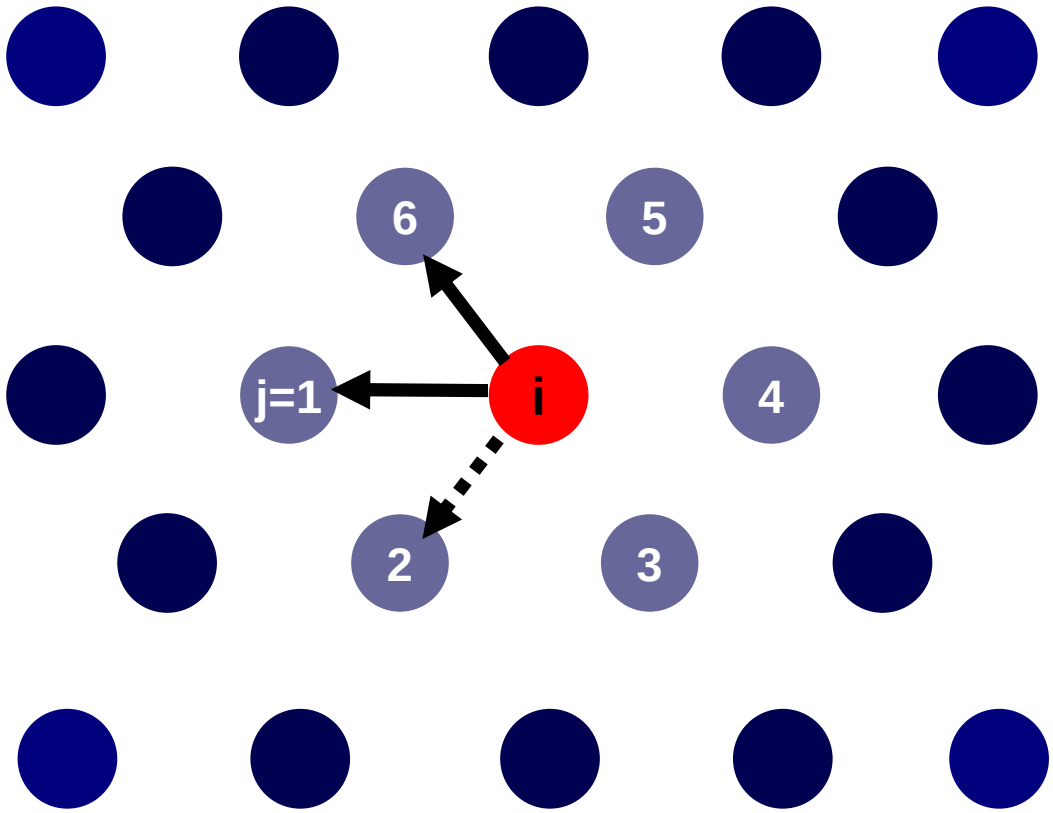
- Consequences:
  - Can not reproduce surface relaxation
  - Cauchy relation

$c_{12} / c_{44} = 1$ Not satisfied in most metals (e.g. Au $c_{12} / c_{44} = 3.7$)

http://www.fisica.uniud.it/~ercolessi/forcematching.html

Modeling attempts: Multi-body potential

- Multi-body potential depend on more than pairs of atoms, but instead also on the environment of each atom
- Important for metals due to the "electron gas"



new

$$\phi_i = \sum_{j=1..N_{neigh}} \frac{1}{2}\varphi(r_{ij}) + F(\rho_i)$$

Pair potential energy

Embedding energy as a function of electron density

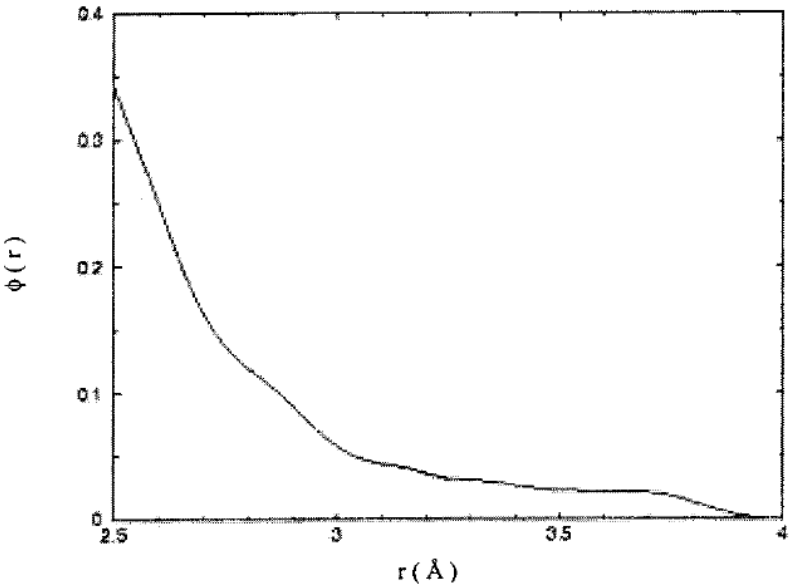
ρ_i Electron density at atom *I* based on a pair potential:

$$\rho_i = \sum_{j=1..N_{neigh}} \pi(r_{ij})$$

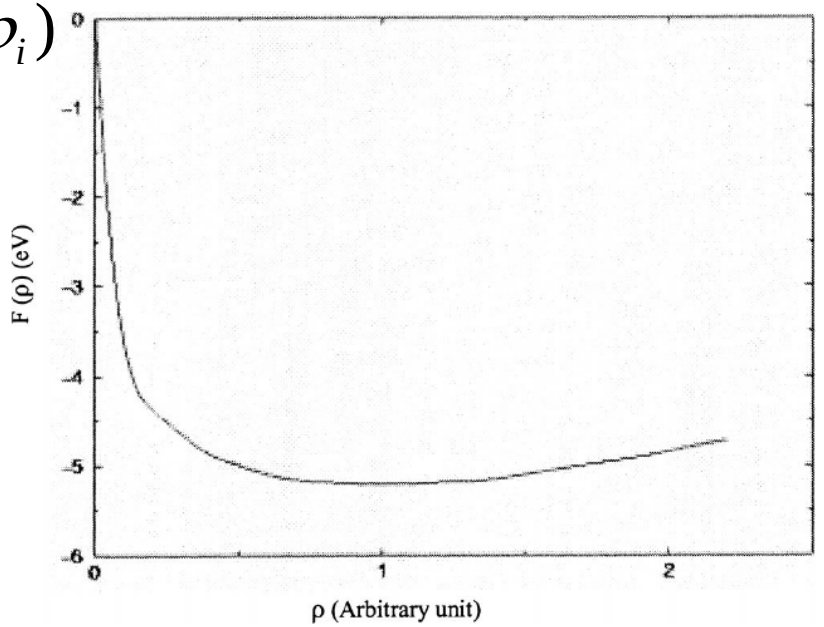
First proposed by Finnis, Sinclair, Daw, Baskes *et al.* (1980s)

Example: EAM potential for Ta

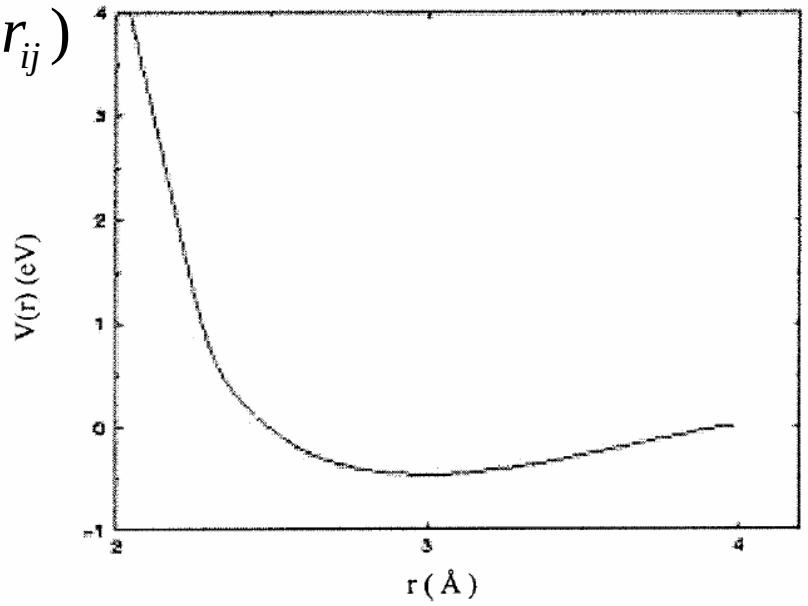
$\pi(r_{ij})$



$F(\rho_i)$



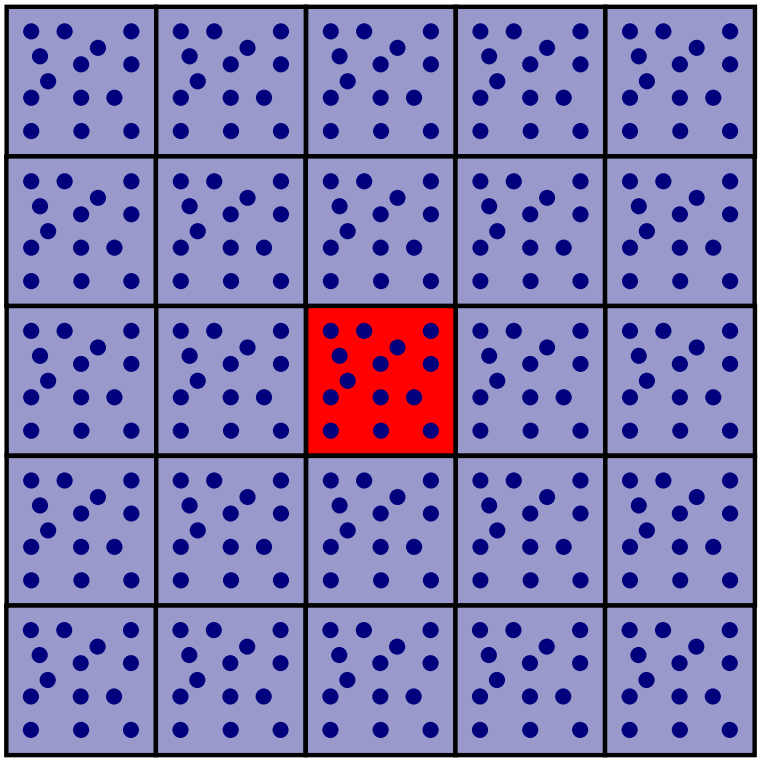
$\varphi(r_{ij})$



http://ceaspub.eas.asu.edu/cms/papers/Ta_final.pdf

Numerical implementation of multi-body EAM potential

- Requires two loops over atoms within each cell



Loop 1:

(i) Pair contributions (derivatives and potential)

(ii) Calculate electron density

Loop 2:

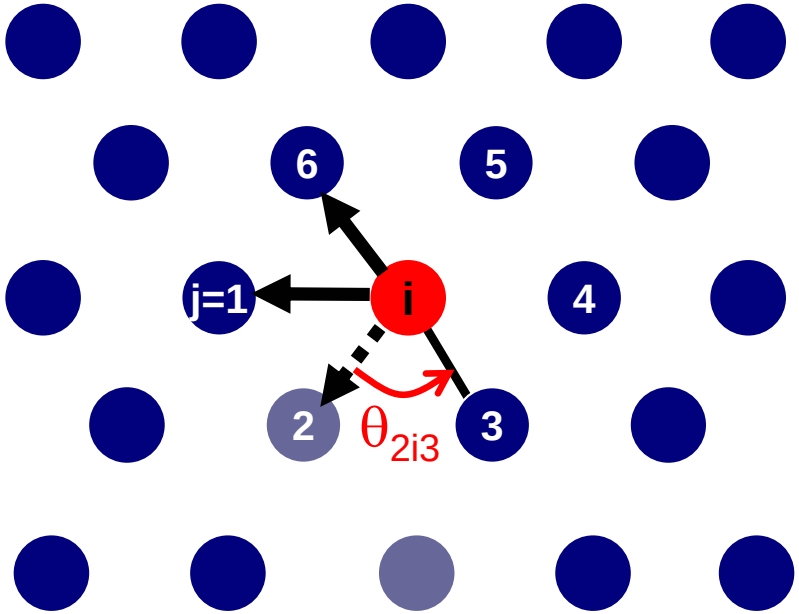
(iii) Calculate embedding function and derivatives

$$\mathbf{F}_i = -\sum_{j \neq i} \left(\phi'(r_{ij}) + [U'(n_i) + U'(n_j)]\rho'(r_{ij}) \right) \frac{\mathbf{r}_{ij}}{r_{ij}}$$

Due to additional (i) calculation of electron density and (ii) embedding contribution EAM potentials are 2-3 times slower than pure pair potentials

Modeling attempts: MEAM method

- MEAM potentials introduce an additional angular term to account for covalent, directional character of bonding, which is critical in some metals (e.g. Ta due to partially filled d-orbitals) and semiconductors (e.g. Si)



$$\phi_i = \underbrace{\sum_{j=1..N_{neigh}} \frac{1}{2}\varphi(r_{ij})}_{\text{Pair potential energy}} + \underbrace{F(\rho_i)}_{\substack{\text{Embedding energy as a function of electron density}}}$$

ρ_i Electron density at atom *i* contains three-body contributions:

$$\rho_i = \frac{2\rho_i^{(0)}}{1+\exp\left[-\sum_{s=1}^{3} t_i^{(s)}\left(\rho_i^{(s)}/\rho_i^{(0)}\right)^2\right]}$$

$$\left(\rho_i^{(s)}\right)^2 = \sum_{j,k\neq i} \rho_j^{a(s)}(r_{ij})\rho_k^{a(s)}(r_{ik})L^{(s)}(\cos\theta_{jik})$$

Loop over triple pairs

angular term

MEAM developed by Baskes *et al.* (1992, 1997), http://www.itap.physik.uni-stuttgart.de/~imd/userguide/meam.html, http://msl.stanford.edu/Files/MEAM.pdf

Derivation or “training” of potentials

- Training of parameters is done so that experimental or quantum mechanical results are reproduced
- The success of training depends on the choice of the potential form (analytical) and its ansatz (e.g. include knowledge from QM about chemical bonding (realized in EAM potentials)

Implementations

- Parameter fitting through a (i) training set of data (pairing desired values and structural information including relative weights to define a cost function) and a (ii) potential formulation with variable parameters
  - Force Matching Method (systematic approach to fit potential to a large database of force data from DFT)
  - Genetic algorithm or other optimization schemes
  - By hand or intuition (less effective)

Notes

- Whole research groups dedicated to the problem of potential derivation
- Means to transport information across the scales (see Lecture 1)

http://www.fisica.uniud.it/~ercolessi/forcematching.html

The force matching method

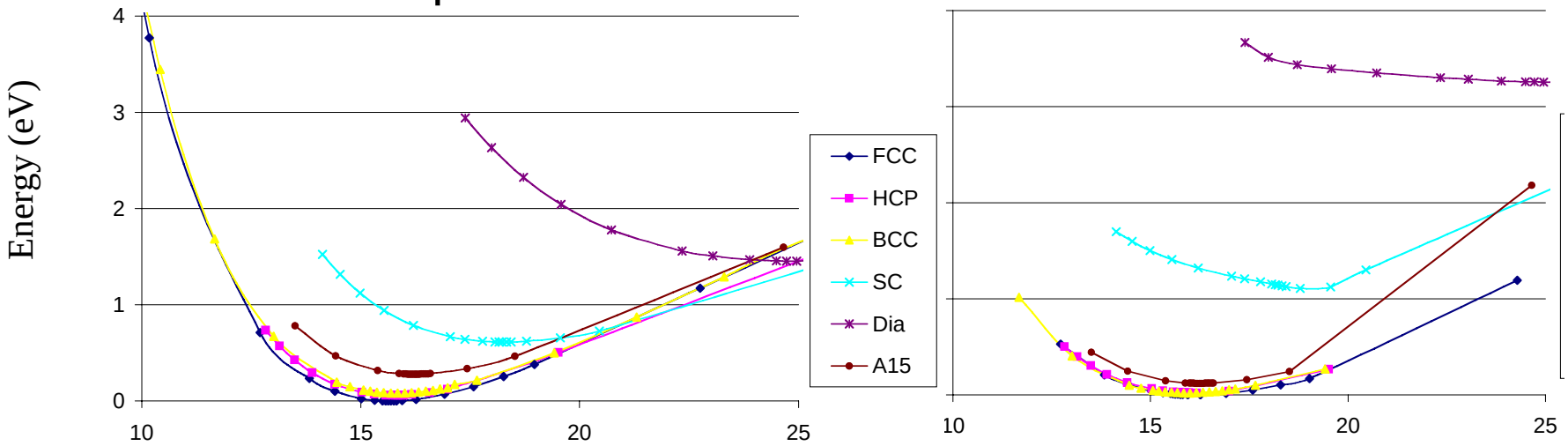
- Developed 1992,1993 at UIUC
- Basic idea: Obtain realistic classical empirical potentials by making use of very large amounts of information obtained by first-principles calculations (EOS, lattice constant, cohesive energy, elastic properties..)
- E.g., as mathematical form use cubic splines to define the potential shape
- Many flavors and similar approaches have been developed in recent years

- Examples for application of force matching method:
  - *Alumuinum, Europhys. Lett.* **26**, 583 (1994)
  - Magnesium, *Modelling and simulation in materials science and engineering* **4**, 293 (1996), by X.-Y. Liu *et al.*

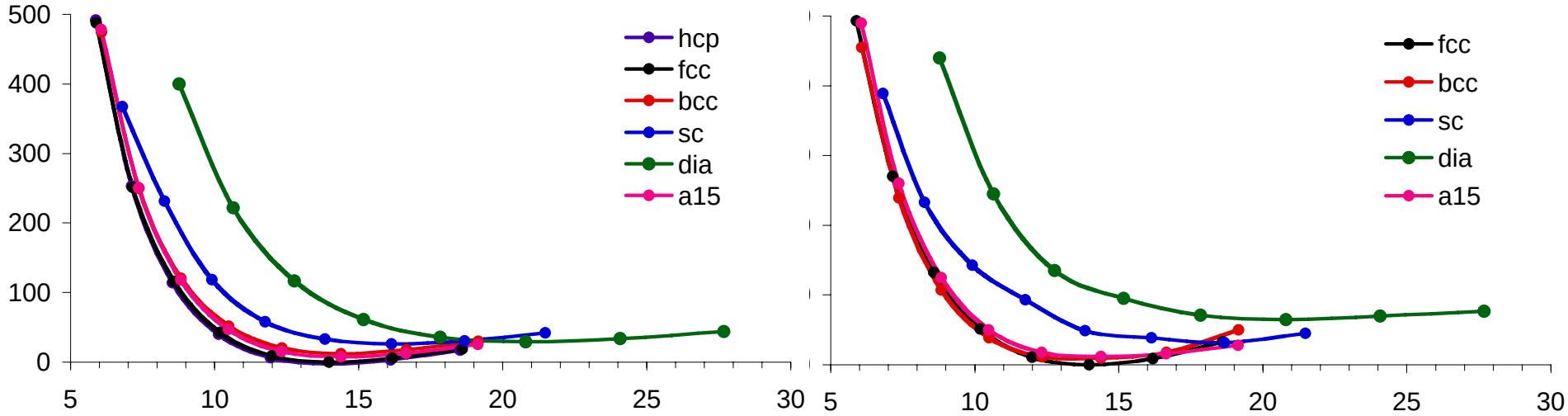
http://www.fisica.uniud.it/~ercolessi/forcematching.html
http://ceaspub.eas.asu.edu/cms/papers/forcem4.pdf
http://ceaspub.eas.asu.edu/cms/papers/Ta_final.pdf

Example: Equation of state for metals

Platinum metal bulk phases



Ruthenium metal bulk phases (van Duin et al.)



QM

ReaxFF

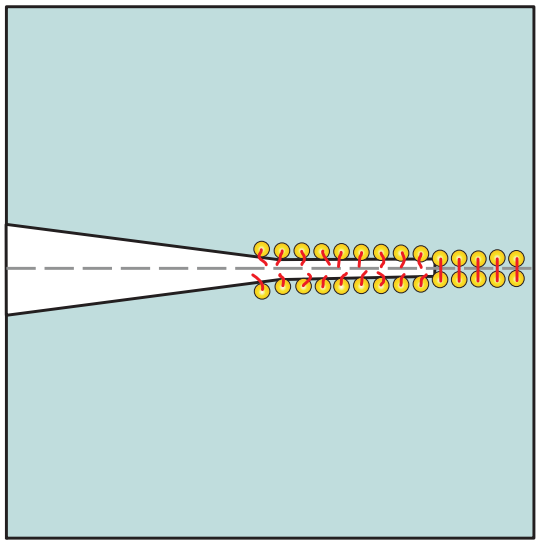
Theoretical concepts and experimental results

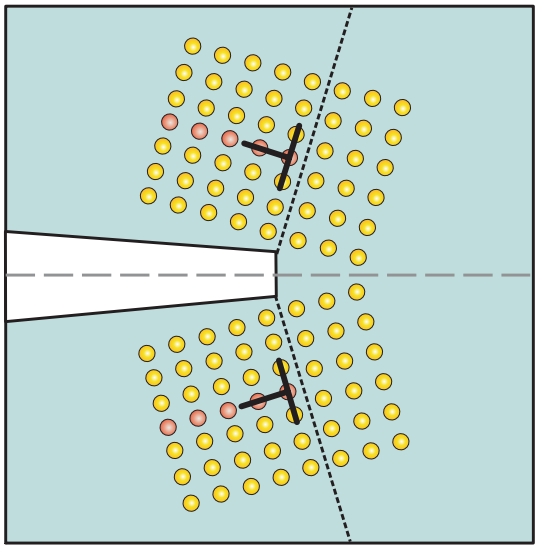
Ductile versus brittle materials

brittle

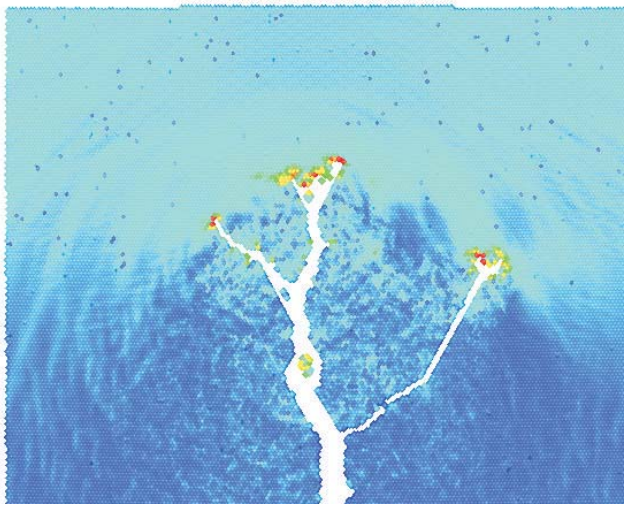
ductile

Propagation of cracks

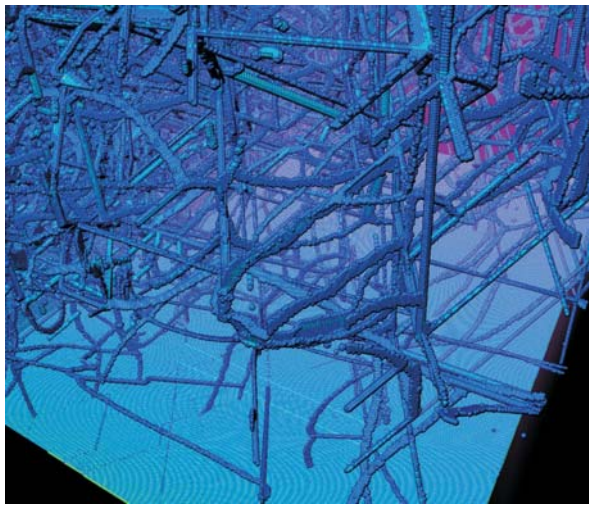




Nucleation of dislocations



(a)

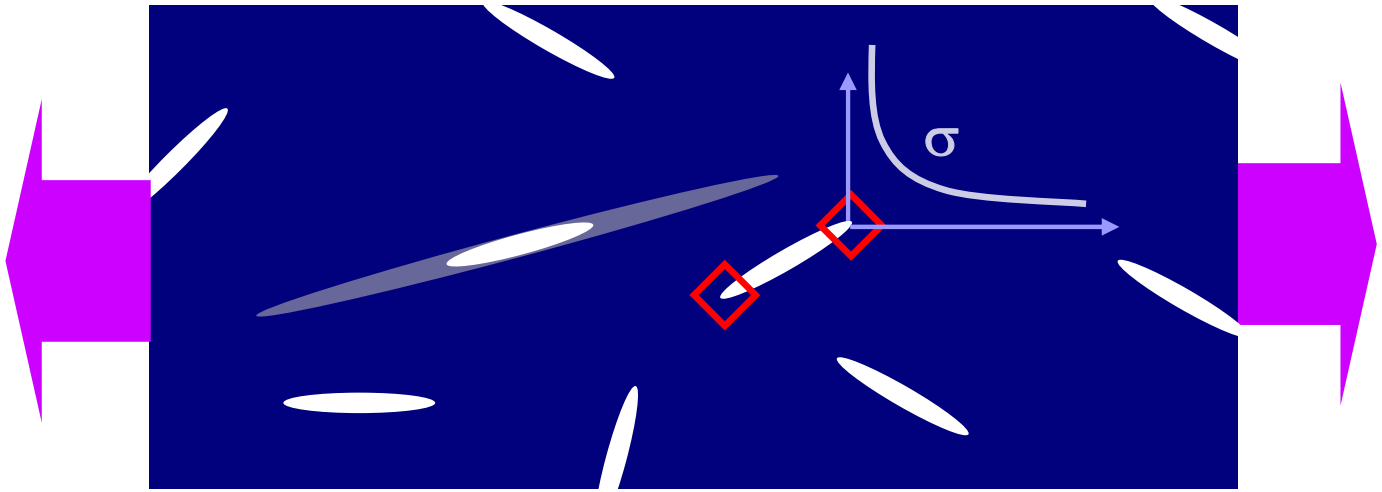


(b)

(Buehler, 2004)

Cracks govern the strength of materials

- The strength of materials is dominated by the existence of cracks or other defects (“flaws”)
- Cracks and similar defects lead to stress concentrations, which in turn lead to nucleation of dislocations or generation of new material surfaces
- Cracks and defects explain the reduced theoretical strength of materials (up to 1,000 compared to theoretical prediction)



Griffith

T.H. Courtney, Mechanical Behavior of Materials, T, Timoshenko, History of strength of materials. New York: McGraw Hill

Review on fracture mechanics: Cracks matter

- To analyze the relationship among stresses, cracks, and fracture toughness, **Fracture Mechanics** was introduced. The first milestone was set by Griffith in his famous 1920 paper that quantitatively relates the flaw size to the fracture stresses.
  Griffith's approach is only suitable for **brittle materials**.

$$\sigma_c = \left(\frac{2E\gamma_s}{\pi a} \right)^{1/2}$$

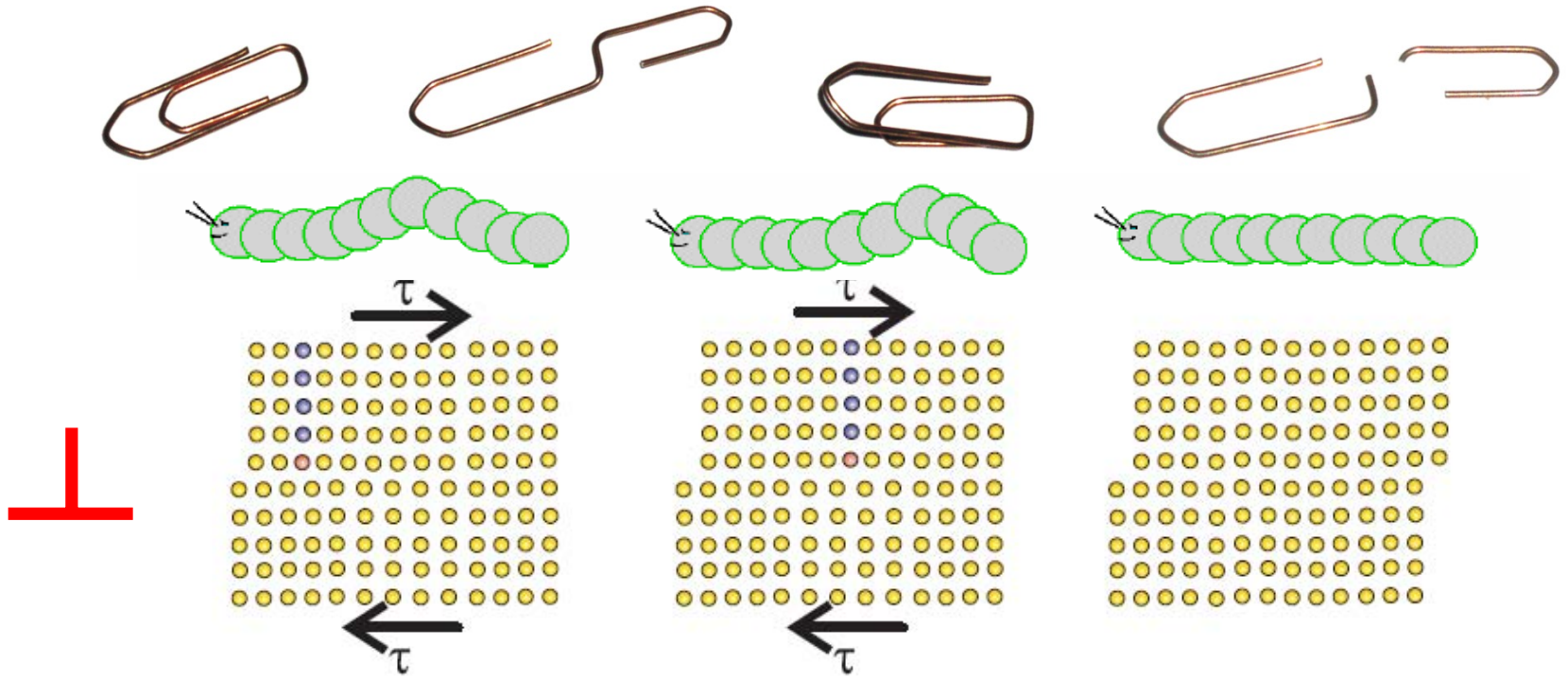
- For **ductile materials**, the milestone did not come about until Irwin developed the concept of **strain energy release rate**, *G*, in 1950s. *G* is defined as the rate of change in potential energy near the crack area for a linear elastic material.

- When the **strain energy release rate** reaches the critical value, G_{cr}, the crack will grow. Later, the strain energy release rate *G* was replaced by the **stress intensity factor** *K* with a similar approach by other researchers.

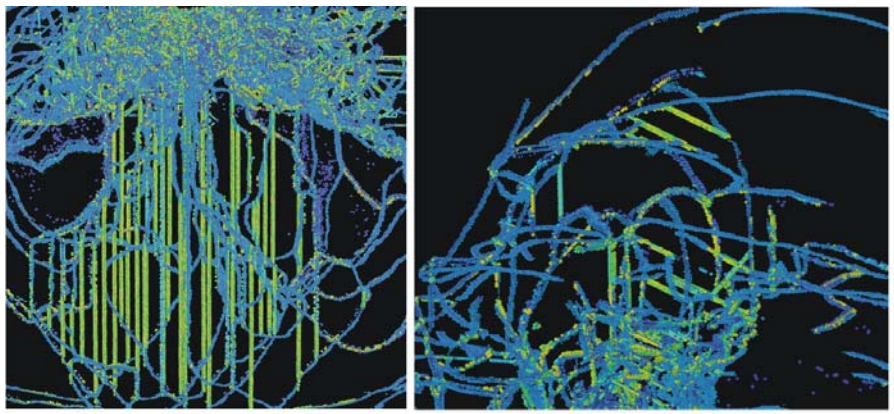
$$G = 2(\gamma_s + \gamma_p) \qquad G = G_I + G_{II} + G_{III} = \frac{1-\upsilon^2}{E}\left(K_I^{\,2} + K_{II}^{\,2} + \frac{K_{III}^{\,2}}{1-\upsilon} \right)$$

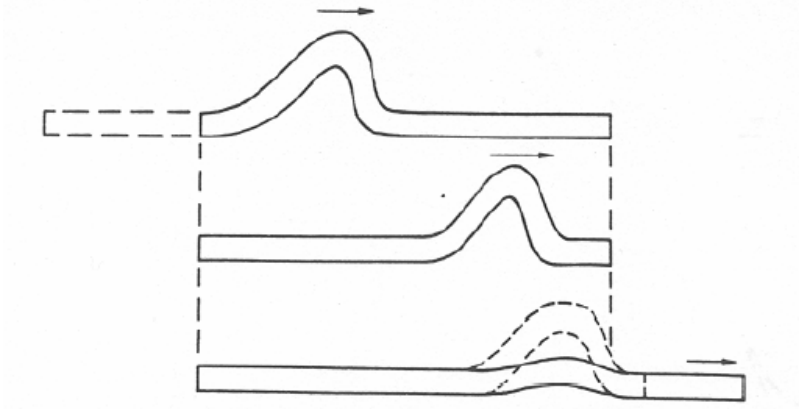
http://www.sv.vt.edu/classes/MSE2094_NoteBook/97ClassProj/anal/grealis/history.html

Ductile materials are governed by the motion of dislocations: Introduction



Dislocations are the entities that carry plastic (permanent) deformation

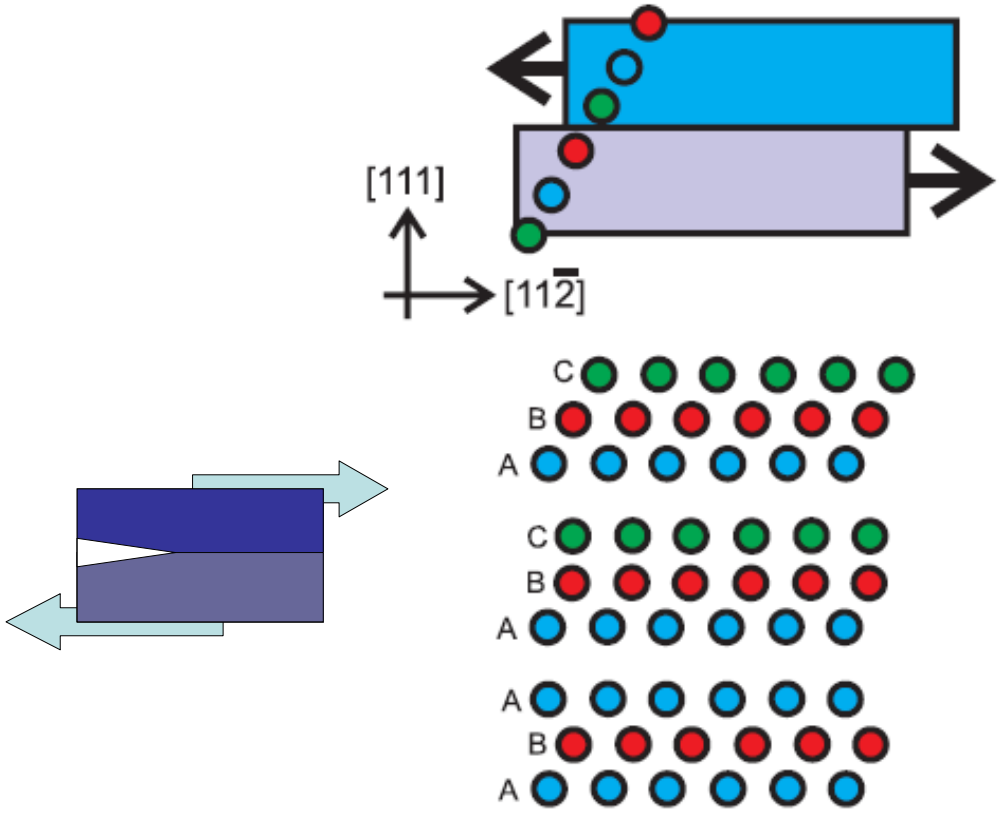


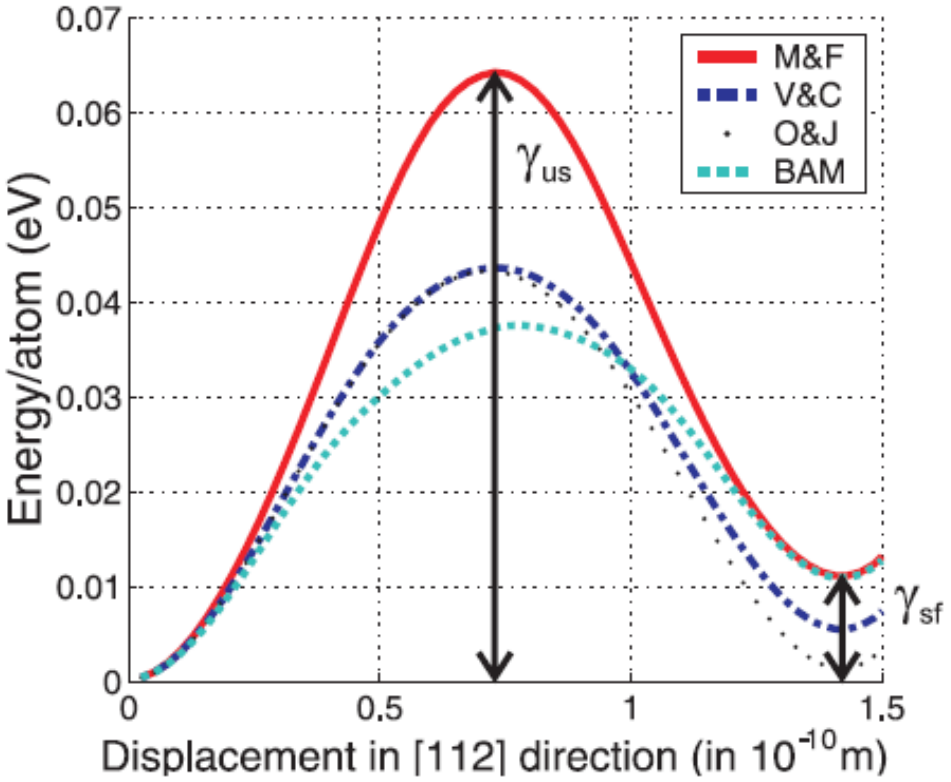


http://www.people.virginia.edu/~lz2n/mse209/Chapter7.pdf

Stacking fault energy

Difficulty of creating a dislocation and moving a dislocation through the crystal

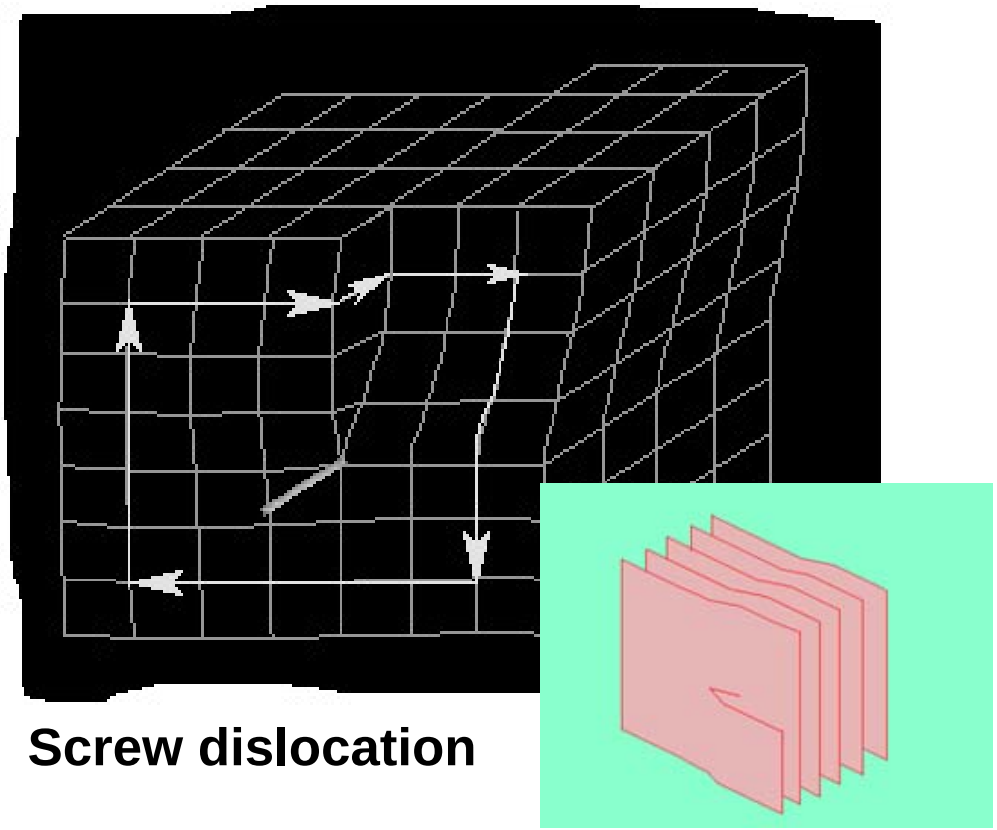




(Buehler, 2006)

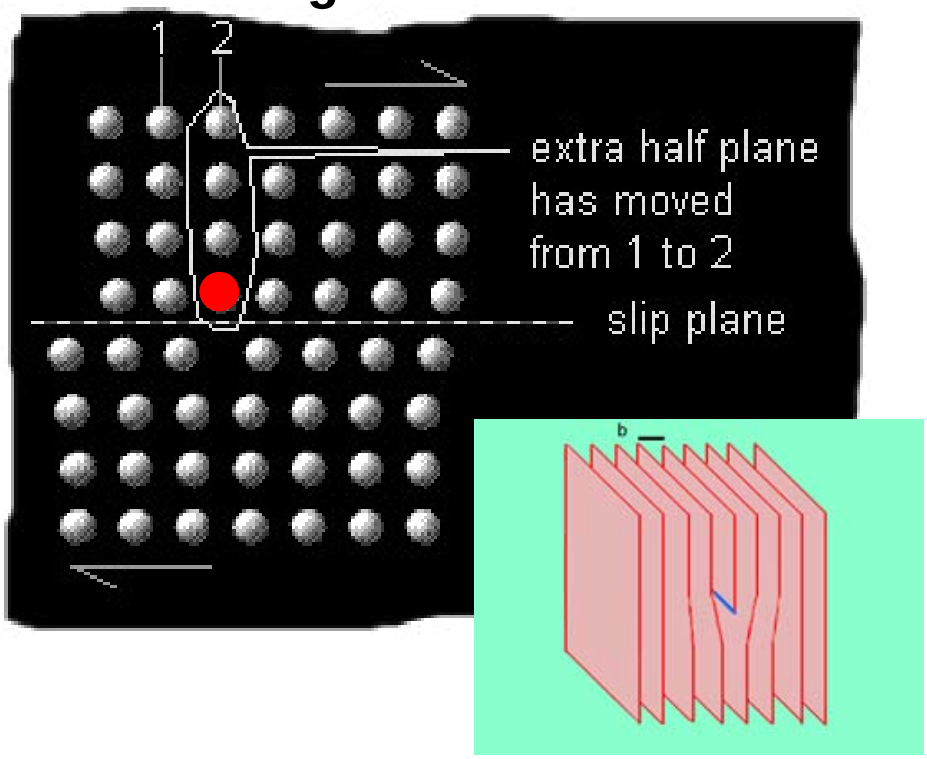
Calculation of stacking fault energy for different interatomic potentials

Edge and screw dislocations



Screw dislocation

Edge dislocation



Dislocation line

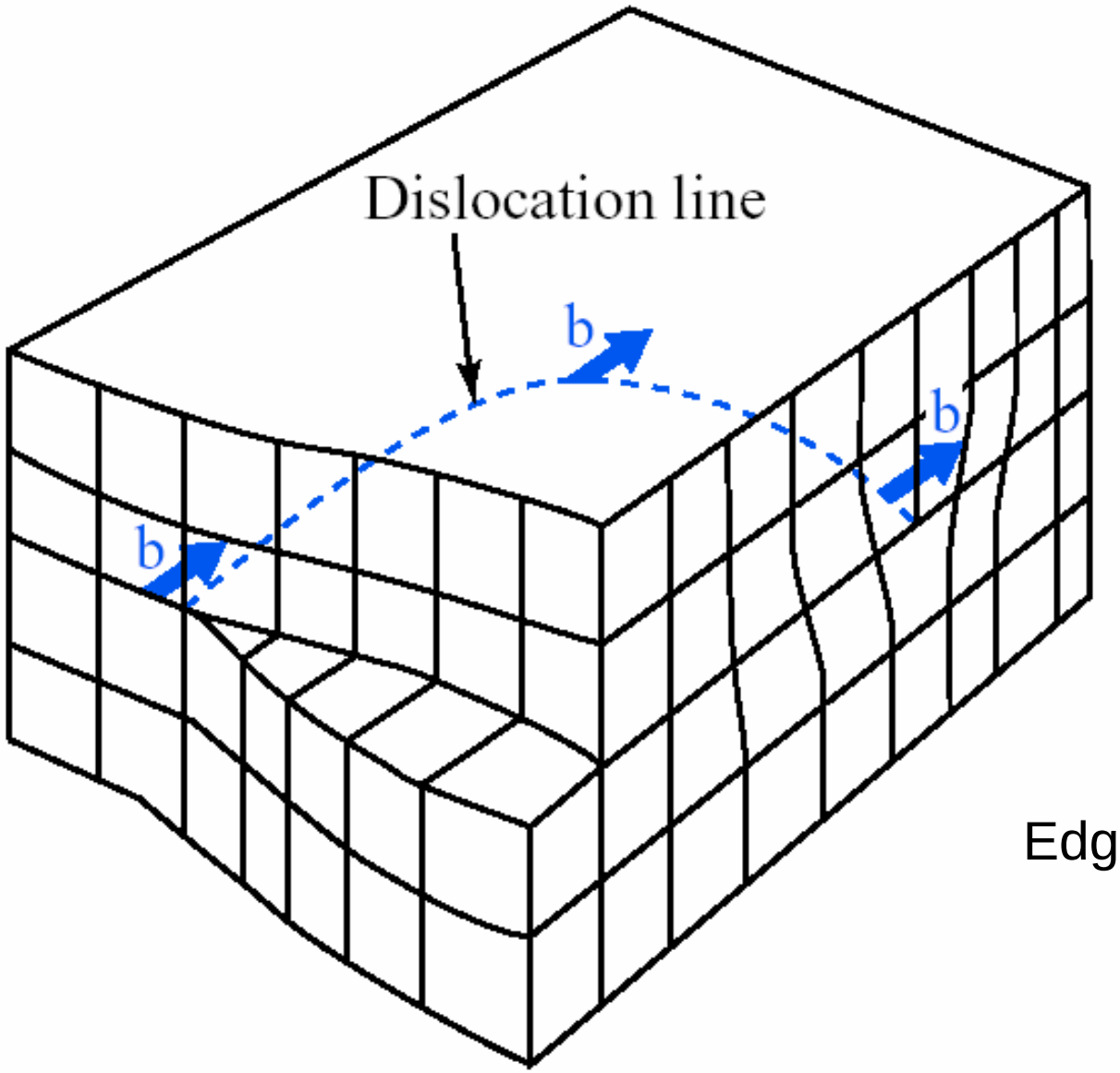
Burgers vector

Screw, edge dislocations

Other crystal defects

Grain boundaries,
vacancies, interstitials

Screw versus edge dislocation

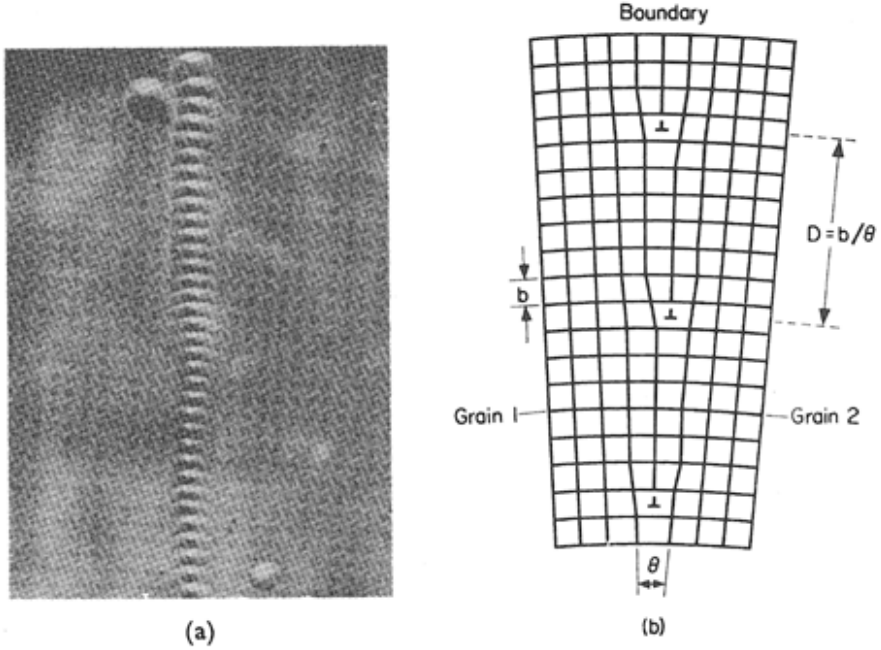


Screw

Edge

Experimental observation

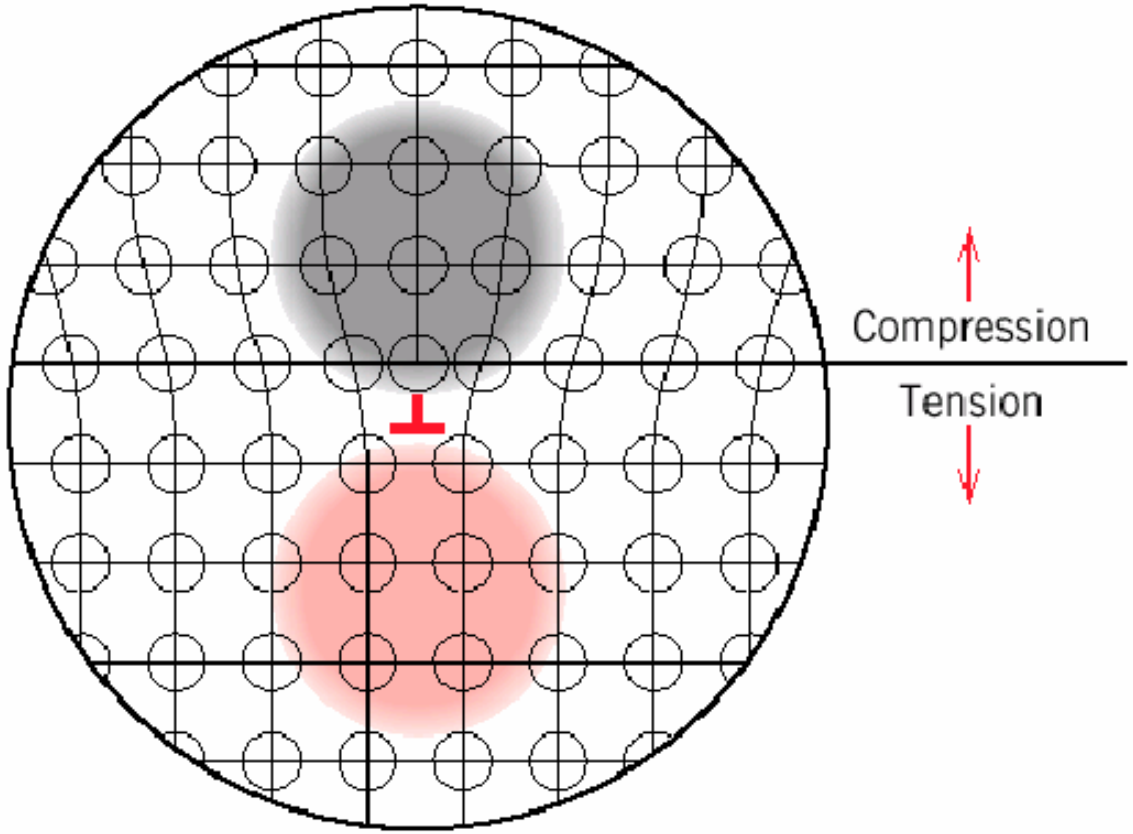
Transmission Electron Micrograph of dislocations (TEM)



GB misfit dislocations

Dieter, G. E. (1988) *Mechanical Metallurgy* ISBN 0071004068
Honeycombe, R.W.K. (1984) *The Plastic Deformation of Metals* ISBN 0713121815
Hull, D. & Bacon, D. J. (1984) *Introduction to Dislocations* ISBN 0080287204
Read, W. T. Jr. (1953) *Dislocations in Crystals* ISBN 1114490660

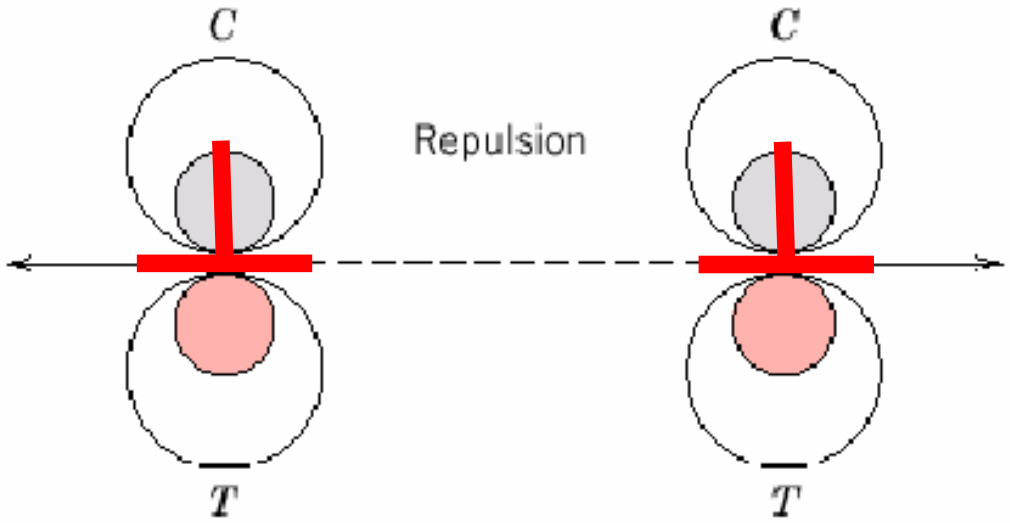
Dislocations: Stress field around a dislocation

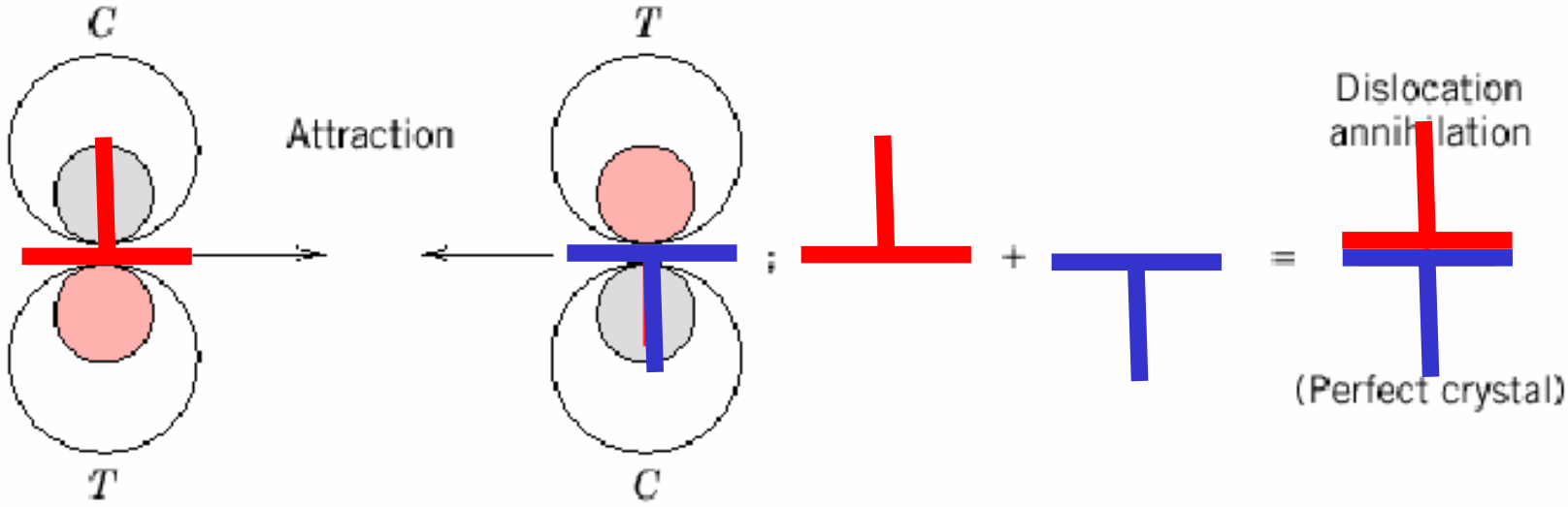


Dislocations lead to a tensile-compressive stress field in their vicinity

Dislocations: Interaction

Important to understand how materials deform





http://dissertations.ub.rug.nl/FILES/faculties/science/2005/s.brinckmann/c2.pdf
http://www.cmat.uni-halle.de/~hsl/Realstruktur/Defects%20VI%20-%20Elasticity%20theory.pdf

Motion of dislocations

$$\vec{F}_d = \left(\sigma \cdot \vec{b}\right) \times \vec{\xi}$$

Peach-Koehler force: Drives dislocation motion

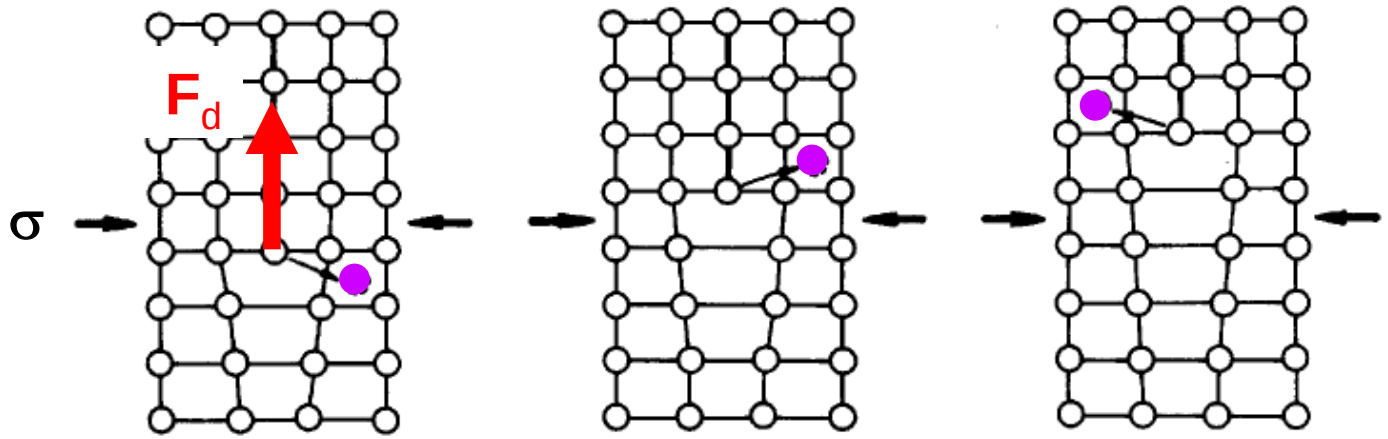
σ Applied stress

Resolved shear stress on dislocation

$\vec{b}$ Burgers vector

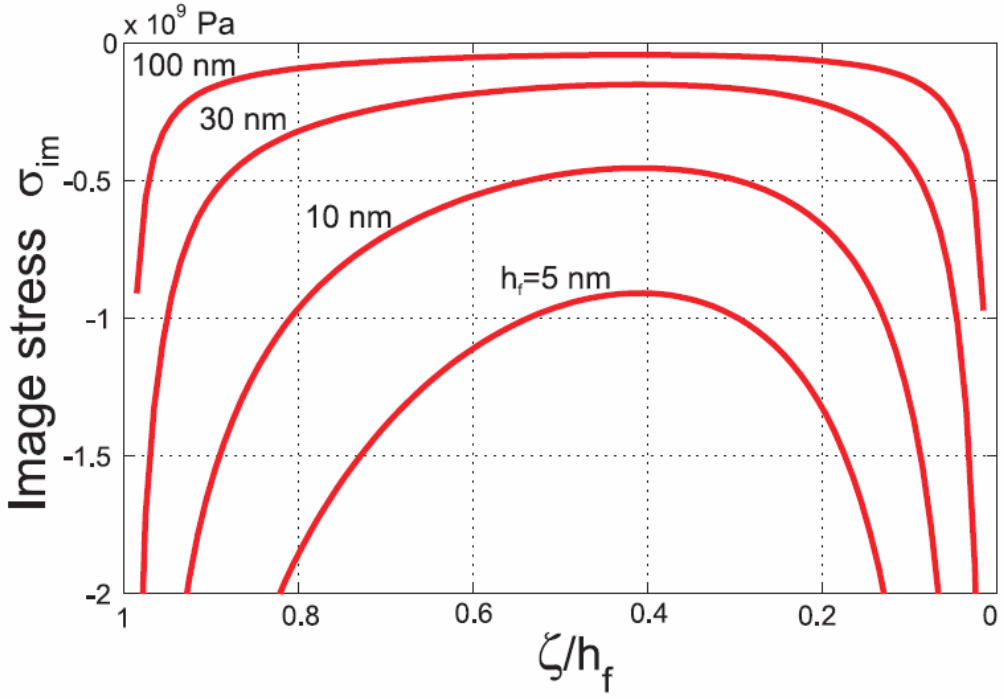
$\vec{\xi}$ Line direction

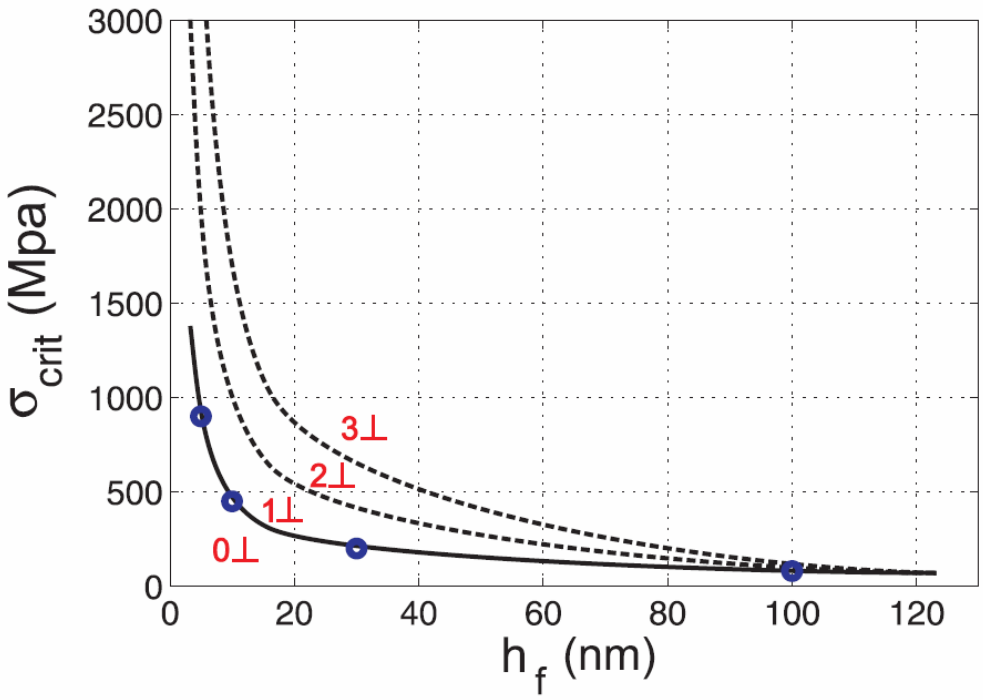
"Climb of dislocations" (nonconservative)

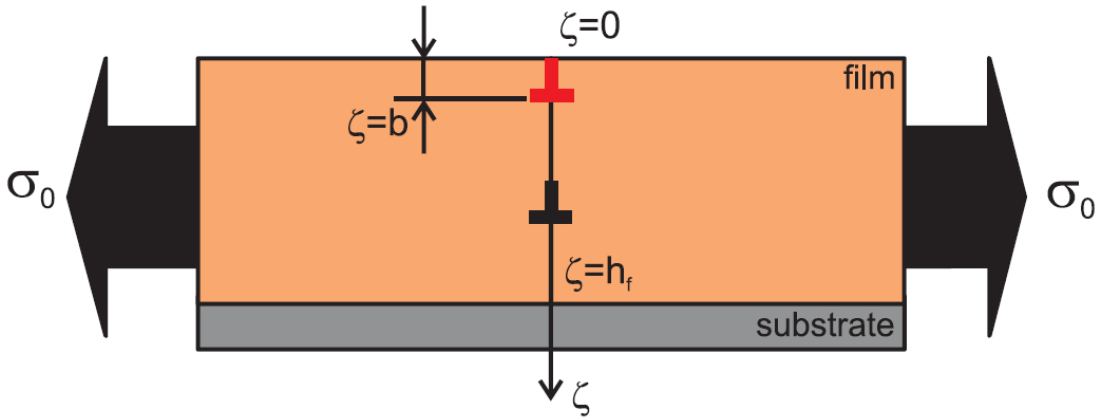


Emission of interstitials during climb

Nano-confinement of dislocations in ultra thin films on substrates



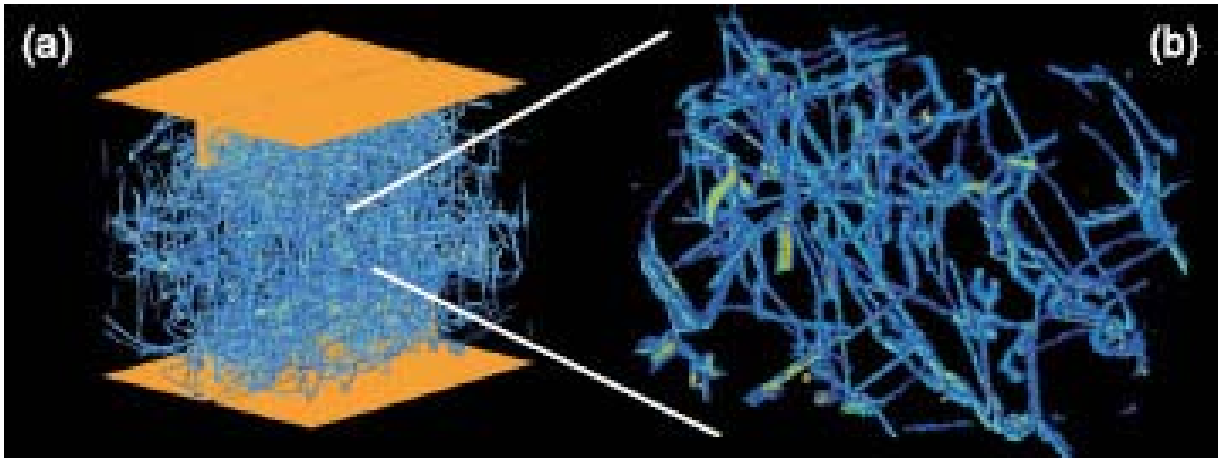


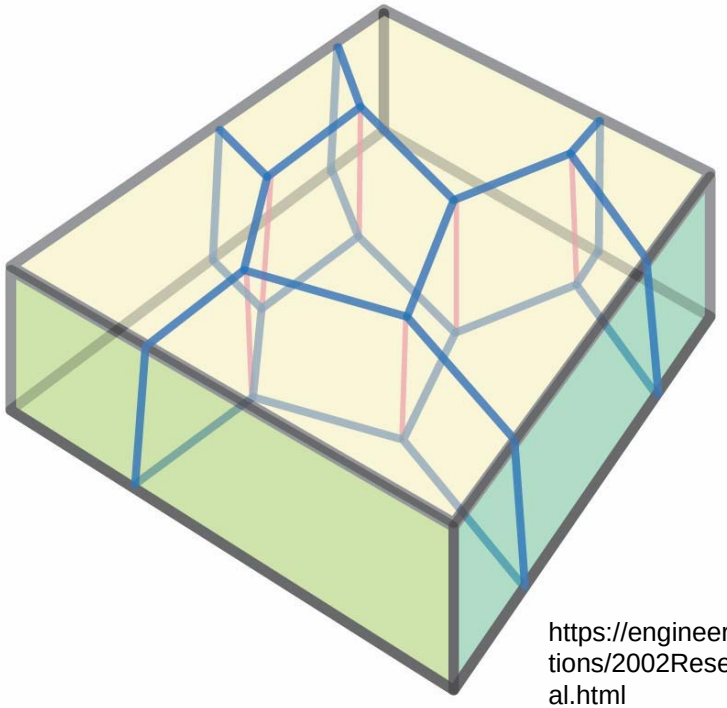


(Buehler *et al*., 2006)

Summary: The nature of dislocations

- Dislocations are complex line defects with complicated interaction with each other and other defects and the crystal lattice
- They are made up out of atoms, but all atoms are not necessary to describe their behavior unless they undergo reactions; long-range interactions
- Dislocations are critical to understand the behavior of many materials, in particular metals
- Modeling of atomistic dislocations with realistic material dimensions of micrometers and beyond has so far been elusive
- Current research efforts e.g. at SNL/LANL are geared towards developing models that describe deformation of materials based on fundamental principles
- Dislocations also appear in molecular crystals; but their role remains unclear

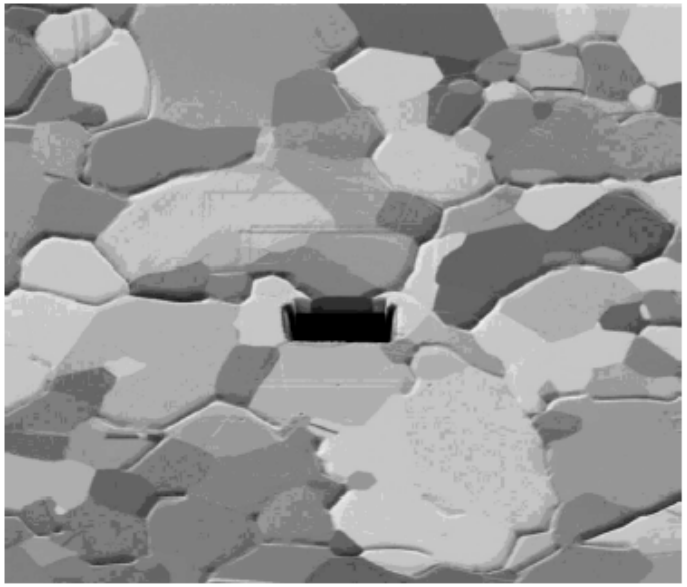




https://engineering.purdue.edu/Engr/Research/Publications/2002ResearchReport/nanotech_spotlight_material.html

Mechanics of ultra thin copper films

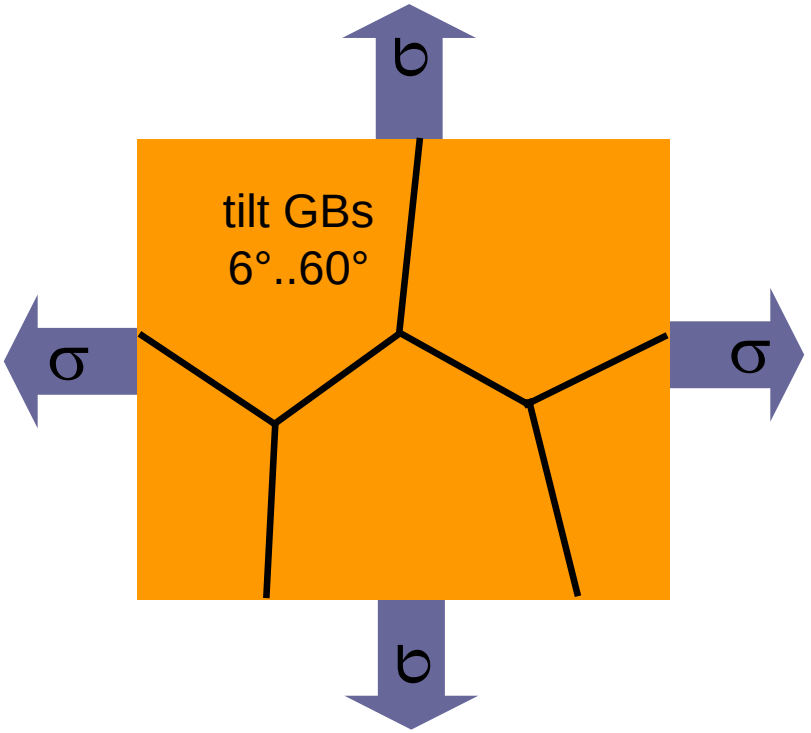
Introduction



Courtesy Dirk Weiss, MIT

Polycrystalline thin metal film of copper grains (111) aligned

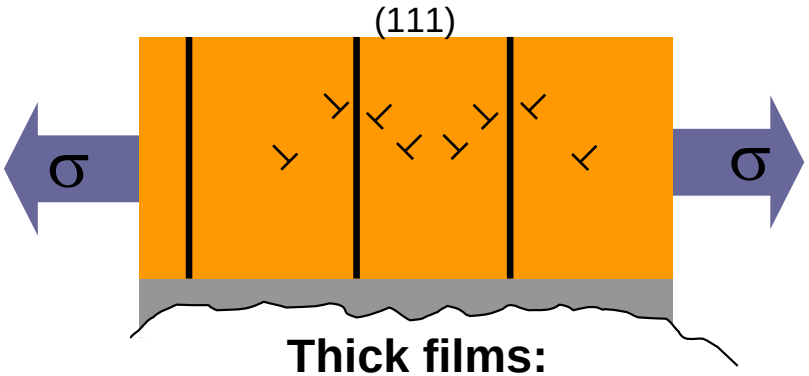
Schematic



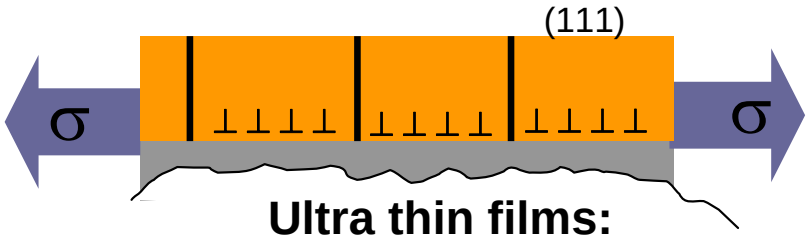
• Biaxial loading by thermal mismatch of film and substrate material: High stresses cause severe problems during operation of the device

• Ultra thin, submicron copper films become critically important in next generation integrated circuits (see, e.g. *Scientific American*, April 2004), MEMS/NEMS

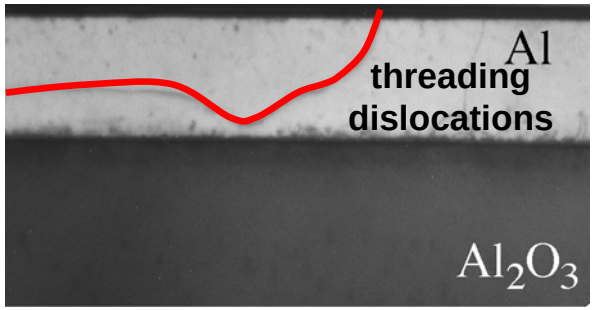
Mechanisms of deformation: Experimental background



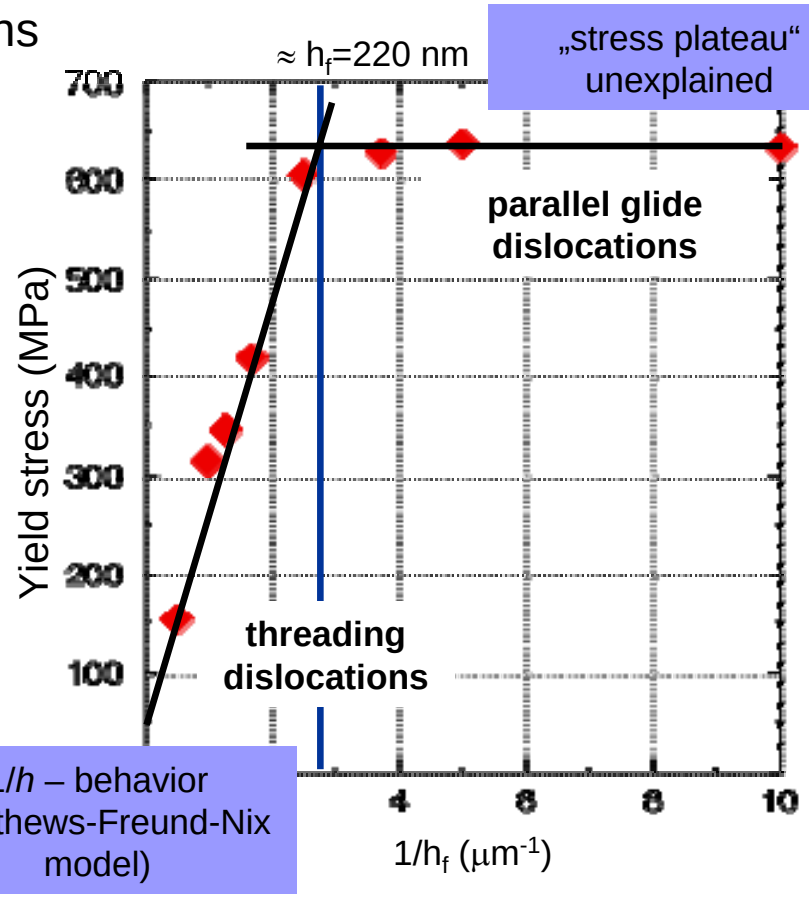
Thick films:
Threading dislocations



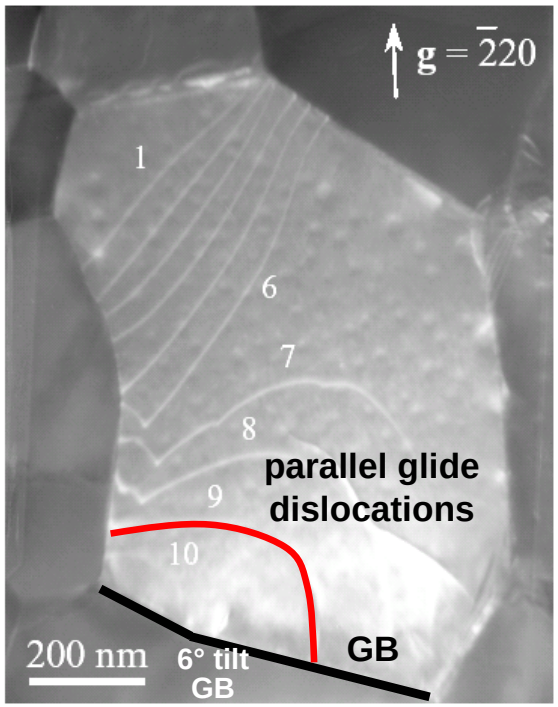
Ultra thin films:
Parallel glide dislocations



(Dehm *et al.* 2002)



1/*h* – behavior (Matthews-Freund-Nix model)

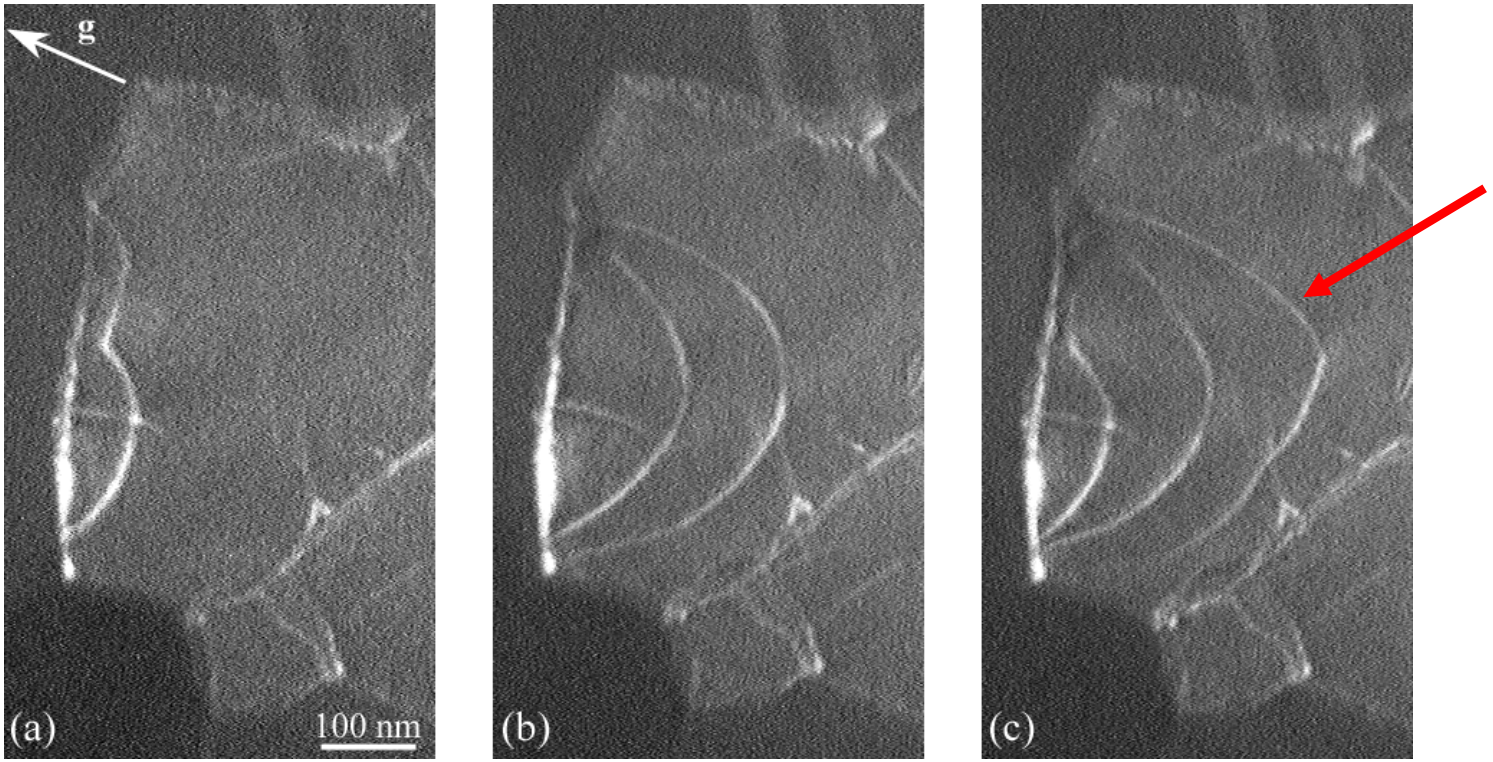


(Balk, Dehm *et al.* 2001, 2002)

Micrometer films

Submicron films

Experimental observation of parallel glide



(Dehm, Balk, von Blanckenhagen, Gumbsch, Arzt, 2002)

Plateau regime (suspected deformation mechanism)

- Surface and grain boundary diffusion with subsequent nucleation of dislocations on parallel slip planes (seen below h=400 nm)
- Sriving force: inhomogeneous stress through grain boundary diffusion (Gao, Zhang, Nix, Thompson, Arzt, 1999)

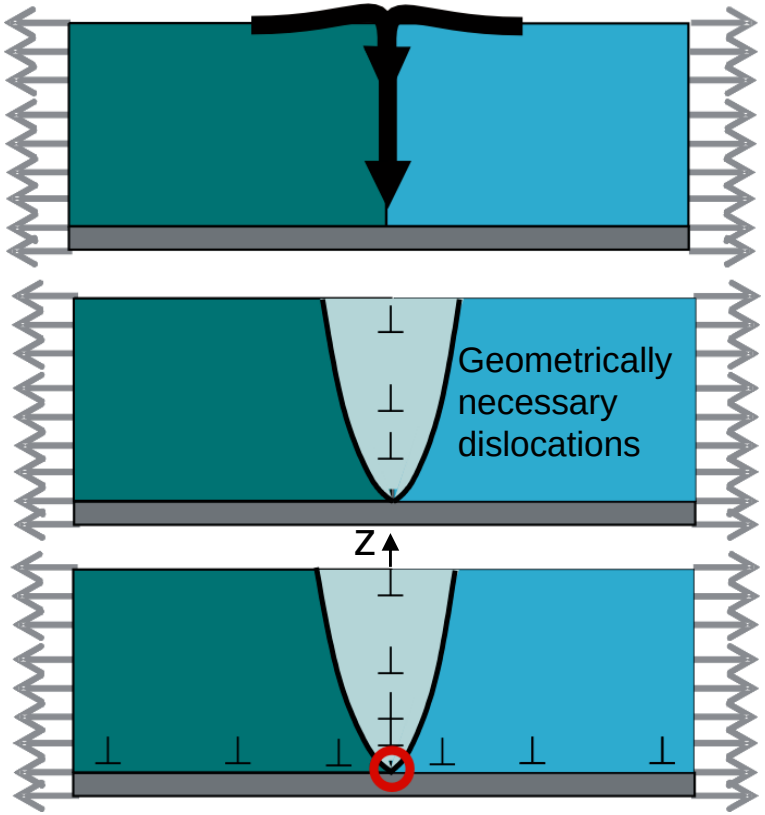
Continuum model: Constrained diffusional creep

Gao *et al., Acta Mat.* (1999):

Step 1: To relax stress, surface atoms diffuse into the grain boundary

Step 2: Form a pileup of climb dislocations
Crack-like diffusion wedge

Step 3: Emission of <u>parallel glide dislocations</u> at the root of the grain boundary



$$\frac{\partial \sigma_{gb}(z,t)}{\partial t} = \frac{E D_{gb} \delta_{gb} \Omega}{4\pi(1-\nu^2)\mathrm{k}T} \int_0^{h_f} S(z,\zeta) \frac{\partial^3 \sigma_{gb}(\zeta,t)}{\partial \zeta^3} \mathrm{d}\zeta$$

Continuum model: Constrained diffusional creep

Gao *et al., Acta Mat.* (1999):

Step 1: To relax stress, surface atoms diffuse into the grain boundary

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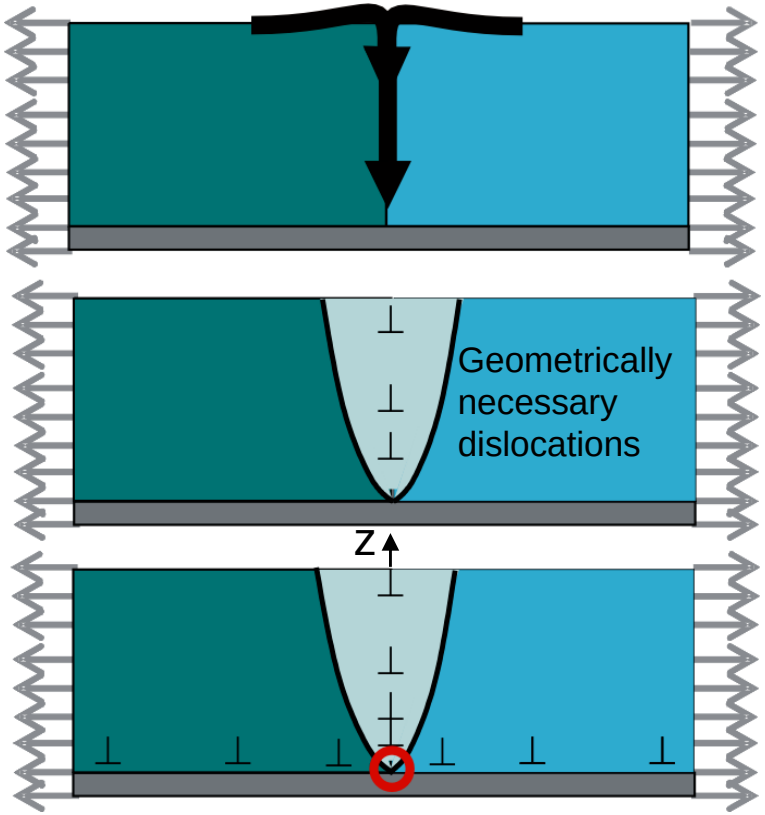
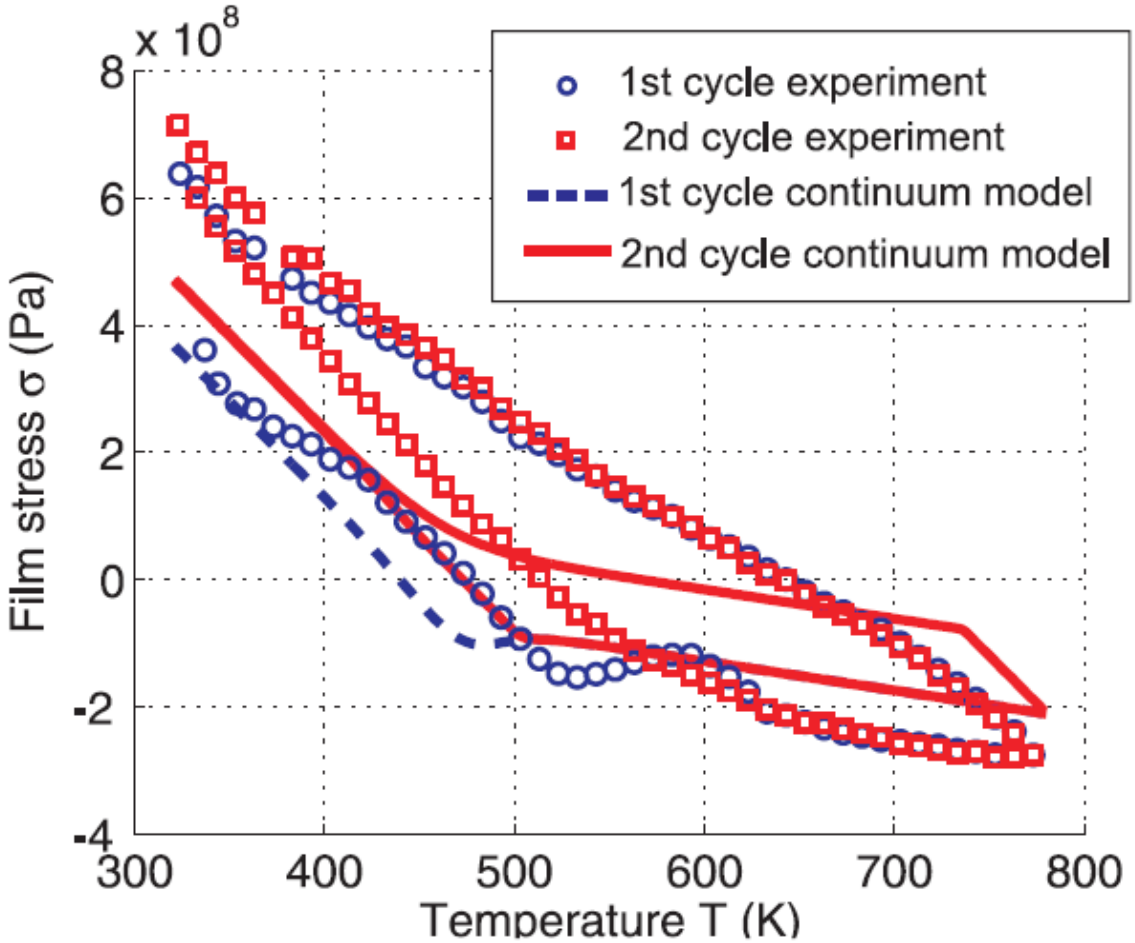
Step 3: Emission of <u>parallel glide dislocations</u> at the root of the grain boundary



Goal: Develop atomistic modeling of these mechanisms to gain further insight into mechanisms

Thermal cycling experiments



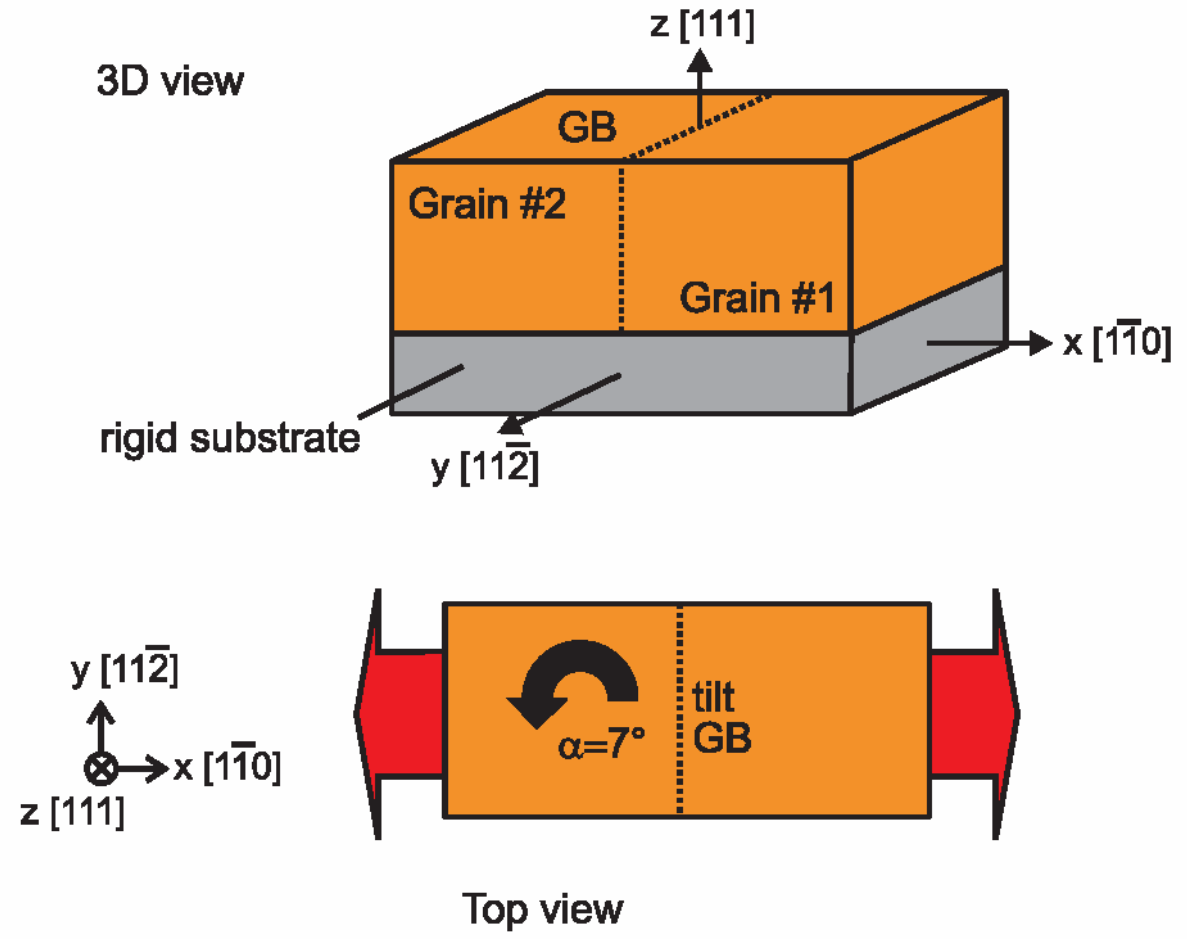
- Compare continuum model with threshold stress to the experimental data of thermal cycling
(Buehler *et al.*)

The film thickness is

h_f = 100 nm

- Measure stress in thin copper film during thermal cycling

Atomistic model

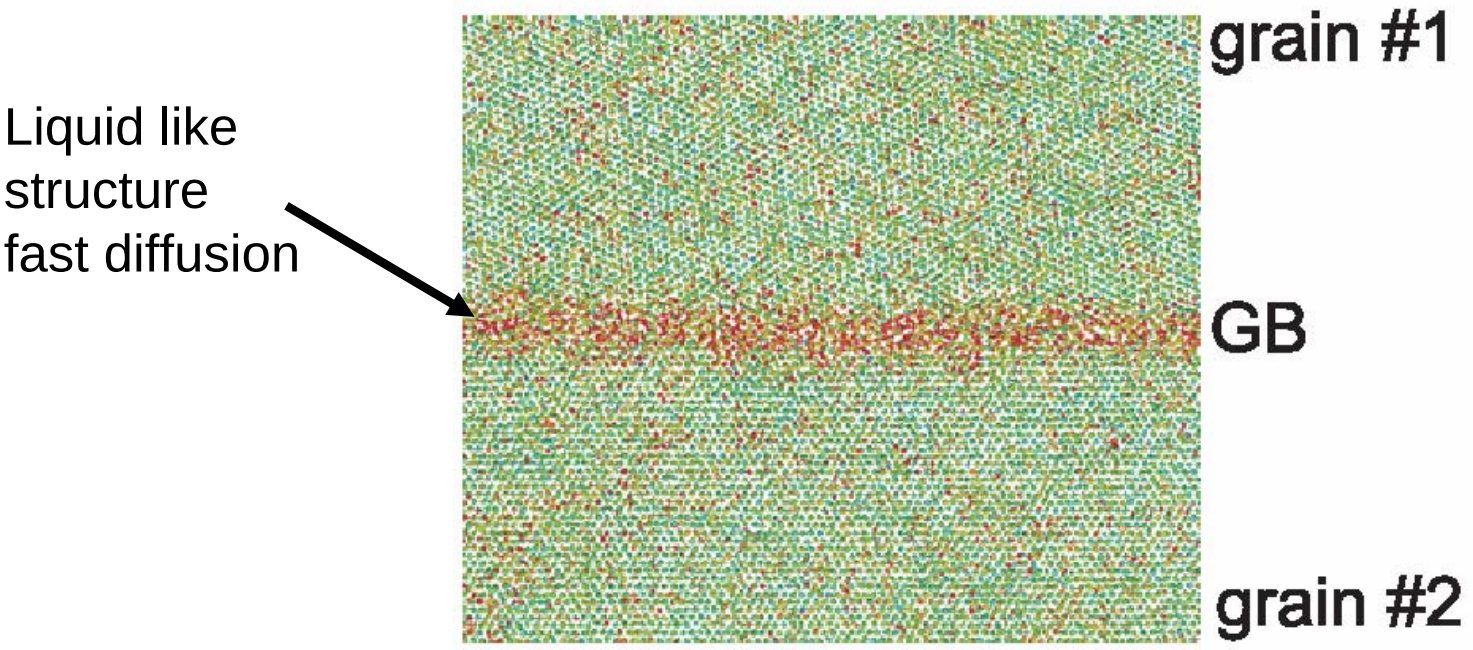


- Copper atoms deposited on a rigid substrate (atoms constrained)
- Use Mishin's EAM potential for copper
- 80%..90% of melting temperature to allow modeling of diffusion with MD at ns timescale (Wolf *et al*., 2001)+ construct high energy GB

Loading applied by displacing the outermost rows of atoms

(Buehler *et al*., MSMSE, 2004)

Liquid-like grain boundary



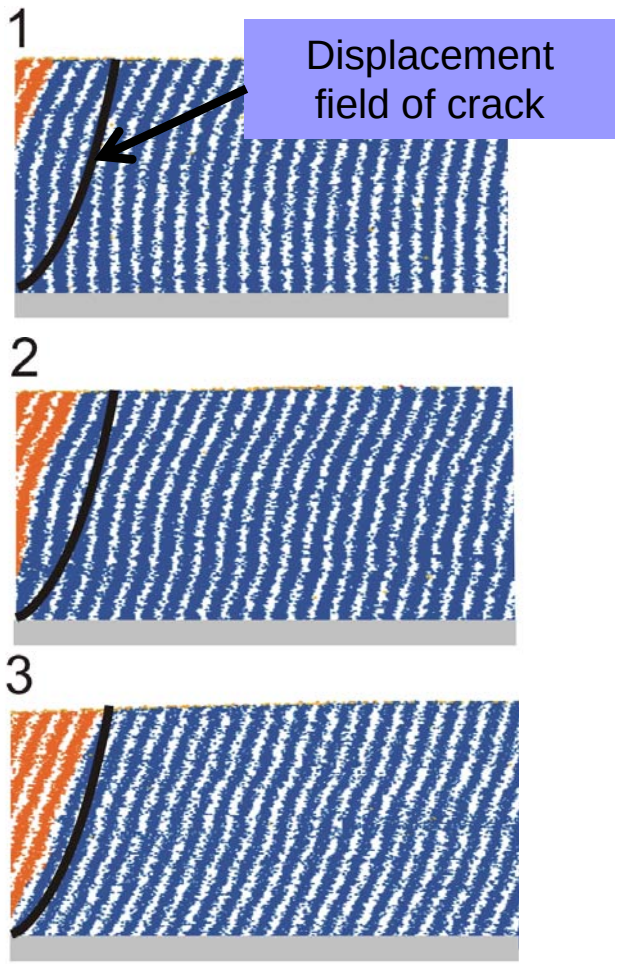
(T=85% of melting temperature)

- We find glassy, liquid-like GB structure at elevated temperatures
- This allows modeling of GB diffusion with molecular dynamics (limited to nanosecond time scale)

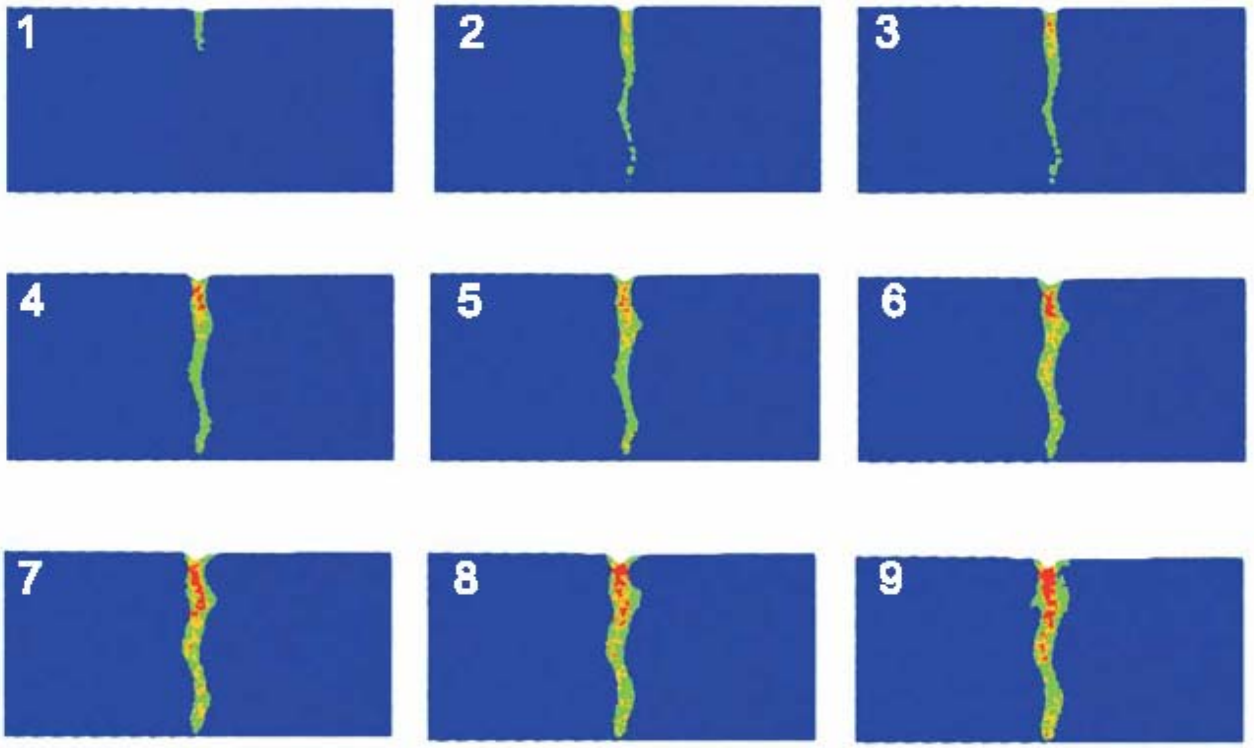
(Buehler, 2004)

Formation of the diffusion wedge

Climb of edge dislocations in the GB



➢ Formation of crack-like field can be correlated with mass transport along GB (towards substrate):

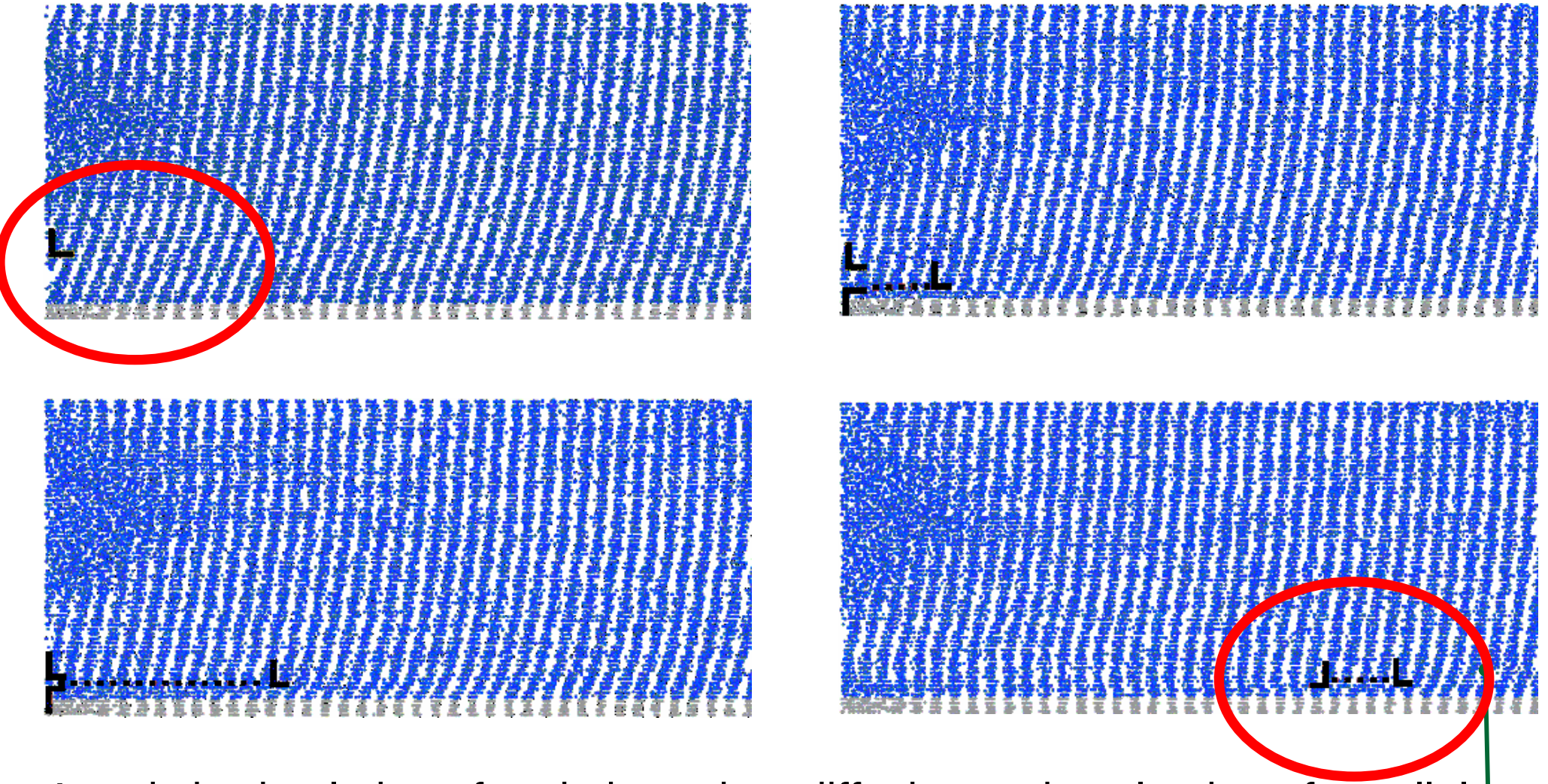


Diffusive displacement along GB toward the substrate

➢ As material is transported into the GB, the field becomes increasingly crack-like

(Buehler *et al*., JMPS, 2003)

Nucleation of PG dislocations

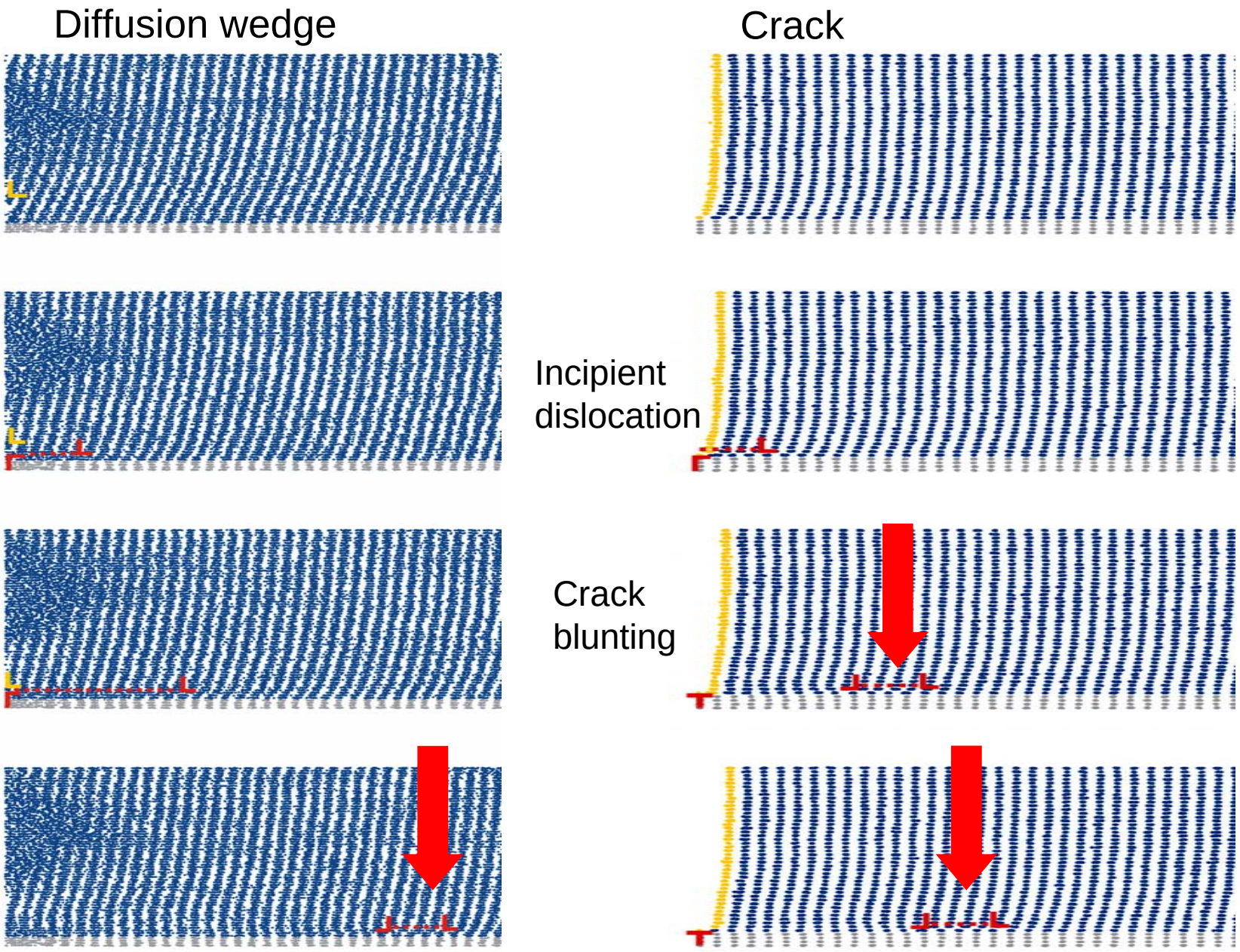


Atomistic simulation of grain boundary diffusion and nucleation of parallel glide dislocations

Lattice planes viewed along [211]

(Buehler *et al*., MSME, 2004)

Nucleation of PG dislocations: Diffusion wedge versus crack



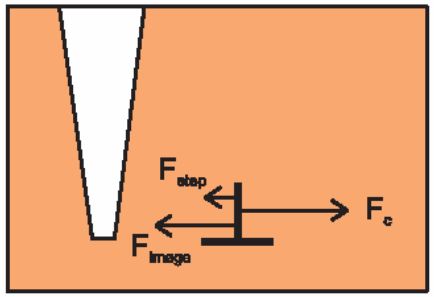
(Buehler *et al.*, JMPS, 2003)

Critical SIF cracks versus diffusion wedge

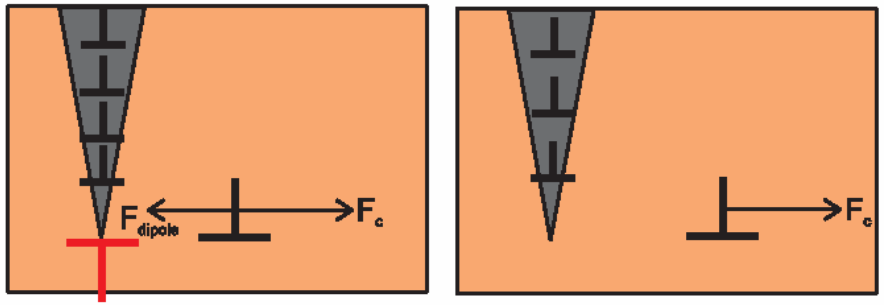
T (K)	h_f (nm)	K^{PG} (MPa × m^s)
Crack		
300	27.2	4.95
Diffusion wedge		
1150	27.2	11.91
1250	27.2	11.35
1250	34.2	11.23

- Concept of SIF is a reasonable concept to link atomistic results to continuum description
- Observe: Critical SIF for diffusion wedge is about twice as large as in the case of a crack

Crack

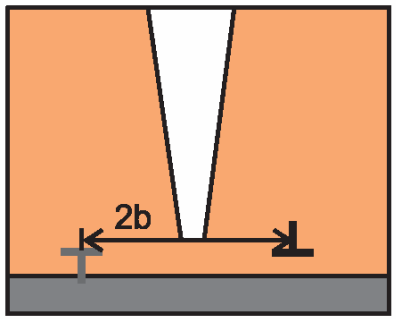


Diffusion wedge

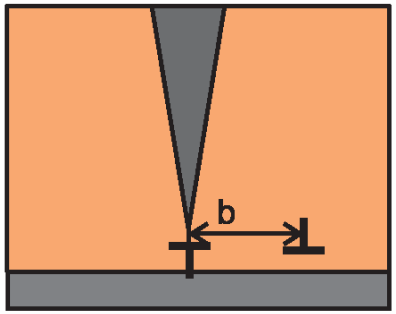


Rice-Thomson model

Crack



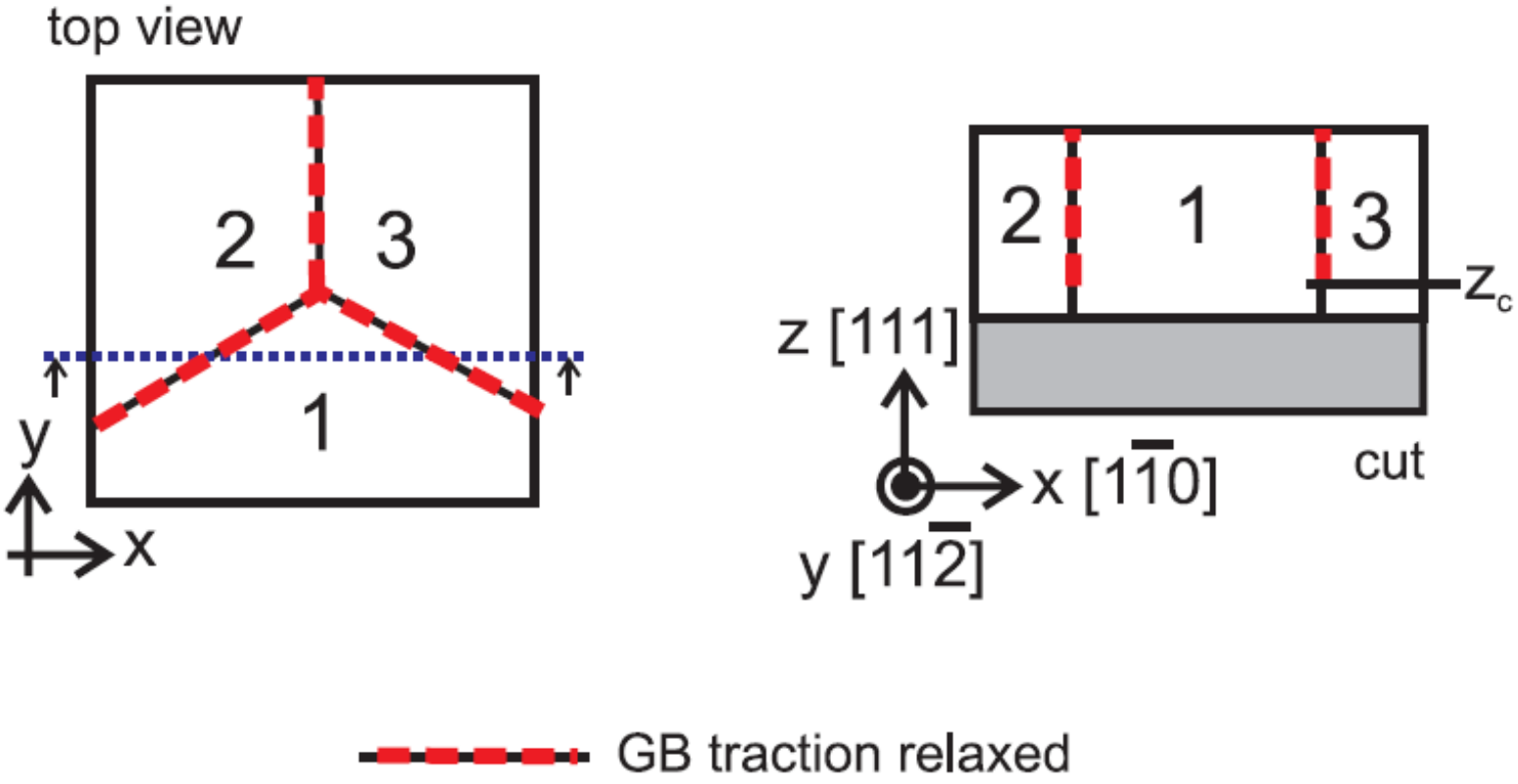
Diffusion wedge



$$K_{\mathrm{cr}}^{\mathrm{PG}} = \frac{E(2\pi b_x)^s}{8\pi(1-\nu^2)} \qquad K_{\mathrm{dw}}^{\mathrm{PG}} = \frac{E(2\pi b_x)^s}{4\pi(1-\nu^2)}$$

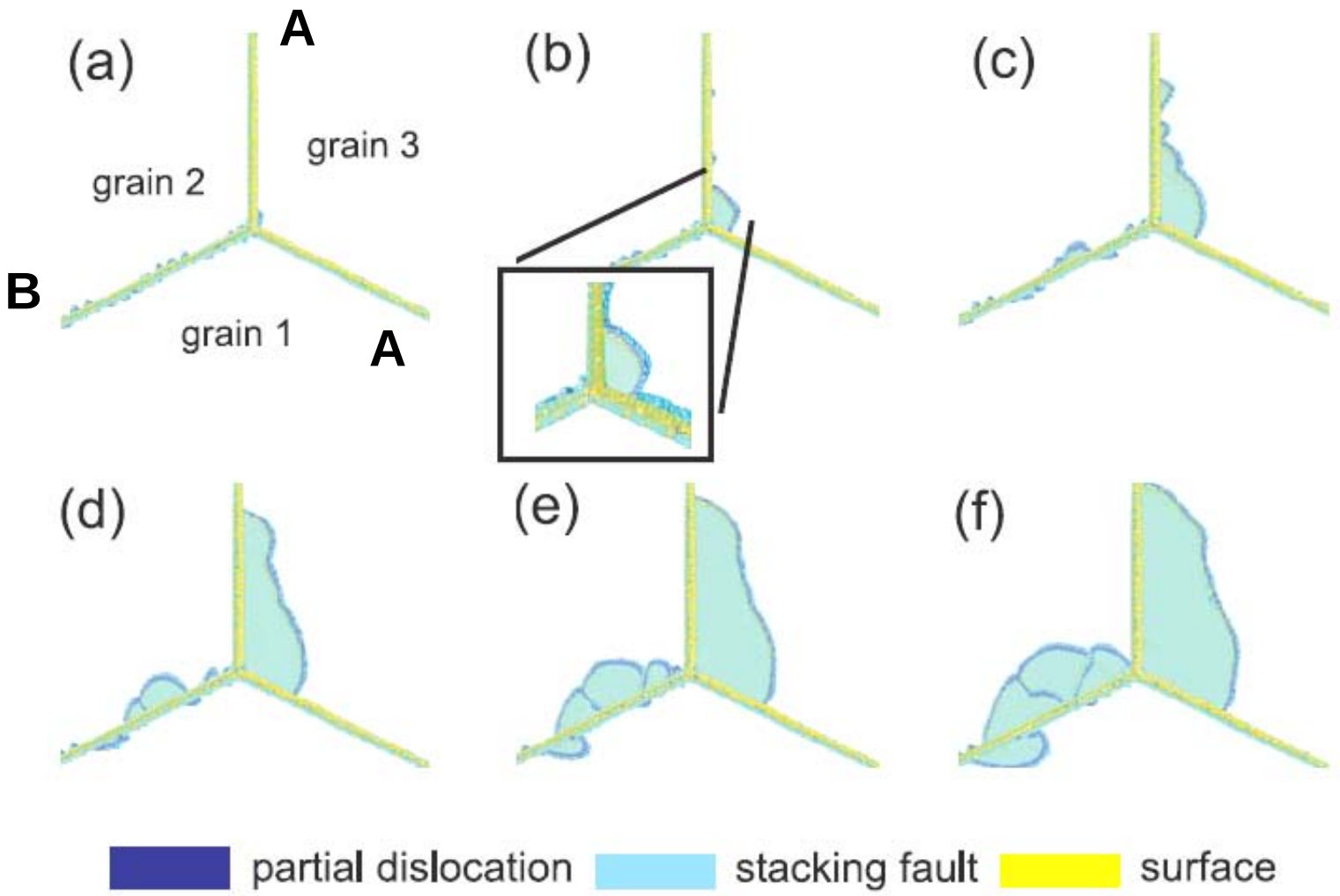
Explains ratio of 2

Extension to triple junction model



Build atomistic model of a triple junction with different types of GBs:
High-energy (disordered)**-A** and low-energy (array of dislocations)**-B**

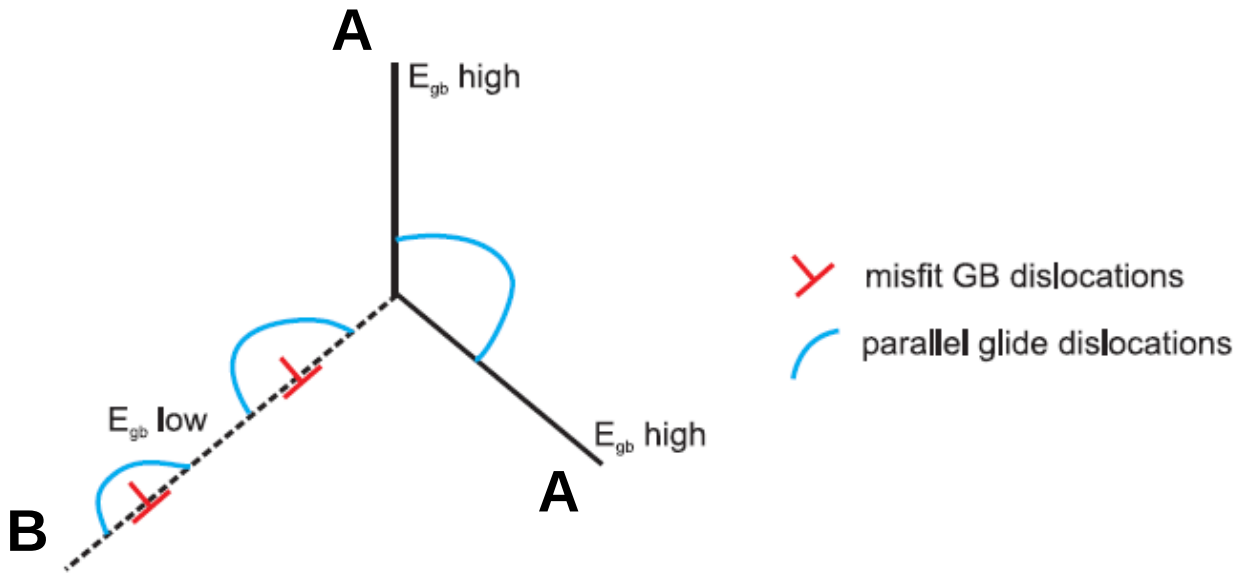
Extension to triple junction model

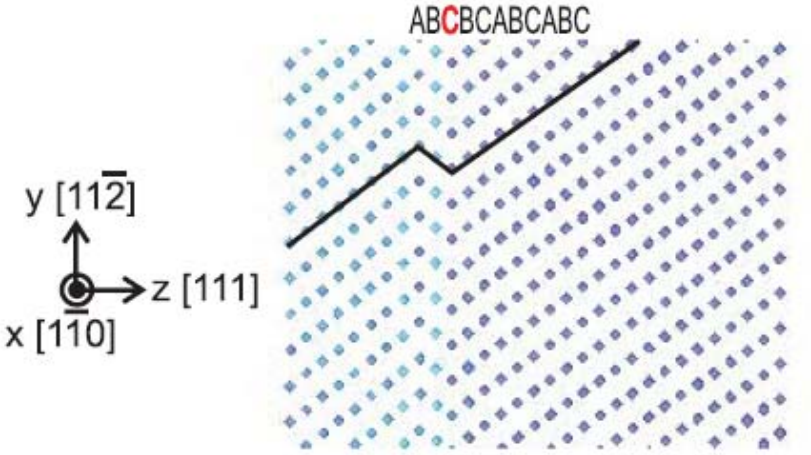


Upon application of biaxial tensile load, observe nucleation of PG dislocations

Misfit GB dislocations to serve as nucleation points for PG dislocations

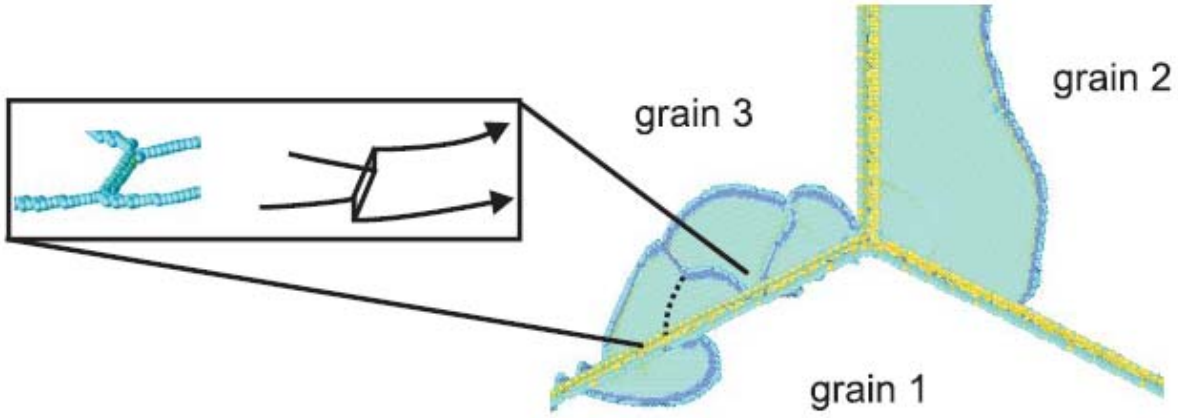
Schematic



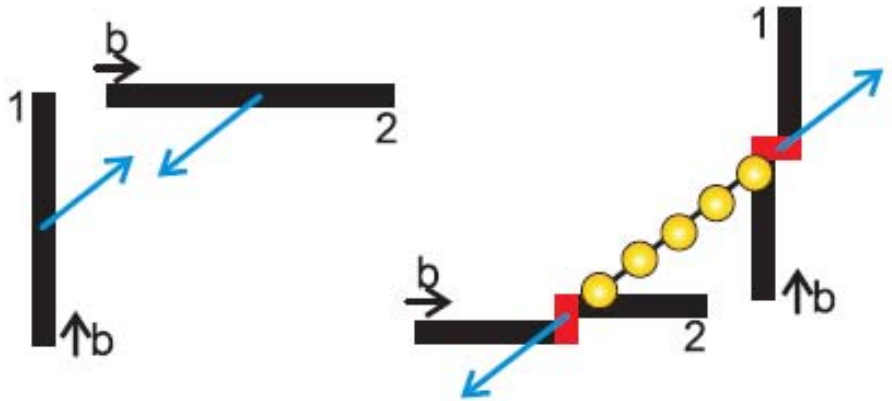


- Deformation twinning by repeated nucleation of partial dislocations.
- Repeated slip of partial dislocations leads to generation of a twin grain boundary.

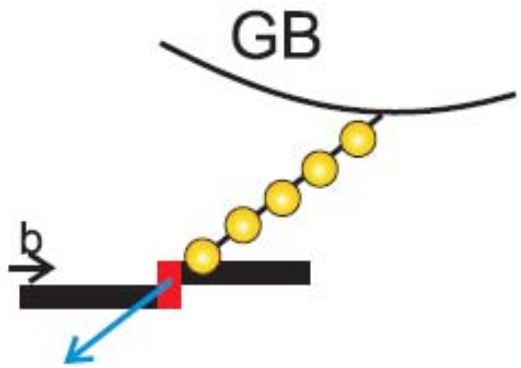
Formation of jogs: Dislocation reactions



- Dislocation junction and bowing of dislocations by jog dragging.
- A trail of point defects is produced at the jog in the leading dislocation, which is then repaired by the following partial dislocation.



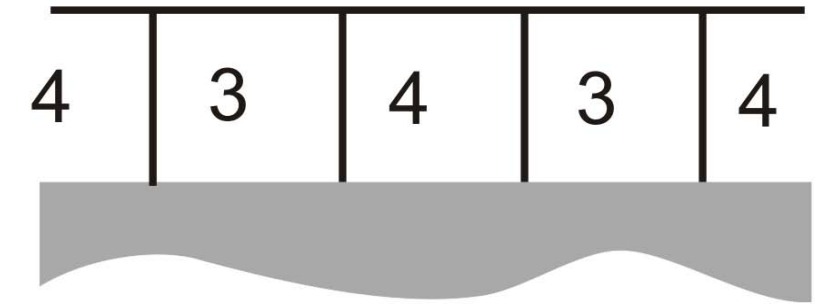
(a)



(b)

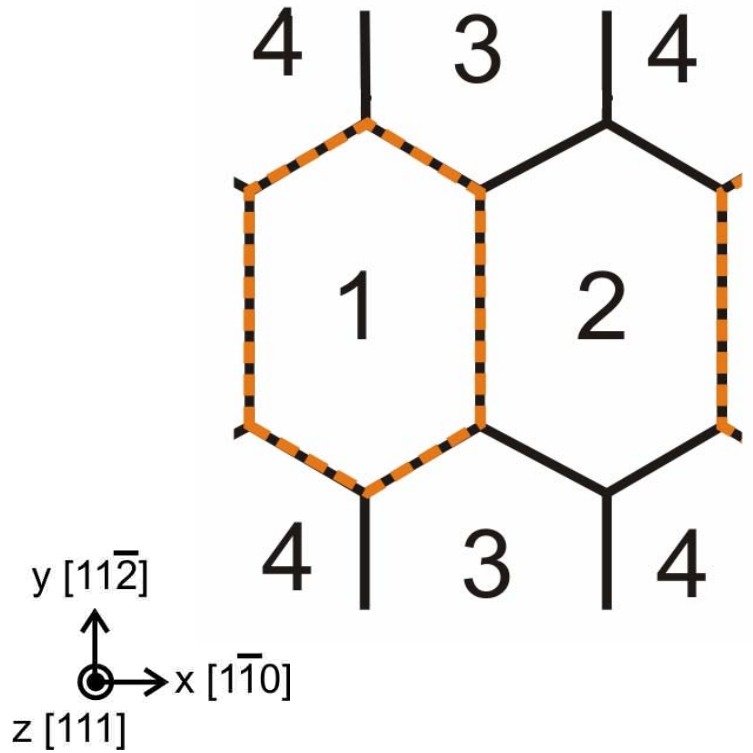
Constrained grain boundary diffusion in polycrystalline models: 3D model

Biaxial loading



High-energy GB

Low-energy GB (misfit dislocations)

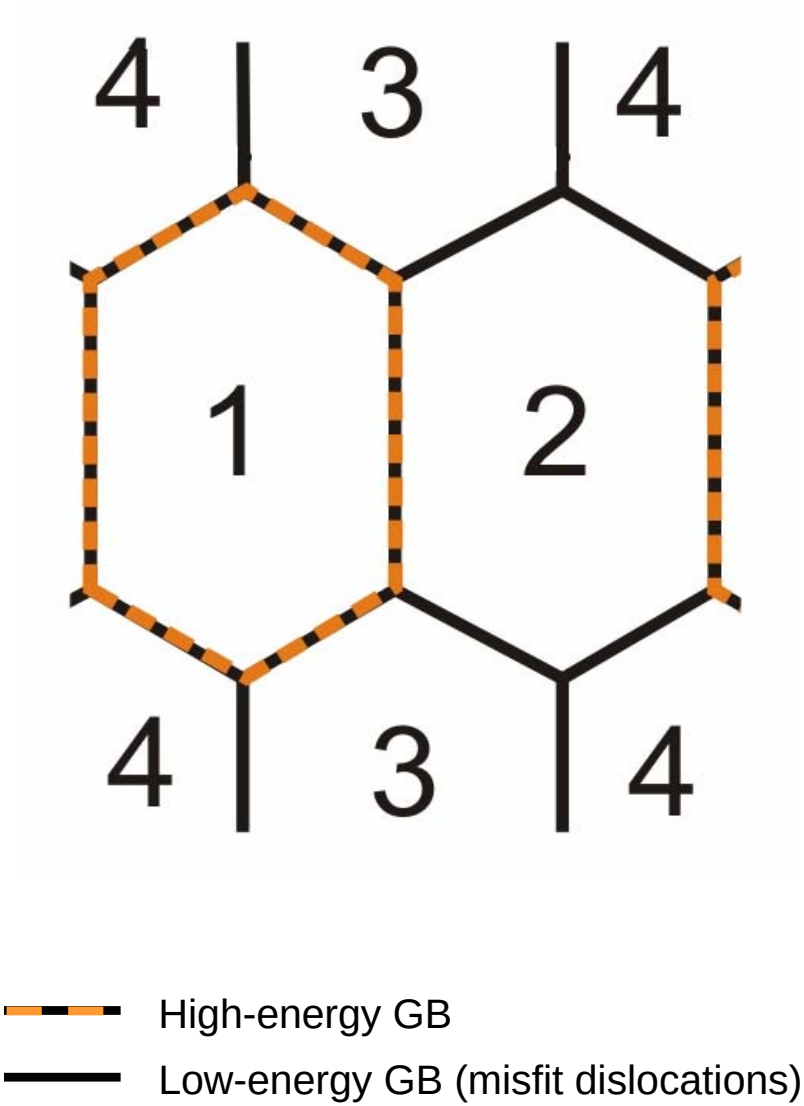


Model:

<u>Polycrystalline sample</u> with low- and high energy grain boundaries (grains rotated around *z* axis, > 2,000,000 atoms, EAM potential for copper- Mishin *et al*., ITAP-IMD code)

• <u>Temperature</u>: About 90 % of melting temperature (similar as Yamakov *et al*.)

Constrained grain boundary diffusion in polycrystalline models

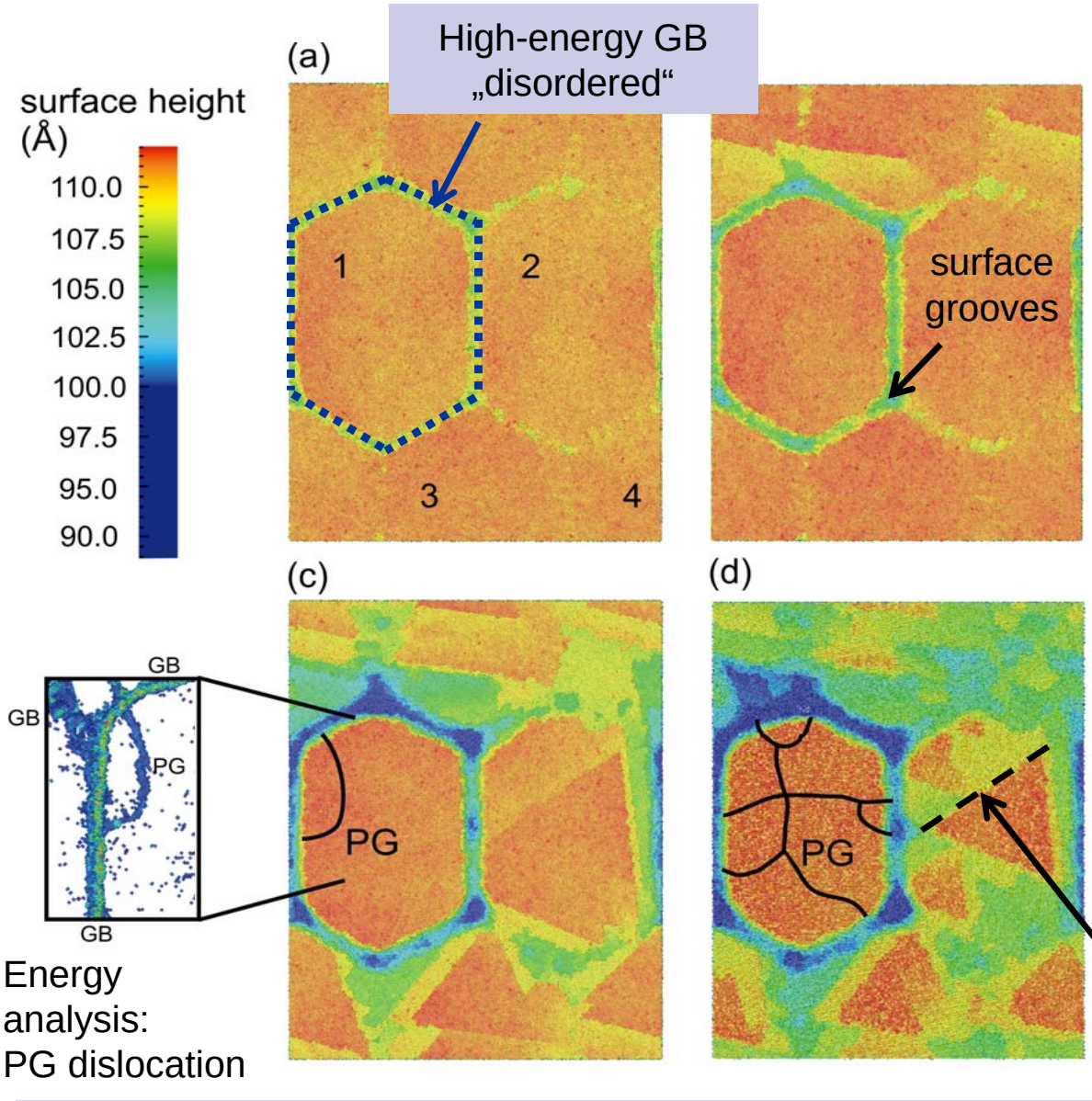


Theoretical predictions

• Diffusional creep strong along high-energy GBs (Wolf *et al.*), should lead to stress relaxation and development of crack-like stress field, leading to PG dislocations according to Gao (1999)

• Along low-energy GBs, threading dislocations should prevail (since no GB traction relaxation possible by diffusion)

Polycrystalline atomistic model



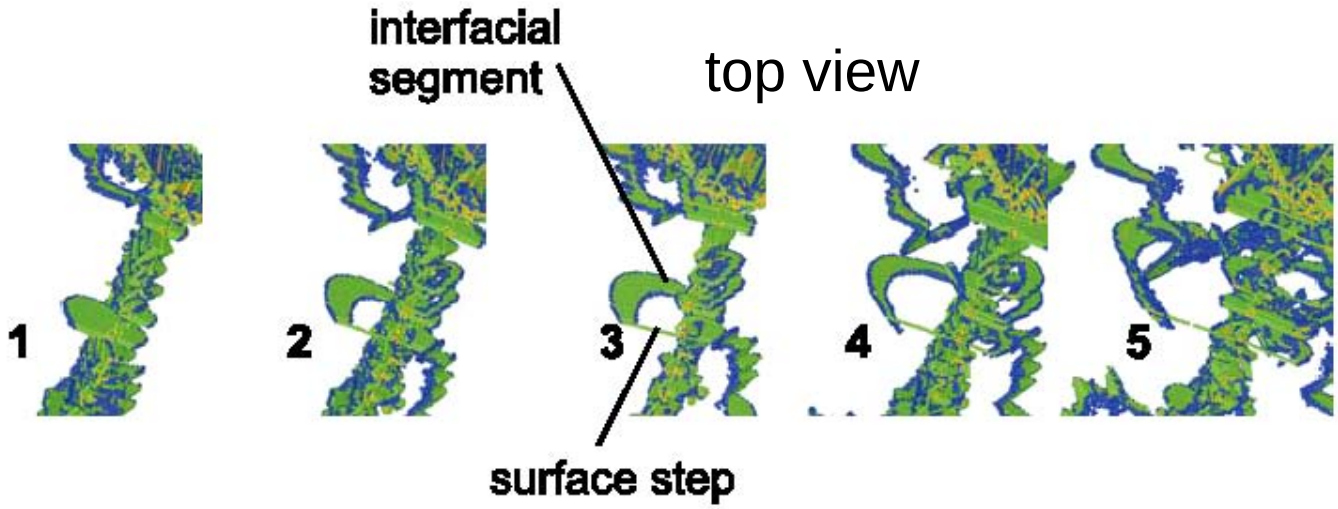
Main results

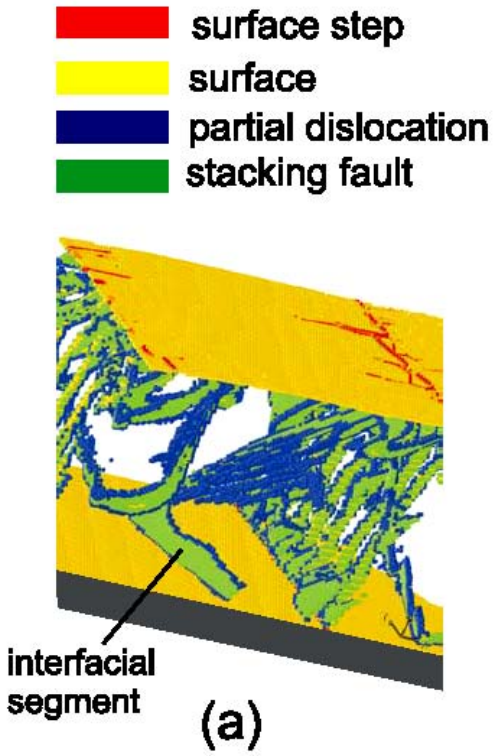
- Diffusion wedges develop preferably at high-energy GBs (fast diffusion paths)
- Diffusion wedges lead to PG dislocations (black lines), otherwise: Threading dislocations.
- No threading dislocations in grain surrounded by high-energy GBs

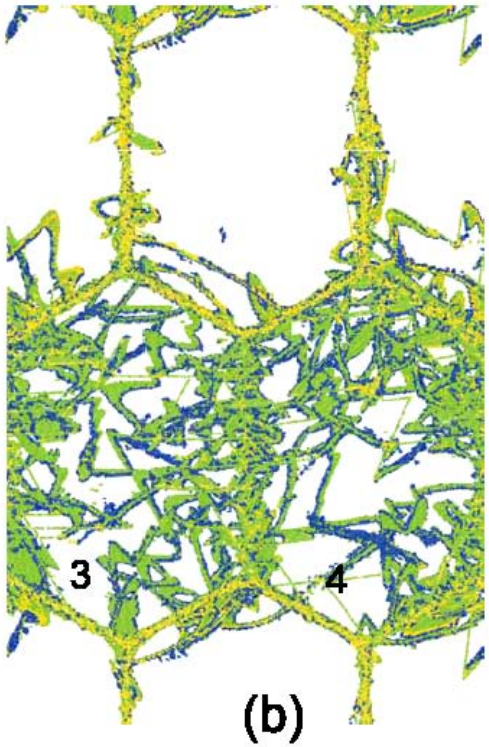
➢ High-energy GBs: Liquid-like structure – fast diffusion paths

Threading and parallel glide dislocations

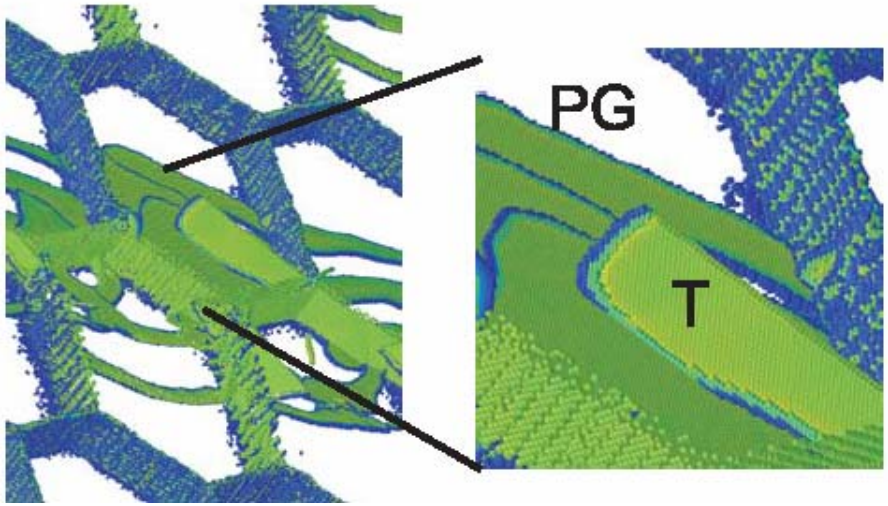
- Nucleation of threading dislocations: Creation of surface steps and interfacial segment



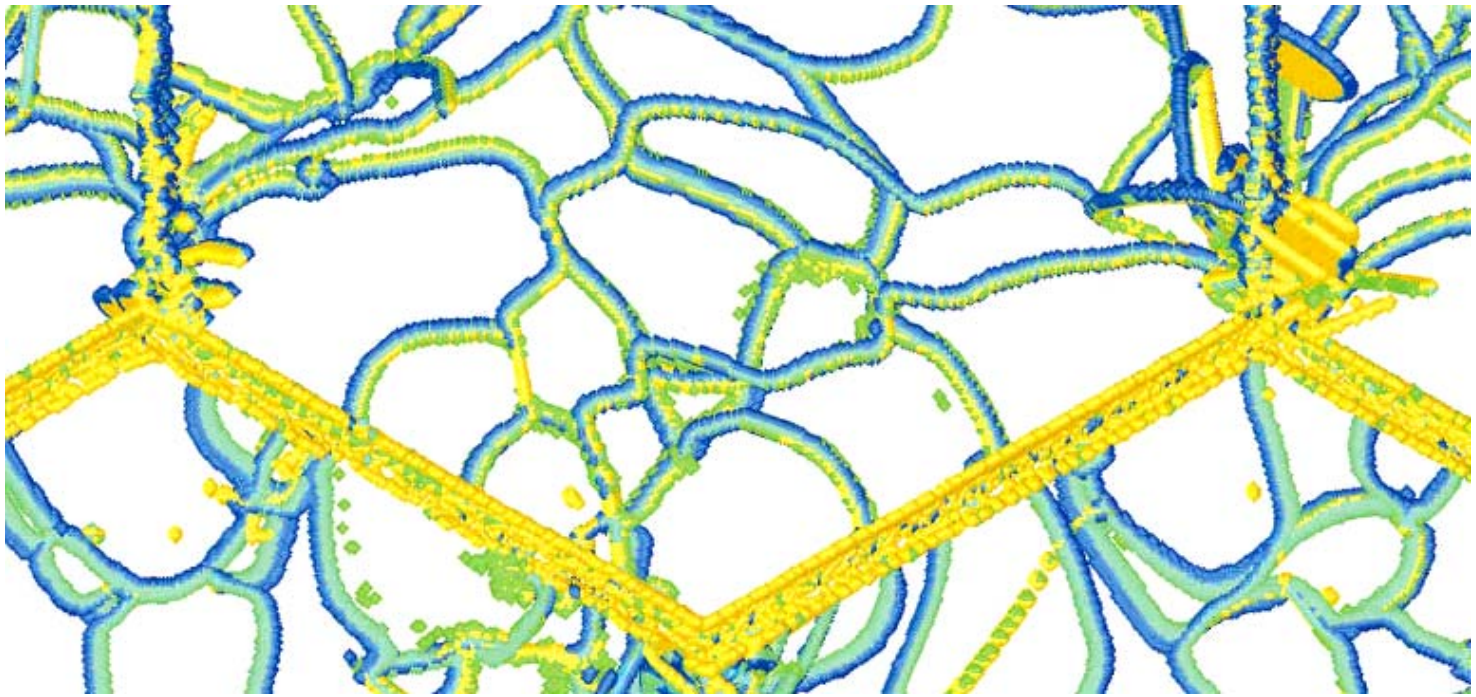




Competition of threading and parallel glide dislocations



Formation of dislocation networks

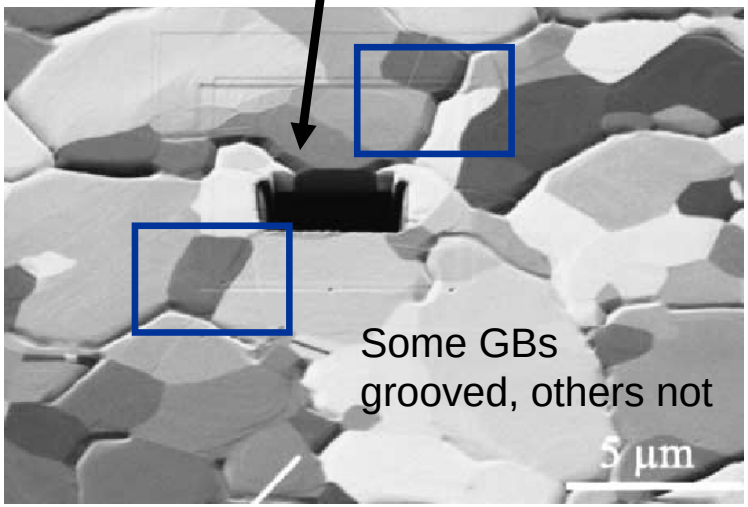


• The plot shows an analysis of the complex dislocation network of partial parallel glide dislocations that develops inside the grains.

• All defects besides stacking fault planes are shown in this plot.

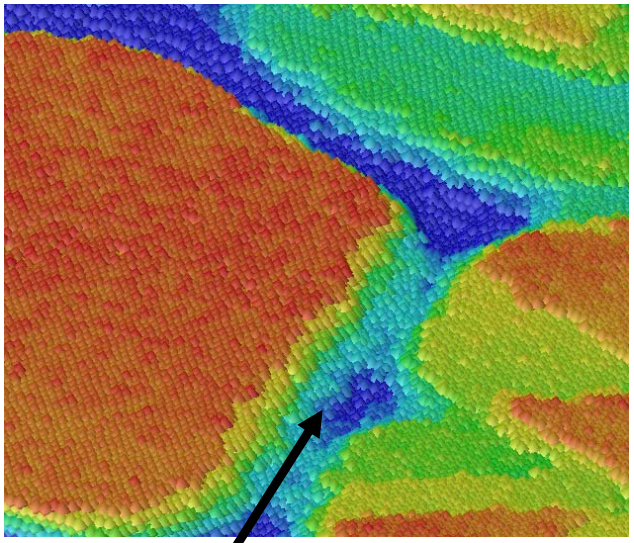
Qualitative comparison of MD results with experiment

Surface grooves

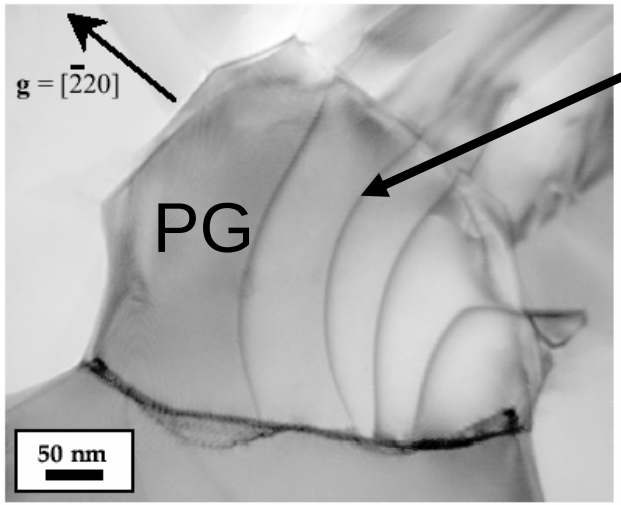


Experiment (Weiss *et al.*)

MD simulation

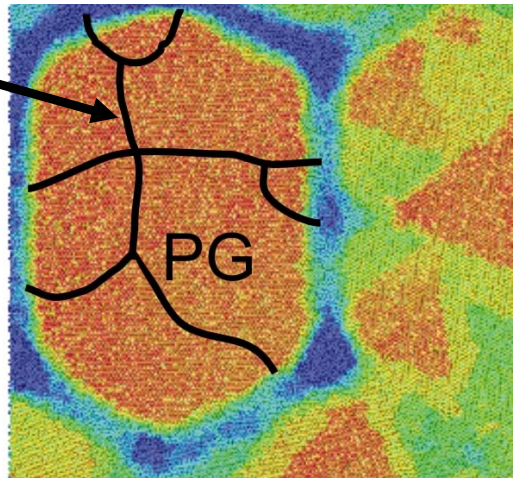


Surface grooves
at specific GBs

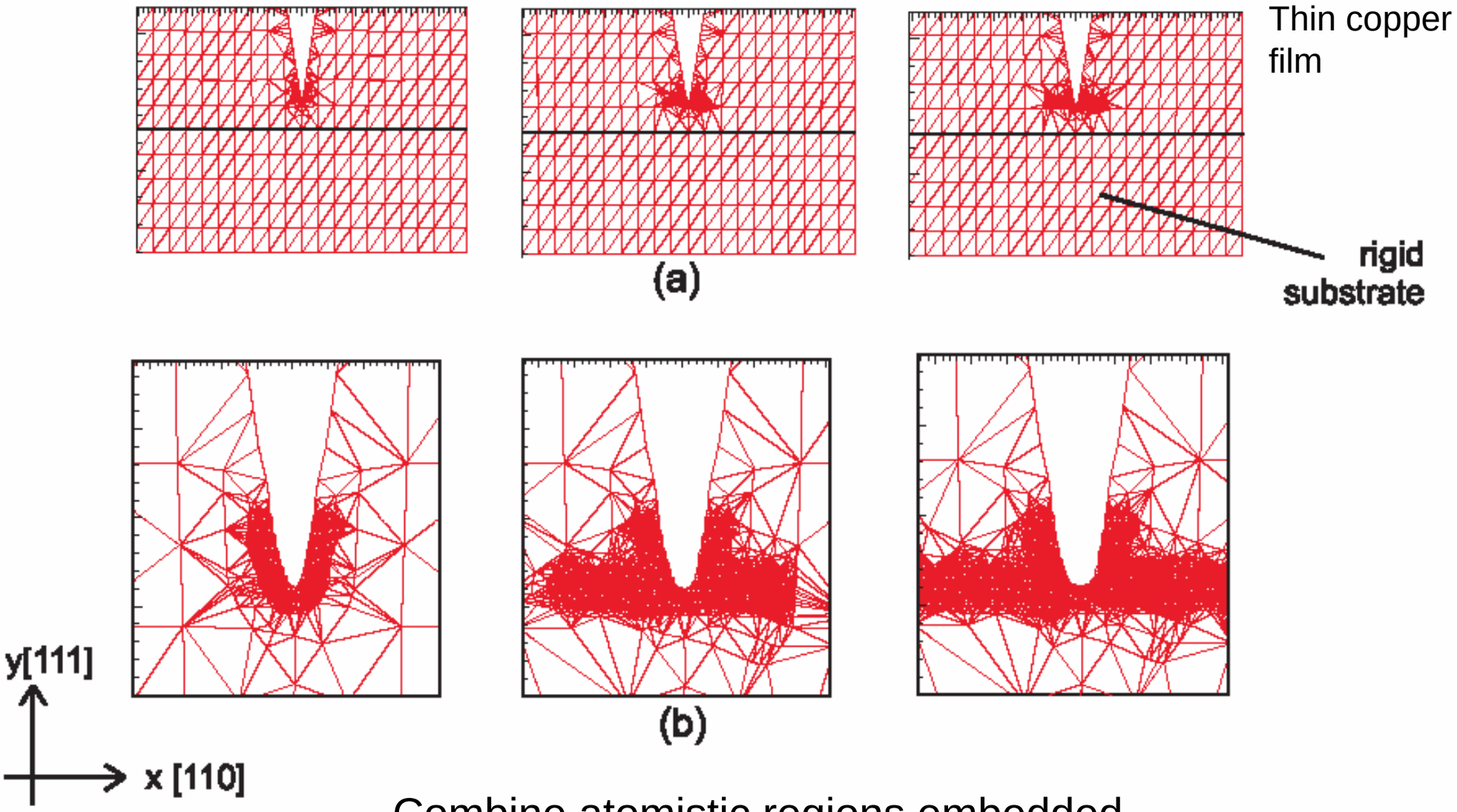


Experiment (Balk *et al.*)

PG
dislocations
in some grains



The Quasi-Continuum (QC) Method

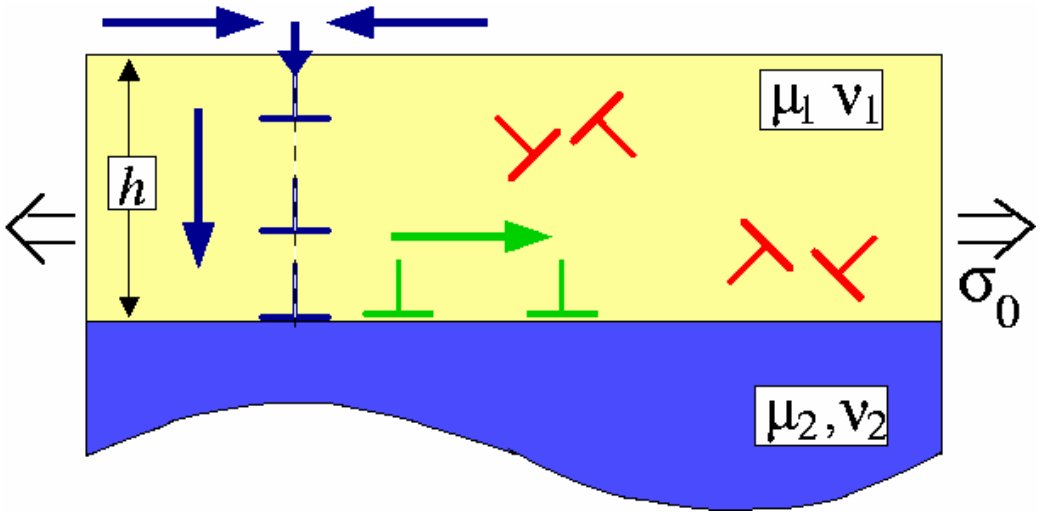


Combine atomistic regions embedded in continuum region

(Buehler *et al*., 2006)

Mesoscopic model

Dislocations: Sources and sinks of plastic strain

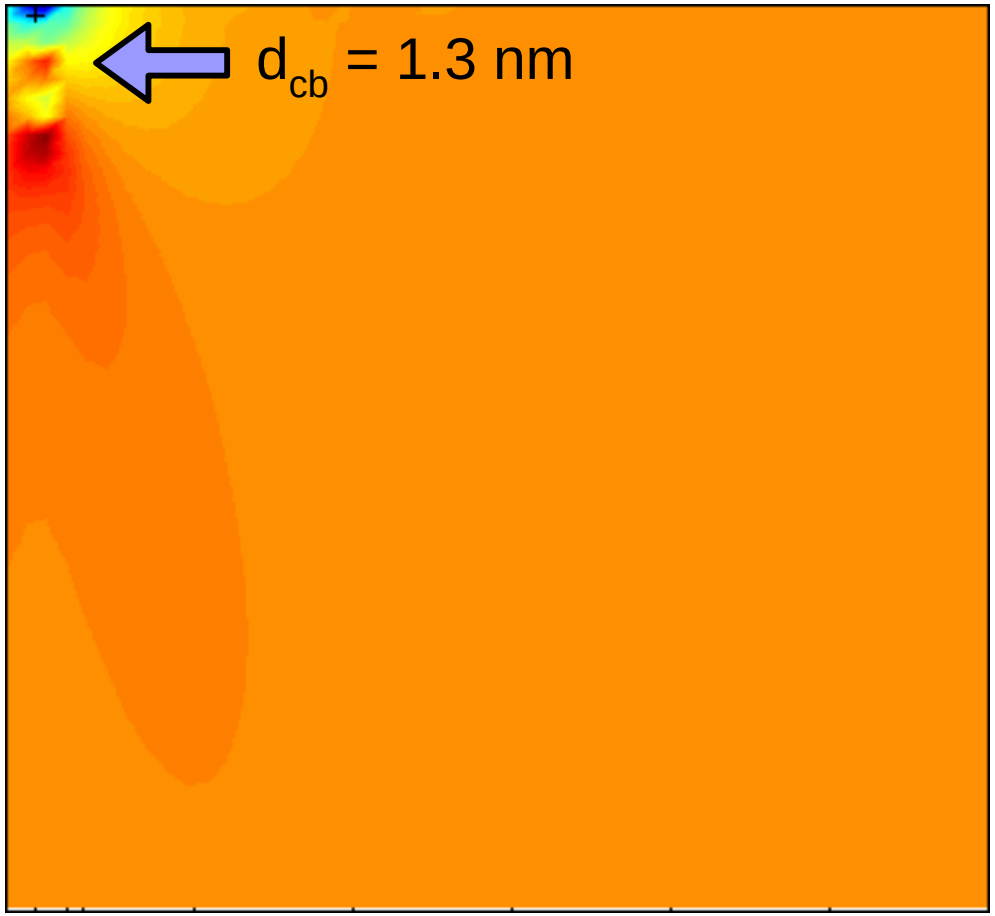


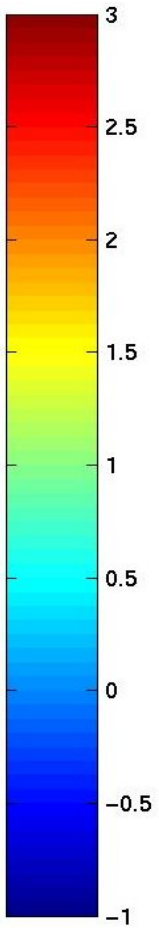
Critical condition for nucleation of PG dislocation from MD simulation:
Critical SIF

- Surface diffusion leads to nucleation of climb dislocations.
- Stress concentration at root of grain boundary drives nucleation of parallel glide dislocations.
- Slip on inclined glide planes is *conventional* deformation mechanism.

(A. Hartmaier, Buehler, Gao, Advanced Engrg. Materials, 2005)

Mesoscopic model: Movie





σ_{xx}

elastic straining to **initial stress level**

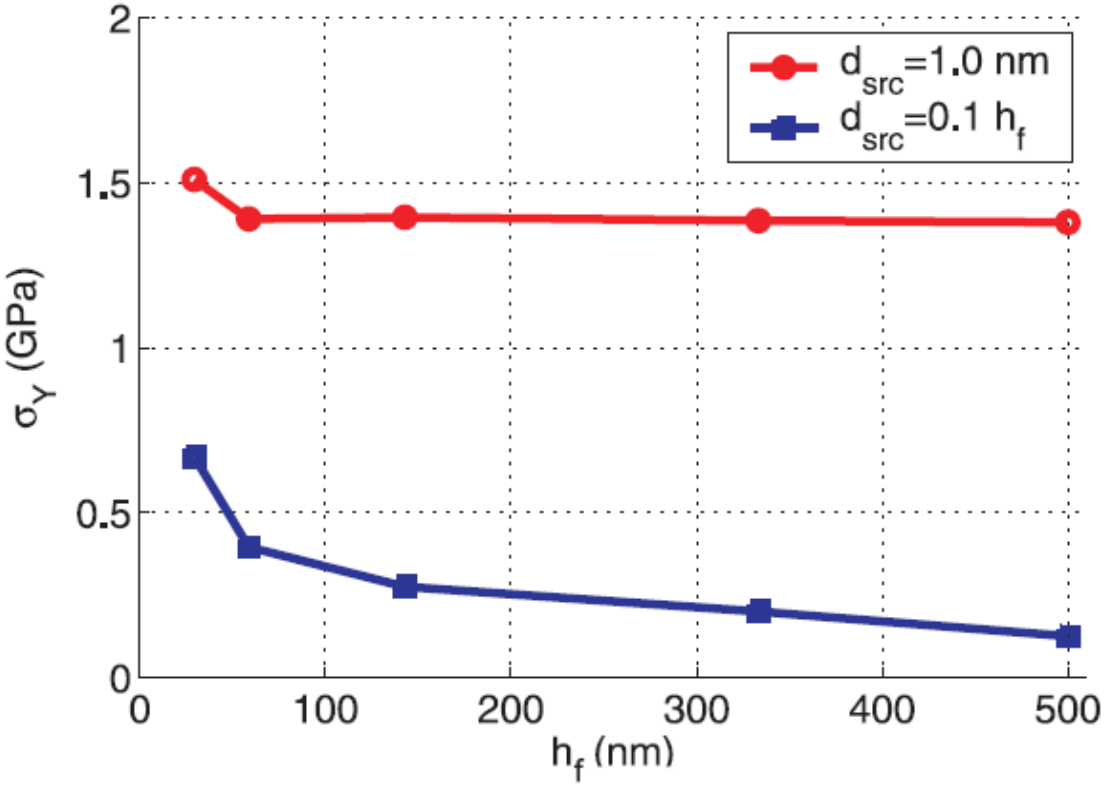
plastic relaxation under constant lateral displacement

Glide source position adapted to MD results

Dislocations are absorbed in grain boundary
(high energy grain boundaries)

(A. Hartmaier, M.J. Buehler, H. Gao, Defect and Diffusion Forum, Advanced Engrg. Materials, 2004, 2005)

Flow stress versus film thickness

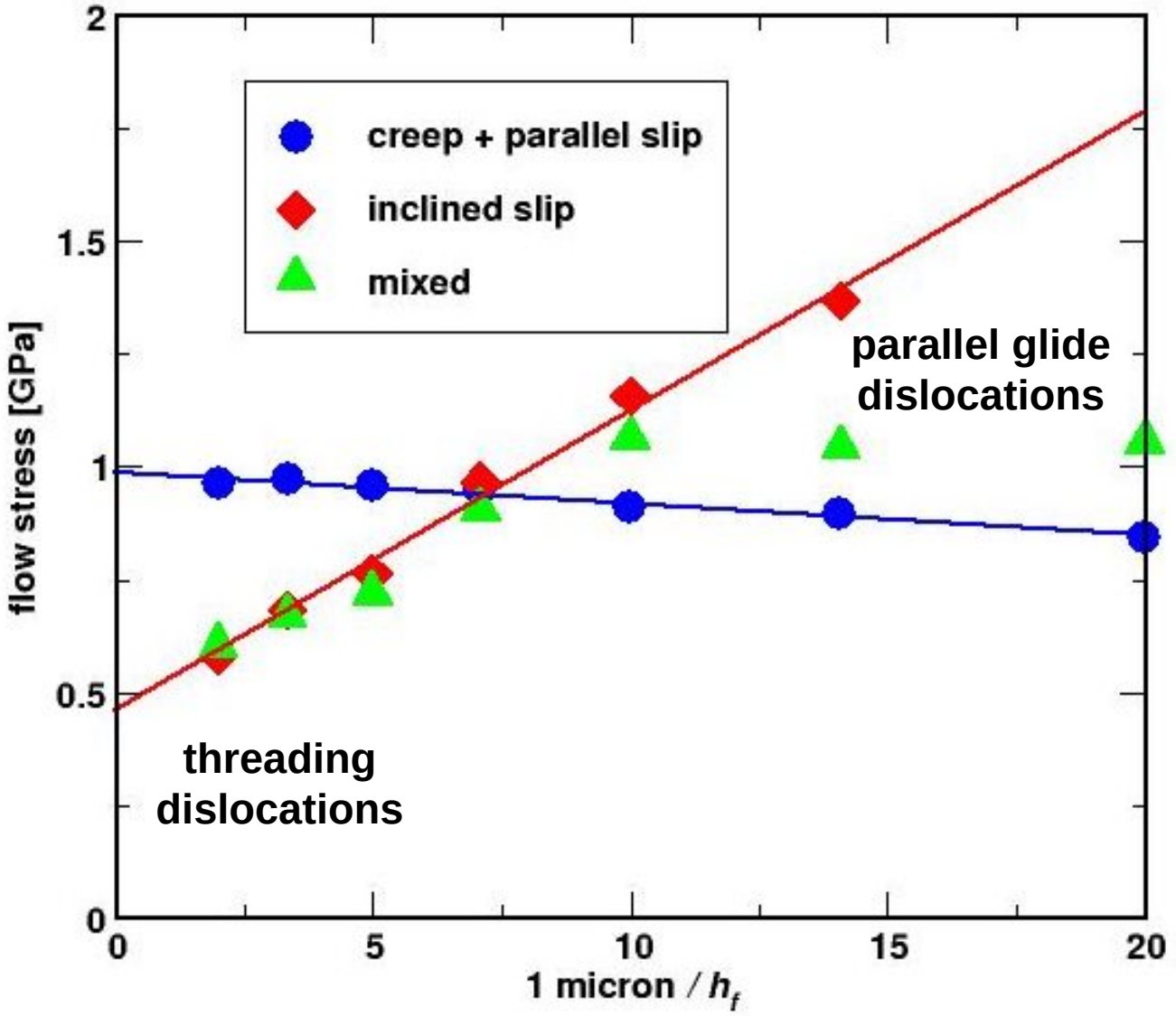


- Flow stress σ_Y versus the film thickness h_f , as obtained from mesoscopic simulations of constrained diffusional creep and parallel glide dislocation nucleation.
- The results are shown for two different initiation criteria for diffusion (constant source and therefore local criterion as proposed in equation, and a film dependent source).
- In the case of a local criterion for diffusion initiation, the yield stress is film-thickness independent as observed in experiment by Balk, Arzt *et al*.

(A. Hartmaier, Buehler, Gao, Advanced Engrg. Materials, 2005)

Competing mechanisms: Slip versus diffusion

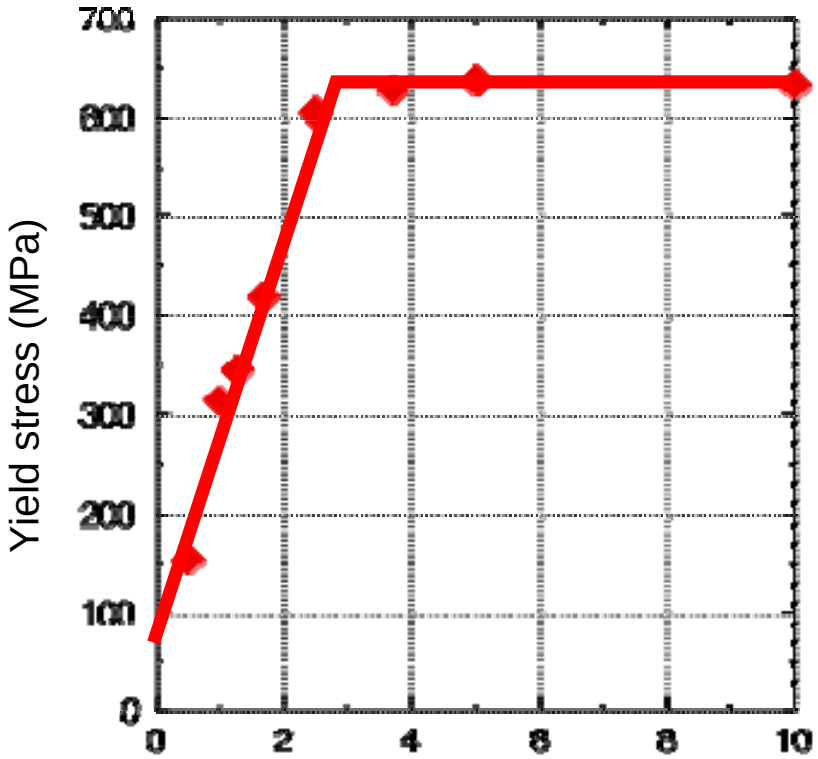
DDD modeling (mesoscale)



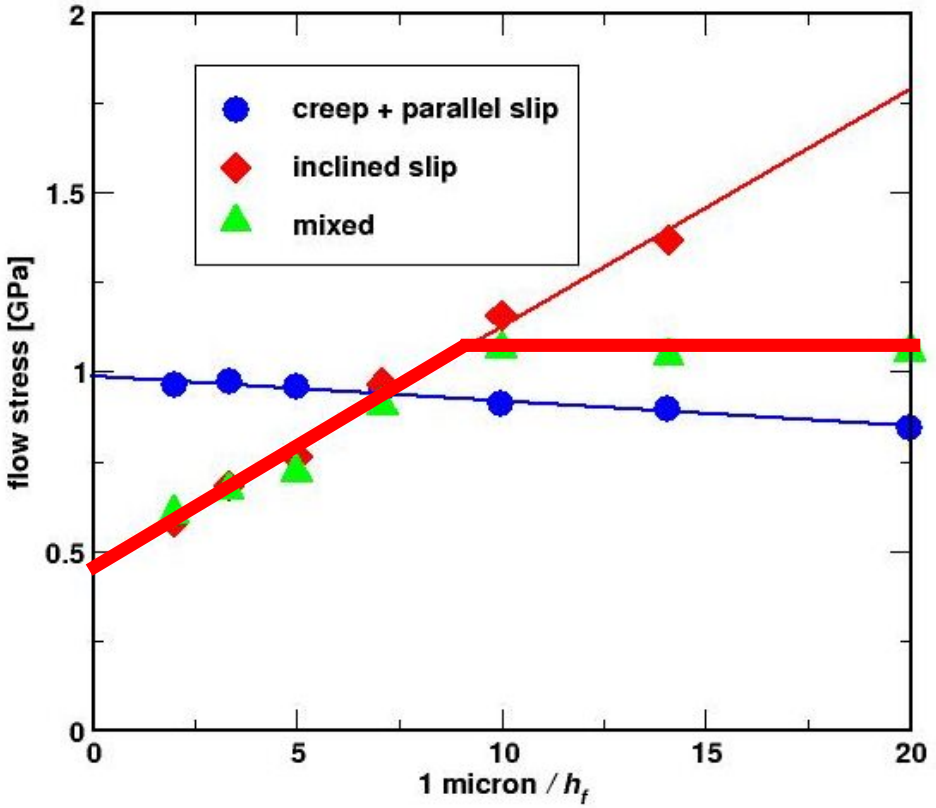
- ✓ Creep mechanism yields constant (or slowly decreasing) flow stress
- ✓ Inclined slip yields linear strengthening with inverse film thickness
- ✓ Deformation mechanisms interact (inclined slip shuts down creep mechanism)

(A. Hartmaier, Buehler, Gao, Advanced Engrg. Materials, 2005)

Comparison: Experiment versus modeling



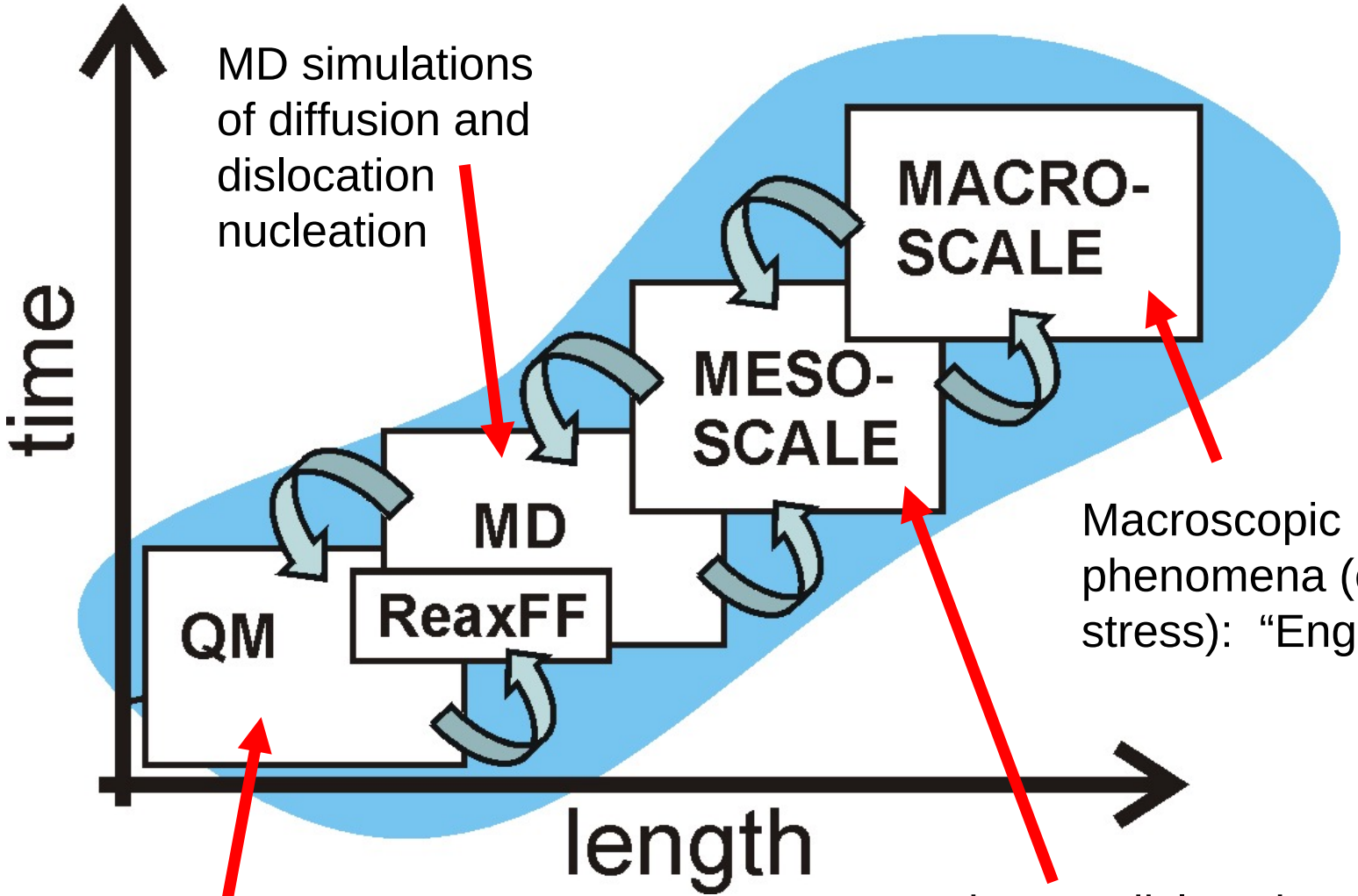
Experiment
(Balk, Dehm, Arzt)



Atomistic based mesoscale model

(A. Hartmaier, Buehler, Gao, Advanced Engrg. Materials, 2005)

Hierarchical multi-scale approach



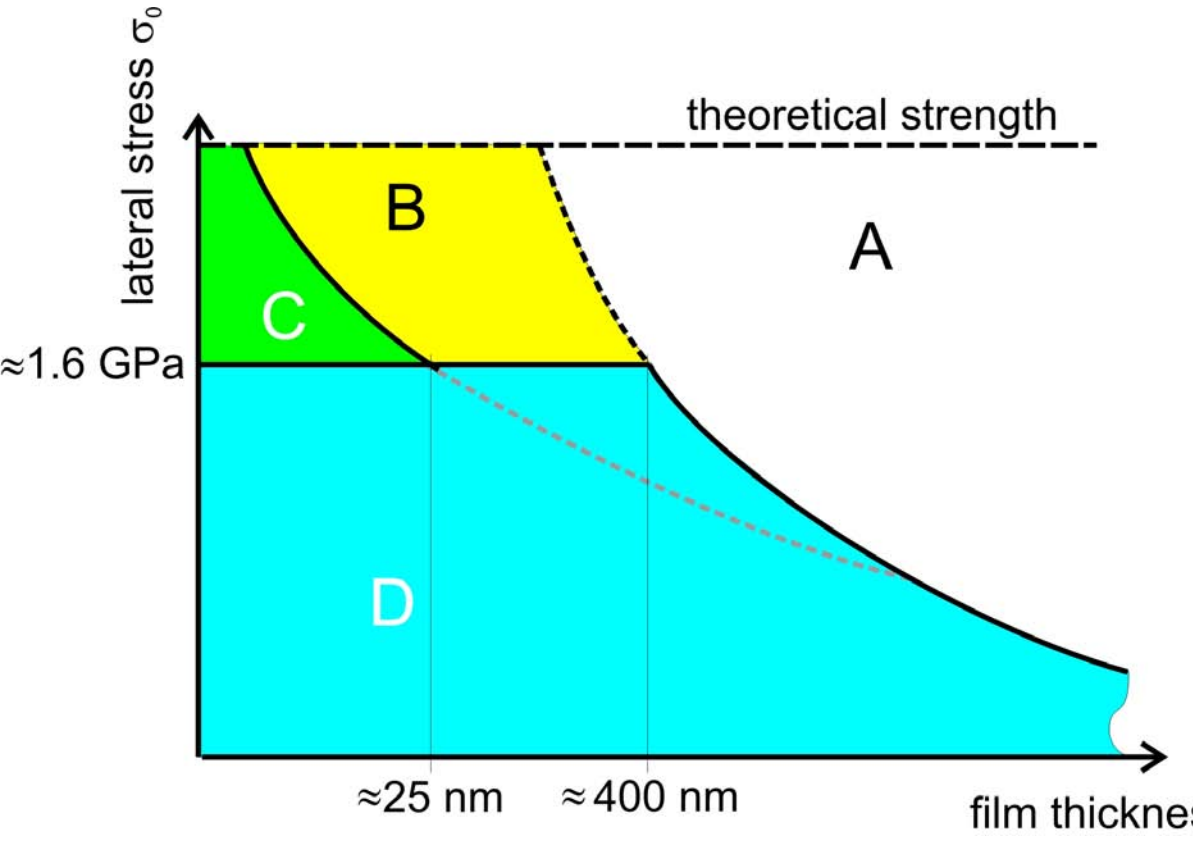
MD simulations of diffusion and dislocation nucleation

Macroscopic phenomena (e.g. yield stress): "Engineering"

Discrete dislocation model (dislocations as particles) model trained based on MD modeling

Force field (EAM) fitting

Deformation map of submicron copper films



Deformation mechanism map *

A-Threading dislocations (Nix)—"classical"

B-Constrained diffusional creep with parallel glide dislocations

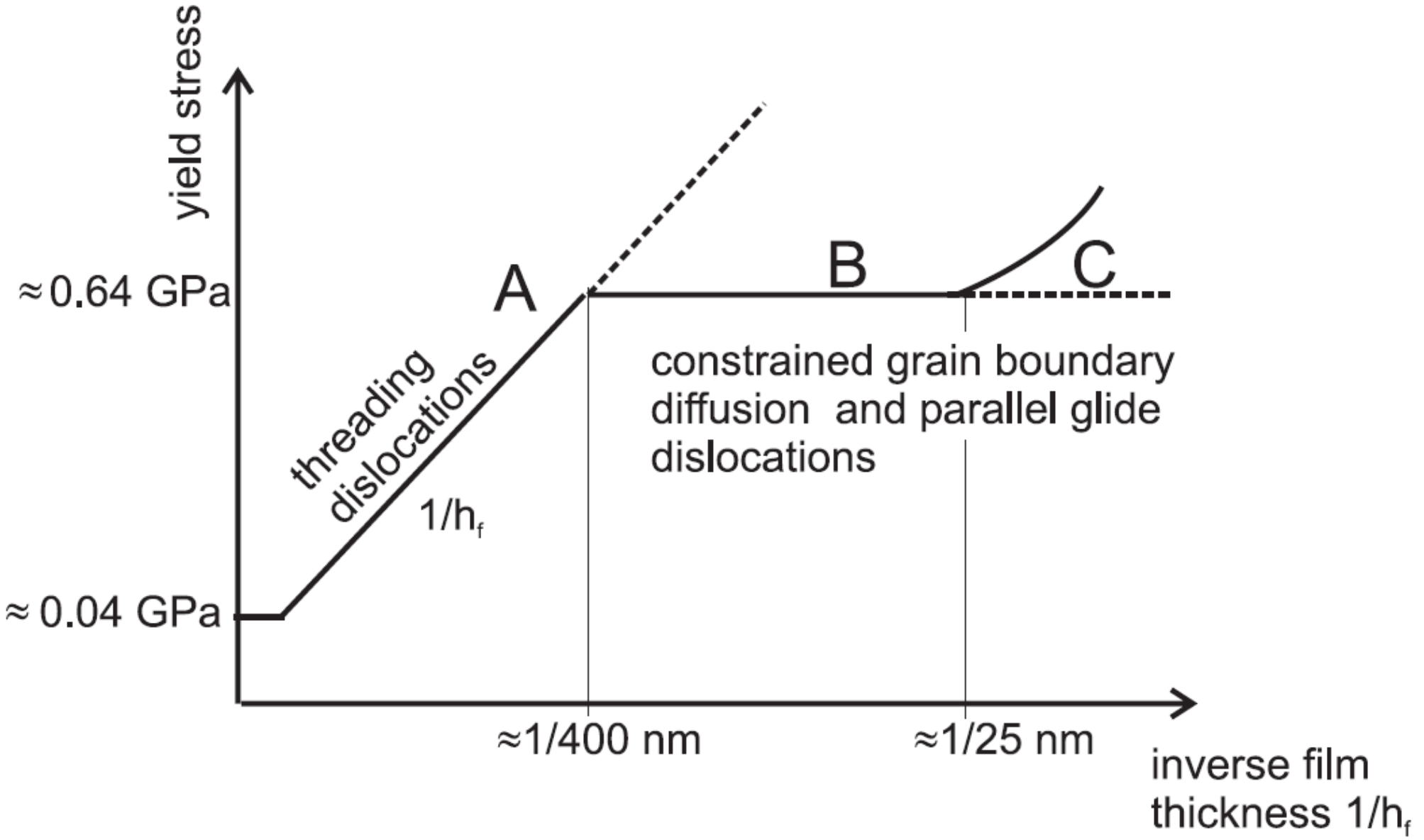
C-Diffusional creep

D-No stress relaxation mechanism

➢ **Conclusion:** In ultra thin copper films without capping layer, constrained grain boundary diffusion and parallel glide dislocations play a governing role

* Results based on MD modeling, experiments, continuum theory and mesoscopic modeling (joint experiment-theory-simulation effort with Prof. Arzt group at MPI-MF)

Deformation map of submicron copper films

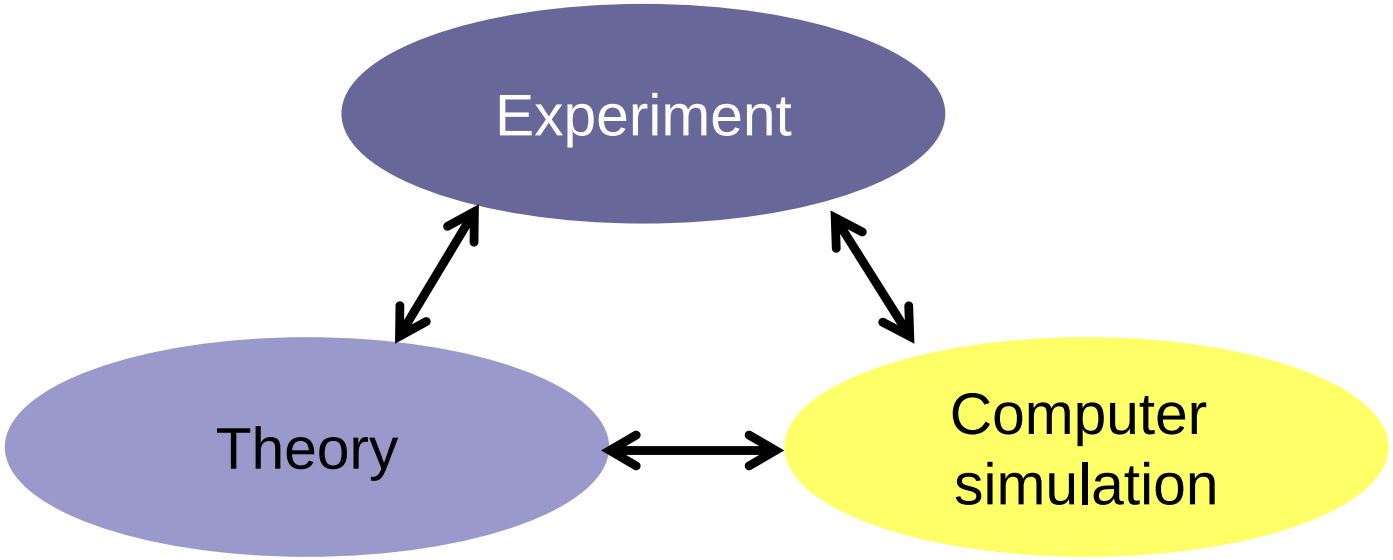


Experiment-theory-simulation

• Atomistic simulations is an increasingly important tool in materials science; it can be used to…

- Advance theory and discover new physical phenomena
- Augment and explain experiment

• With its **limitations** understood, MD simulation is an ideal tool to study small-scale dynamics materials phenomena; gain insight into mechanisms



Discussion and conclusion

- MD methods for metals are quite advanced and have found many applications
- This is true partly because the metallic bonding can reasonably well be described using semi-empirical potentials (EAM, MEAM); many models have been suggested in the past decades
- With increase in computing power this enables studies of billions of particles, allowing to reach the critical length scales of micrometers with “first principles” dislocation mechanics
- We have applied these techniques to gain insight into the deformation mechanisms of ultra thin copper films deposited on substrates
- We have discovered that diffusional processes play an increasingly important role at nanoscale and that the deformation mechanism of ultra thin copper films is characterized by parallel glide dislocations rather than threading dislocations

Lecture topics: Outline

Fall 2005

- Oct. 27, 1 PM, Room 1-134: Introduction to atomistic modeling techniques: Do we need atoms to describe how materials behave?
- Nov. 3, 1 PM, Room 1-134: Methods and techniques for modeling metals and their alloys and application to the mechanics of thin metal films
- Nov. 17, 1 PM, Room 1-134: Scale coupling techniques: From nano to macro
- Dec. 5, 1 PM, Room 1-150: Reactive versus nonreactive potentials: Towards unifying chemistry and mechanics in organic and inorganic systems

IAP 2006: From nano to macro: Introduction to atomistic modeling techniques and application in a case study of modeling fracture of copper (1.978 PDF)

- Jan. 9 (Monday): Introduction to classical molecular dynamics: Brittle versus ductile materials behavior
- Jan. 11 (Wednesday): Deformation of ductile materials like metals using billion-atom simulations with massively parallelized computing techniques
- Jan. 13 (Friday): Dynamic fracture of brittle materials: How nonlinear elasticity and geometric confinement governs crack dynamics
- Jan. 16 (Monday): Size effects in deformation of materials: Smaller is stronger
- Jan. 18 (Wednesday): Introduction to the problem set: Atomistic modeling of fracture of copper
- The IAP activity can be taken for credit. Both undergraduate and graduate level students are welcome to participate. Details will be posted on the IAP website (http://web.mit.edu/iap/).

Spring 2006

- TBD. Atomistic modeling of biological and natural materials: Mechanics of protein crystals and collagen
- TBD. Mechanical properties of carbon nanotubes: Scale effects and self-folding mechanisms
- TBD. Atomistic and multi-scale modeling in civil and environmental engineering: Current status and future development

http://web.mit.edu/mbuehler/www/Teaching/LS/