From nano to macro: Introduction to atomistic modeling techniques

IAP 2006

Deformation of ductile materials using billion-atom simulations with massively parallelized computing techniques

Lecture 2

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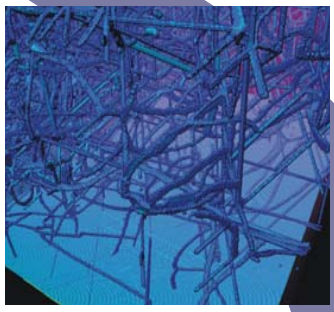
Behavior of different "kinds" of materials

"brittle": Materials that experience little, if any, plastic deformation before the onset of fracture

(Buehler *et al*., *Nature*, 2003, 2006)

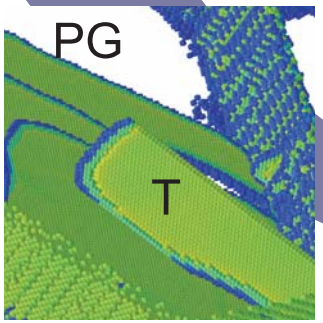
"ductile": Materials that experience significant plastic deformation before the onset of fracture



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

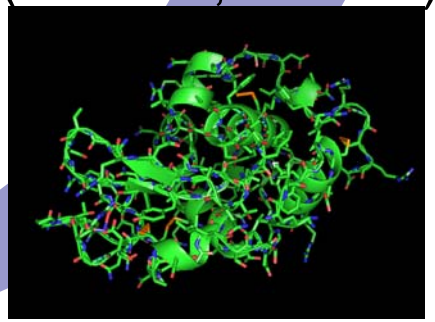
How to use large-scale computing in multi-scale modeling in order to develop fundamental understanding

"geometric confinement"
Nanostructured materials, carbon nanotubes



(Buehler *et al*., *JMPS*, 2002)

"biological materials"
(Proteins, DNA …)



(Buehler *et al*., *MRS Proceedings*, 2004)

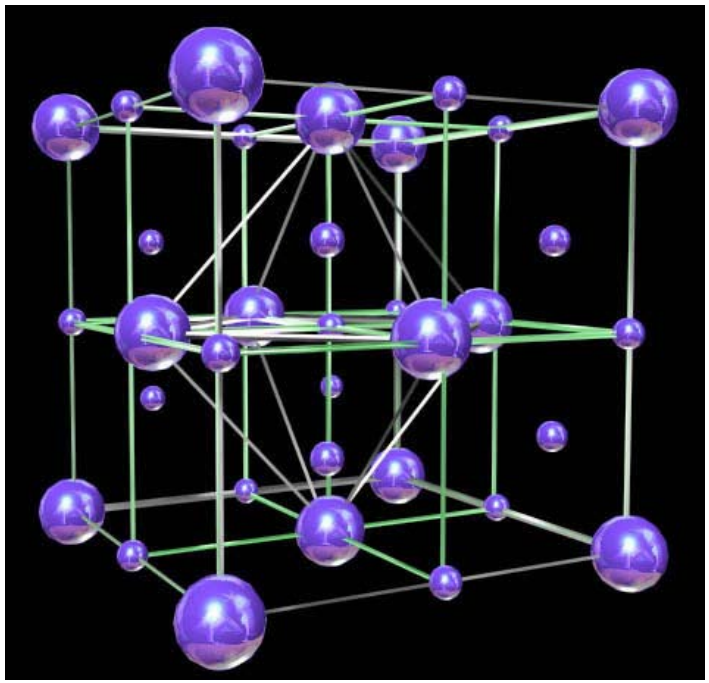
Outline

- Large-scale computing strategies and resources
  - Parallelization
  - TOP 500 list of fastest supercomputers
  - Usefulness of supercomputing
- Introduction to ductile materials and their deformation mechanisms, including
  - Dislocations (sources, geometry, interaction)
  - Mechanisms of hardening of materials
- **Objective:**

  Demonstration of how large-large molecular dynamics can be applied to model ductile deformation

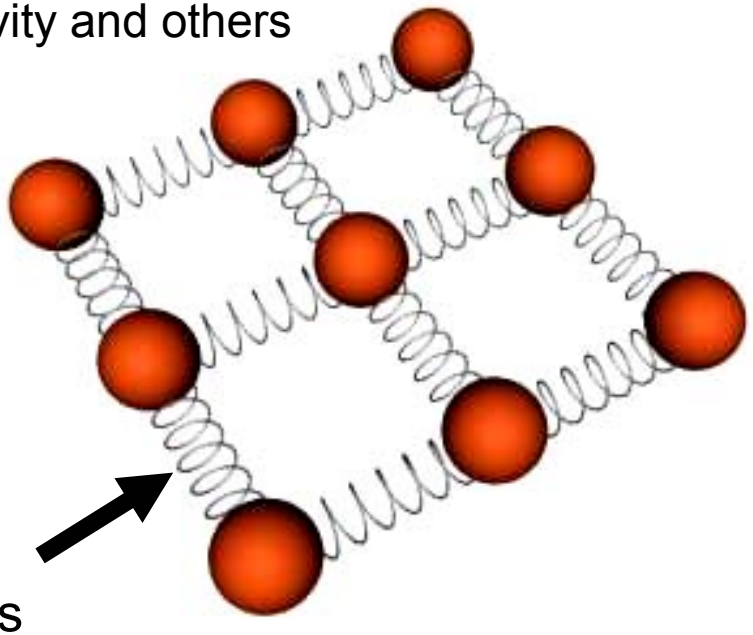
The problem to solve

- 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…

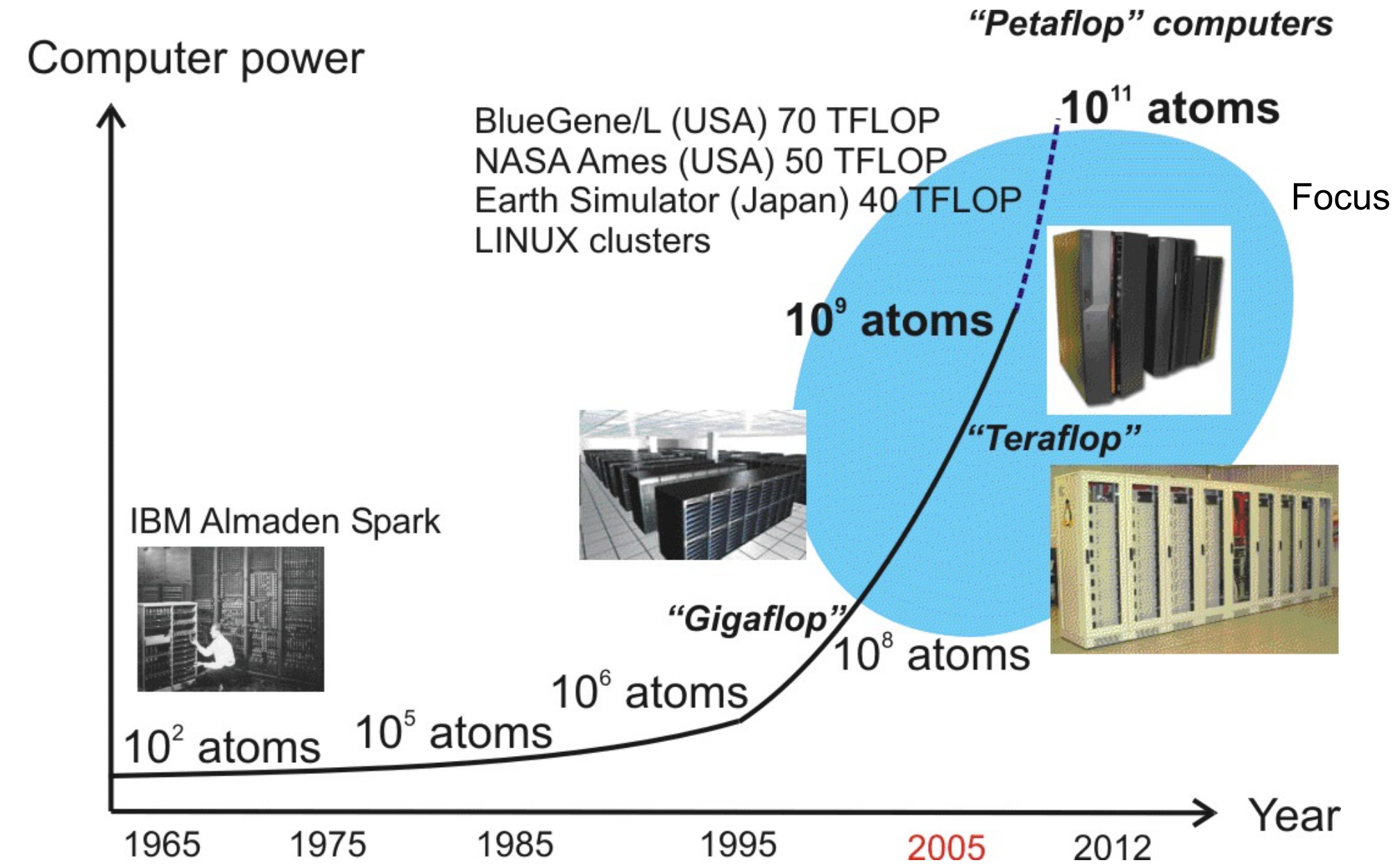
http://www.sr.bham.ac.uk/xmm/images/structures/spherespring_300_248.jpg

The problem to solve

- Molecular dynamics of mechanics applications can be computationally challenging, due to
  - Complexities of force field expressions (calculation of atomic forces)
  - Large number of atoms and thus large number of degrees of freedom in the system (3N)
- To model realistic (macro-engineering) dimensions of materials with microstructural features: Need system sizes with ~10^{23} atoms
- This results in challenges for data analysis and visualization, or just for data handling and storage
- Much research has been done to advance data analysis techniques and visualization schemes

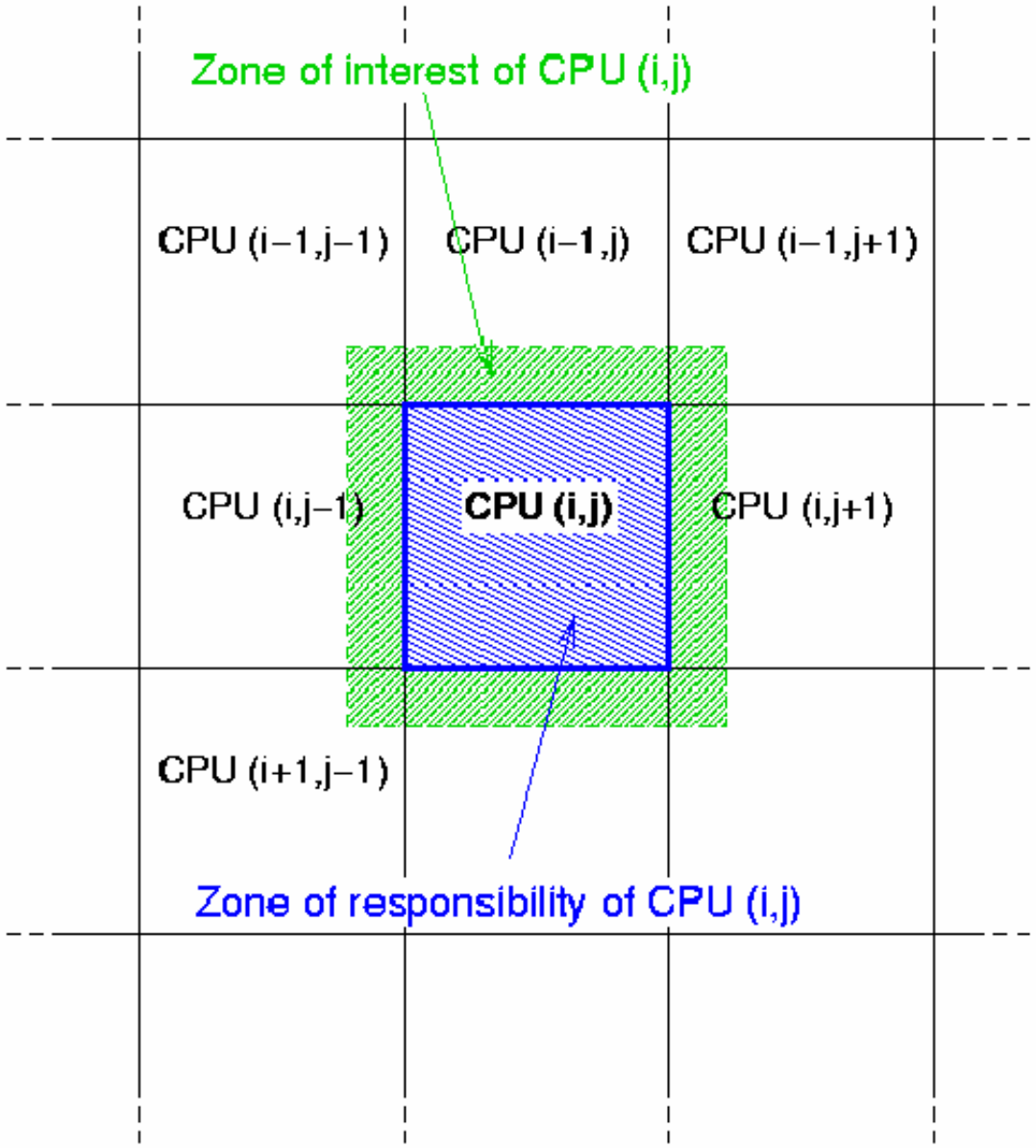
  (e.g., Vashishsta and coworkers at USC's center for Advanced Computing and Simulation, http://cacs.usc.edu)

Increase in computing power
Classical molecular dynamics



(Buehler *et al*., to appear 2006)

Parallel Molecular Dynamics



(after Schiotz)

Concept:

Divide the workload

No (immediate) long range interaction (only via dynamics)

- Each CPU is responsible for part of the problem
- Atoms can move into other CPUs (migration)
- Need to know topology or the geometric environment on other CPUs (green region)
- 1,000,000,000 particles on 1,000 CPUs: Only 1,000,000 atoms/CPU

Implementation of parallelization

- Shared memory systems (all CPUs “see” same memory)
  - OpenMP (easy to implement, allows incremental parallelization)
  - POSIX threads
- Distributed memory systems
  - MPI (=Message Passing Interface)
    Most widely accepted and used, very portable, but need to parallelize whole code at once
- Parallelization can be very tedious and time-consuming and may distract from solving the actual problem; debugging difficult
- **Challenges:** Load balancing, different platforms, input/output, compilers and libraries, modifications and updates to codes, “think parallel” as manager
- Strategy for your own code: Find similar code and implement your own problem

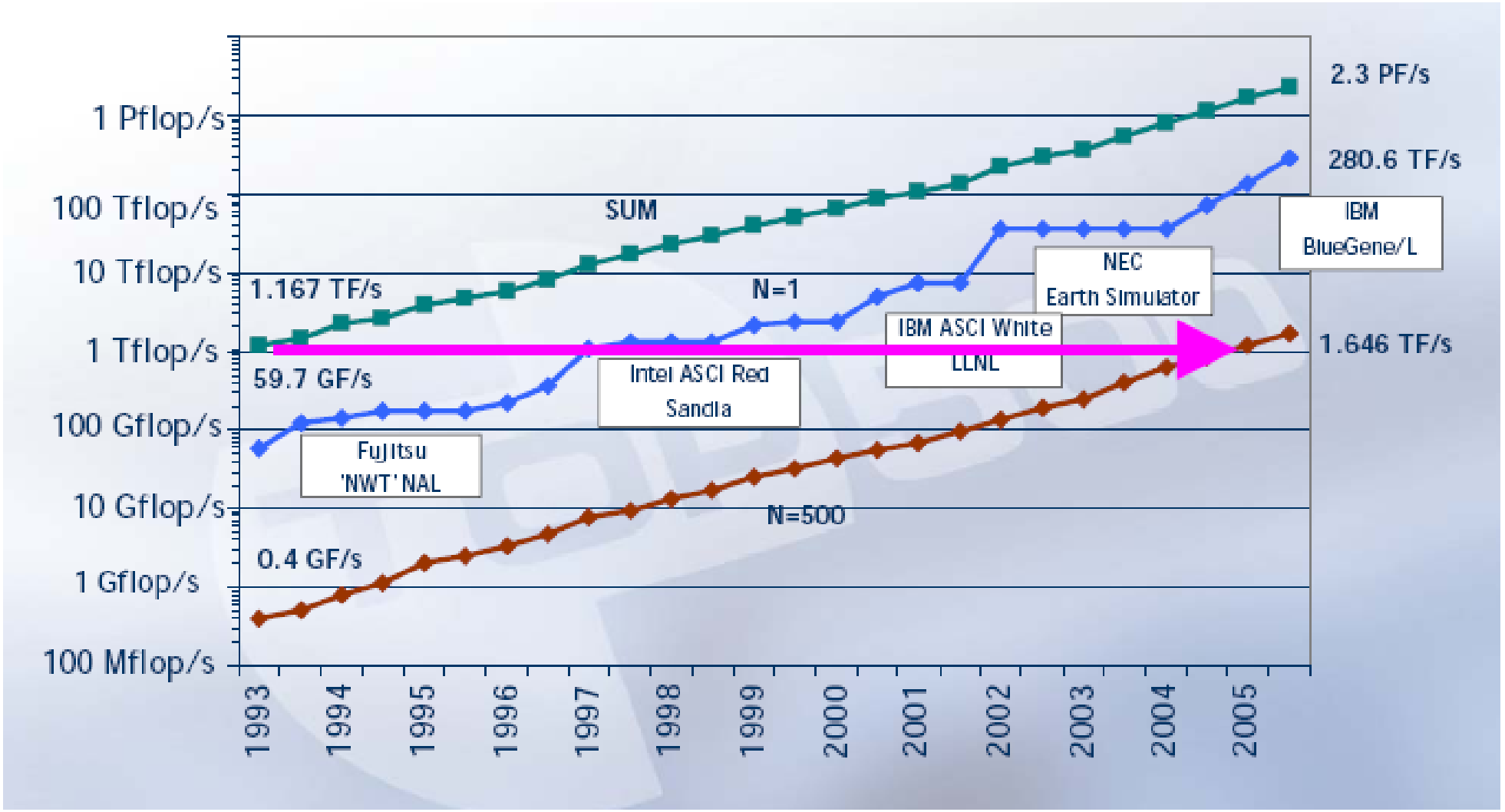
http://nf.apac.edu.au/training/MPIProg/slides/index.html, http://www.openmp.org/, http://www.eecs.umich.edu/~qstout/parallel.html

TOP500 List Fall 2005
The world's fastest supercomputers

	Manufacturer	Computer	Rmax [TF/s]	Installation Site	Country	Year	#Proc
1	IBM	BlueGene/L eServer Blue Gene	280.6	DOE/NNSA/LLNL	USA	2005	131072
2	IBM	BGW eServer Blue Gene	91.29	IBM Thomas Watson	USA	2005	40960
3	IBM	ASC Purple eServer pSeries p575	63.39	DOE/NNSA/LLNL	USA	2005	10240
4 ~~3~~	SGI	Columbia Altix, Infiniband	51.87	NASA Ames	USA	2004	10160
5	Dell	Thunderbird	38.27	Sandia	USA	2005	8000
6 ~~10~~	Cray	Red Storm Cray XT3	36.19	Sandia	USA	2005	10880
7 ~~4~~	NEC	Earth-Simulator	35.86	Earth Simulator Center	Japan	2002	5120
8 ~~5~~	IBM	MareNostrum BladeCenter JS20, Myrinet	27.91	Barcelona Supercomputer Center	Spain	2005	4800
9 ~~6~~	IBM	eServer Blue Gene	27.45	ASTRON University Groningen	Netherlands	2005	12288
10	Cray	Jaguar Cray XT3	20.53	Oak Ridge National Lab	USA	2005	5200

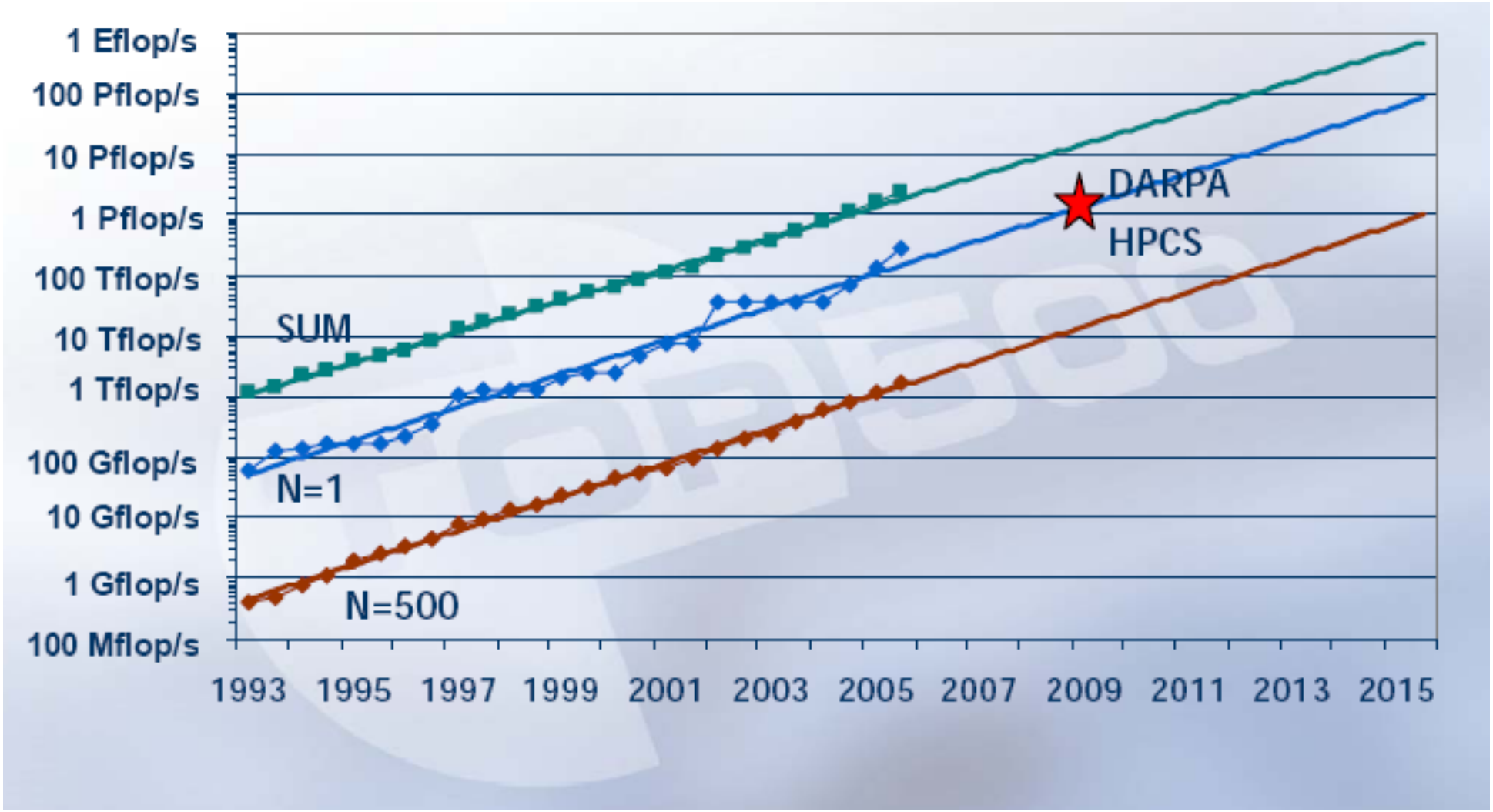
http://www.top500.org/lists/2005/11/TOP10_Nov2005.pdf

Performance history



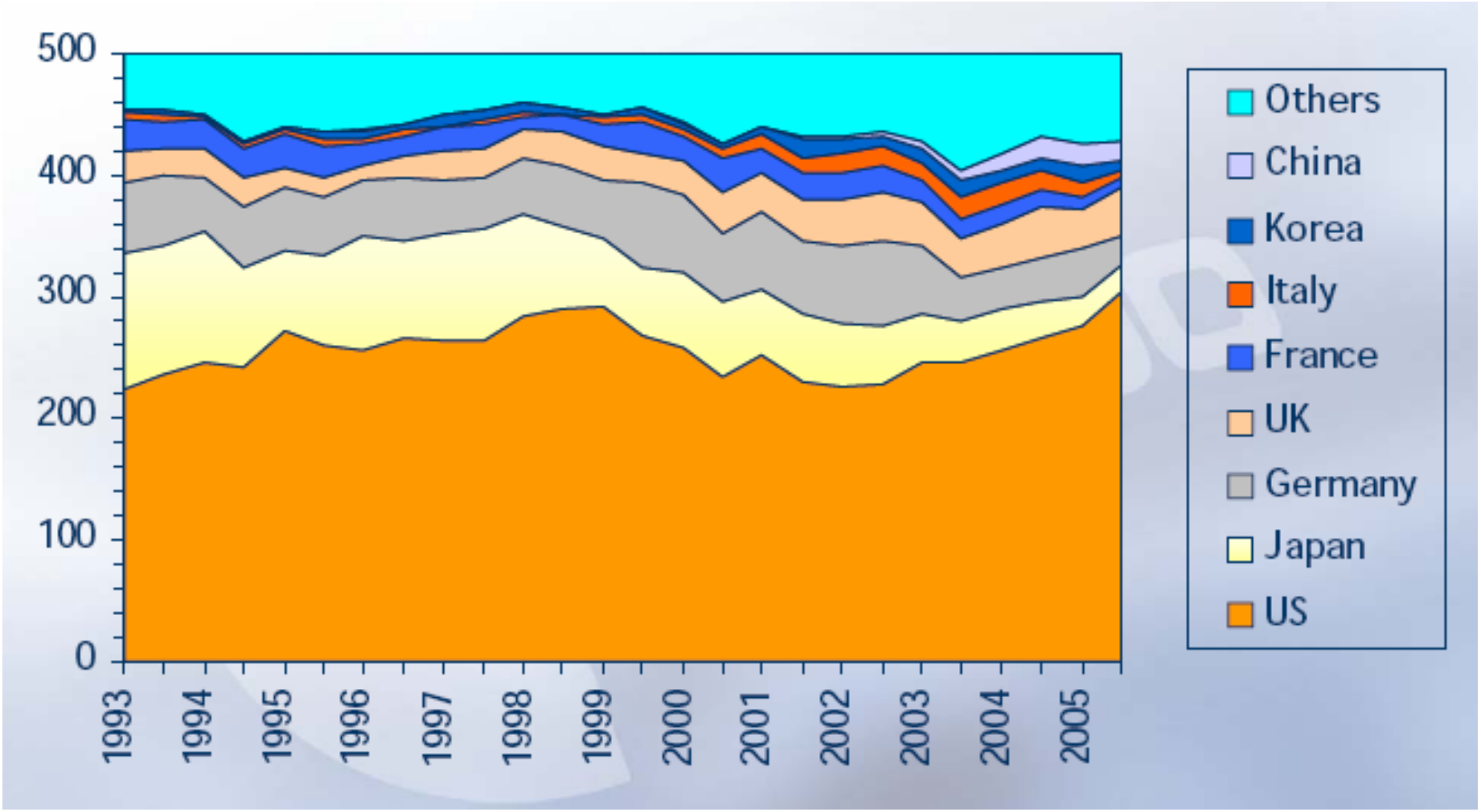
http://www.top500.org/lists/2005/11/TOP500_Nov2005_Highlights.pdf

Performance projection



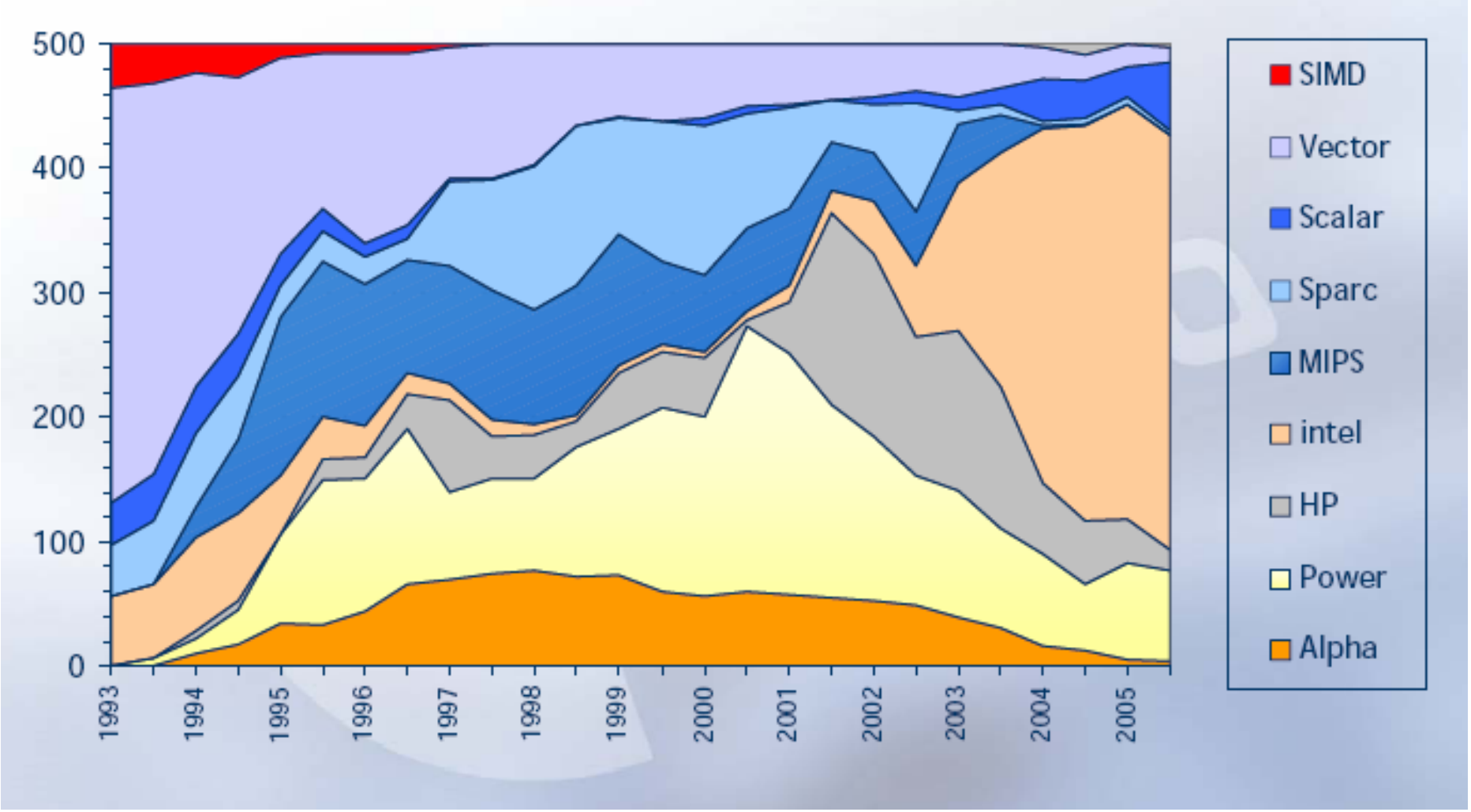
http://www.top500.org/lists/2005/11/TOP500_Nov2005_Highlights.pdf

Computing capacity distribution worldwide



http://www.top500.org/lists/2005/11/TOP500_Nov2005_Highlights.pdf

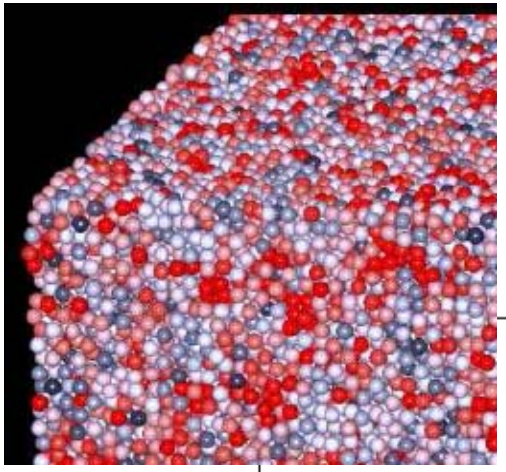
Architecture distribution

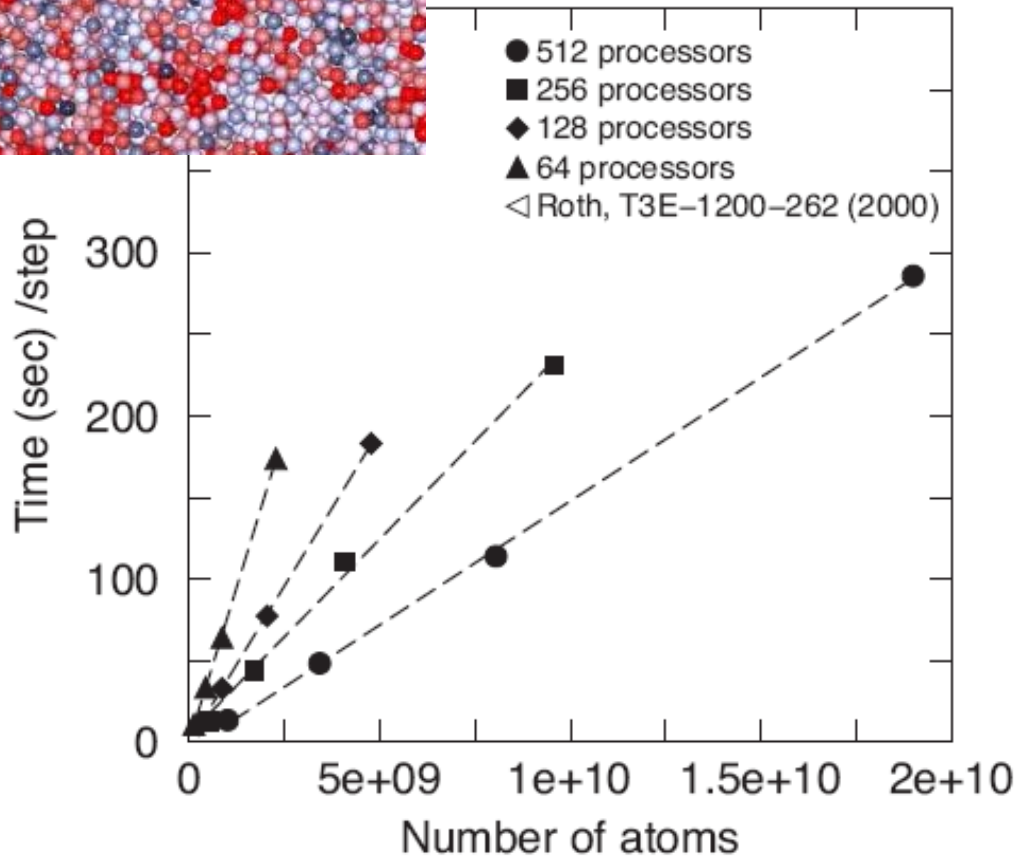


Dominance of LINUX clusters

World's largest MD simulation

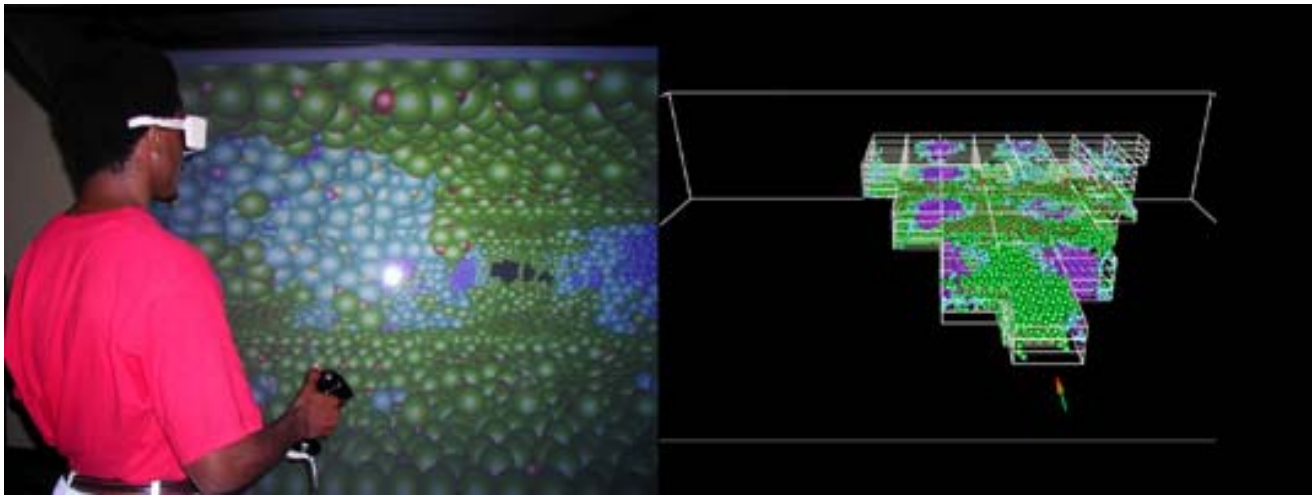
- Largest MD simulation: 19,000,000,000 atoms by Kai Kadau
- The memory needed to save one configuration of one billion atoms in single precision is more than 15 GByte (regular PC: 1 GByte), which makes it inconvenient to save all the raw data and analyze the data in a postprocessing fashion, even on modern platforms with Tbytes of hard-disc capacity
- Covential analysis techniques don't work any more



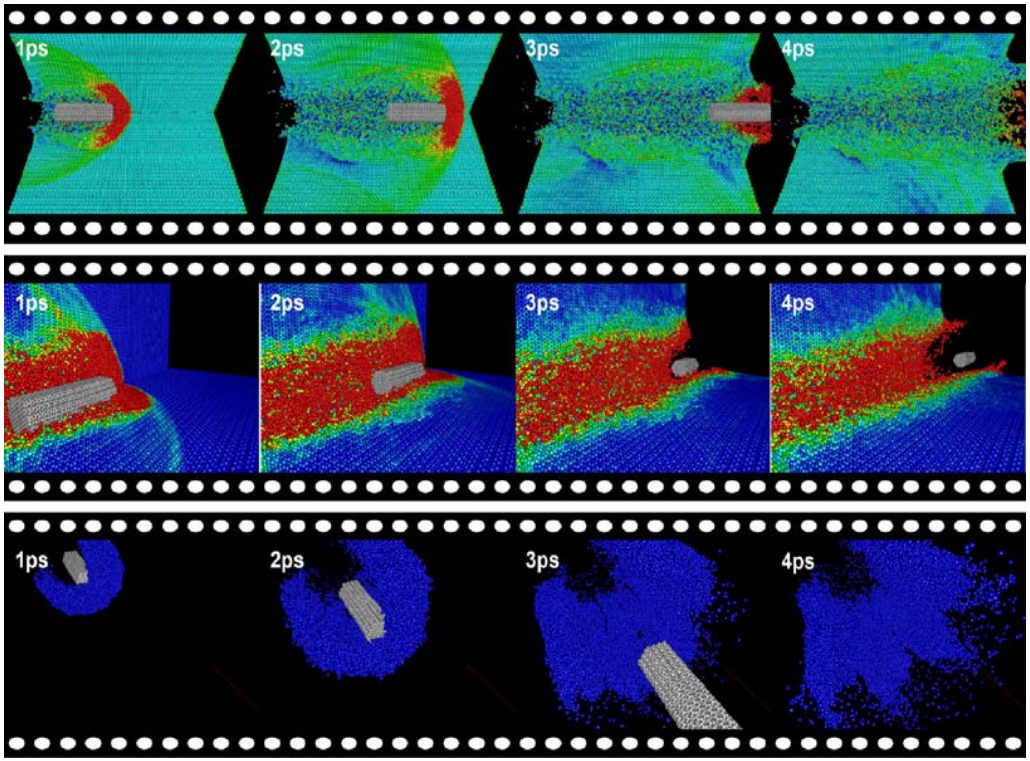


http://www.lanl.gov/orgs/t/publications/research_highlights_2005/docs/SF05_Kadau_WorldRecord.pdf
http://www.thp.uni-duisburg.de/~kai/IJMPC-19bil.pdf

More examples..



Immersive and interactive visualization of large datasets to achieve billion-atom walkthrough.



Molecular modeling of fracture and projectile impact

Vashishta, Kalia, Nakano *et al*., USC

Why is large-scale modeling useful?

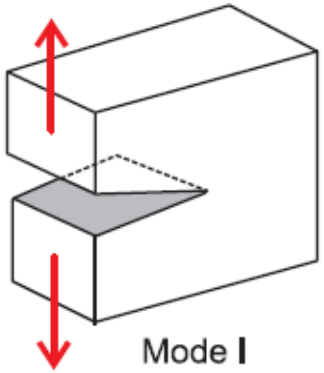
- Bridging length scales by direct numerical simulation (DNS)
- Understand the behavior of complex many-particle systems, without imposing constraints or boundary conditions
- Discover new physical phenomena, e.g. collective events that involve a large number of particles

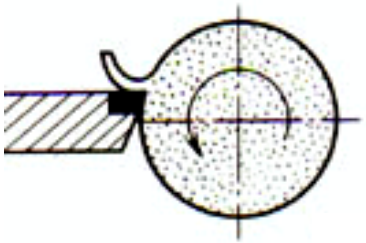
Caution:

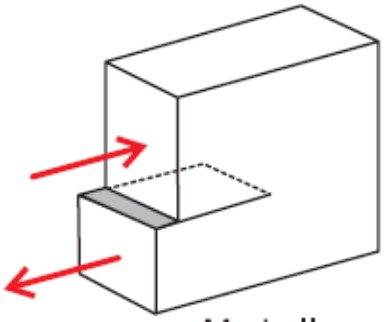
- Need to make sure that model produces useful results, *i.e.* includes new scientific content and discoveries
- Pictures may be pretty, but what do we learn?

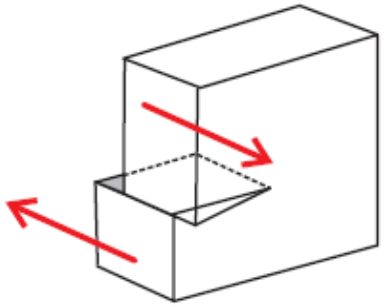
How “stuff” deforms?

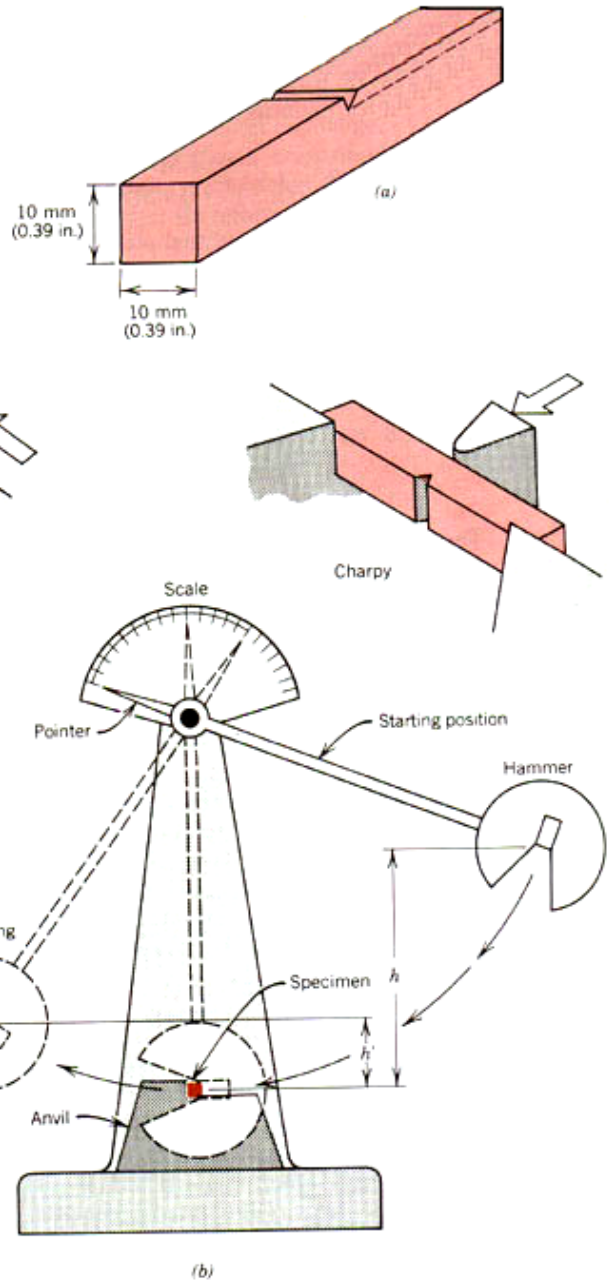
Modes of loading











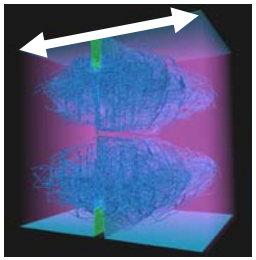
Increase in computing power: Parallelization

Modeling of mechanical behavior of materials is highly demanding and requires models with millions and billions of atoms

2000
1,000,000,000 particles
10 TFLOP computers

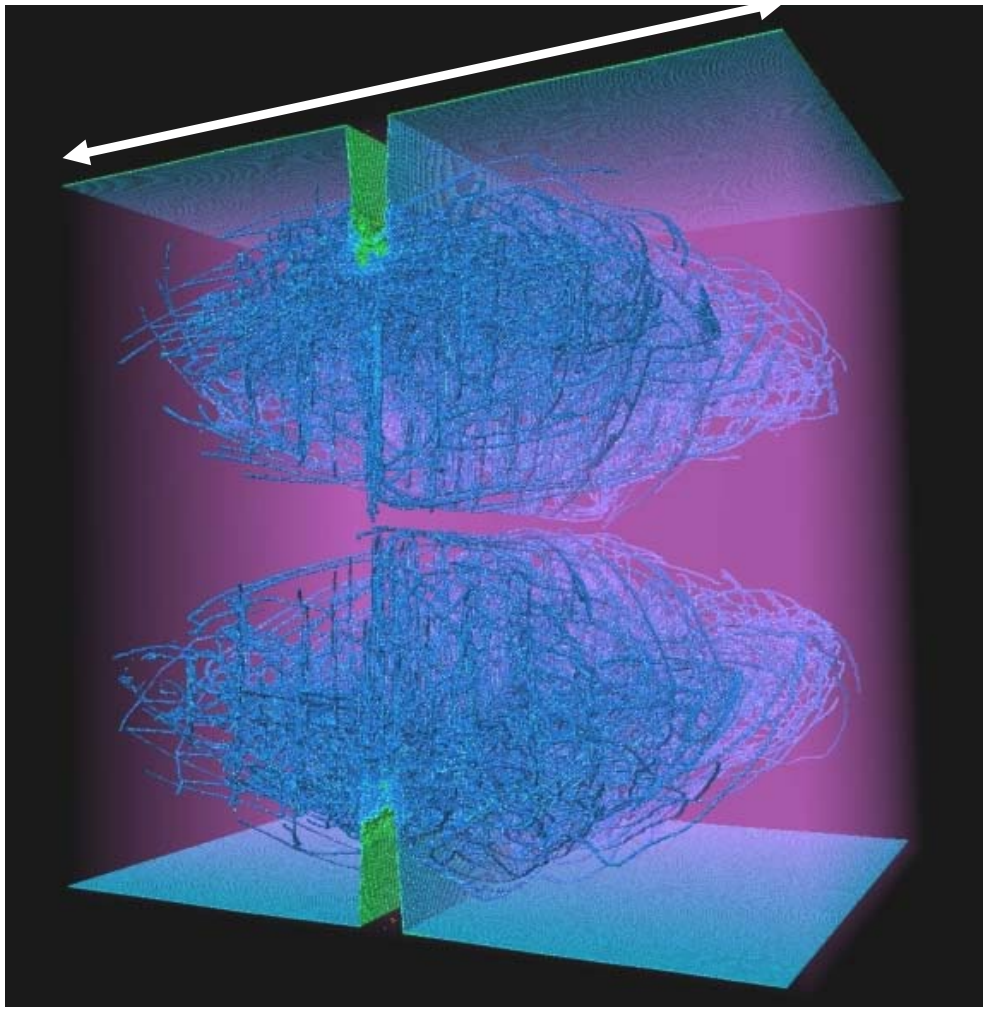
0.3 μm

2005
70,000,000,000 particles
70 TFLOP computers



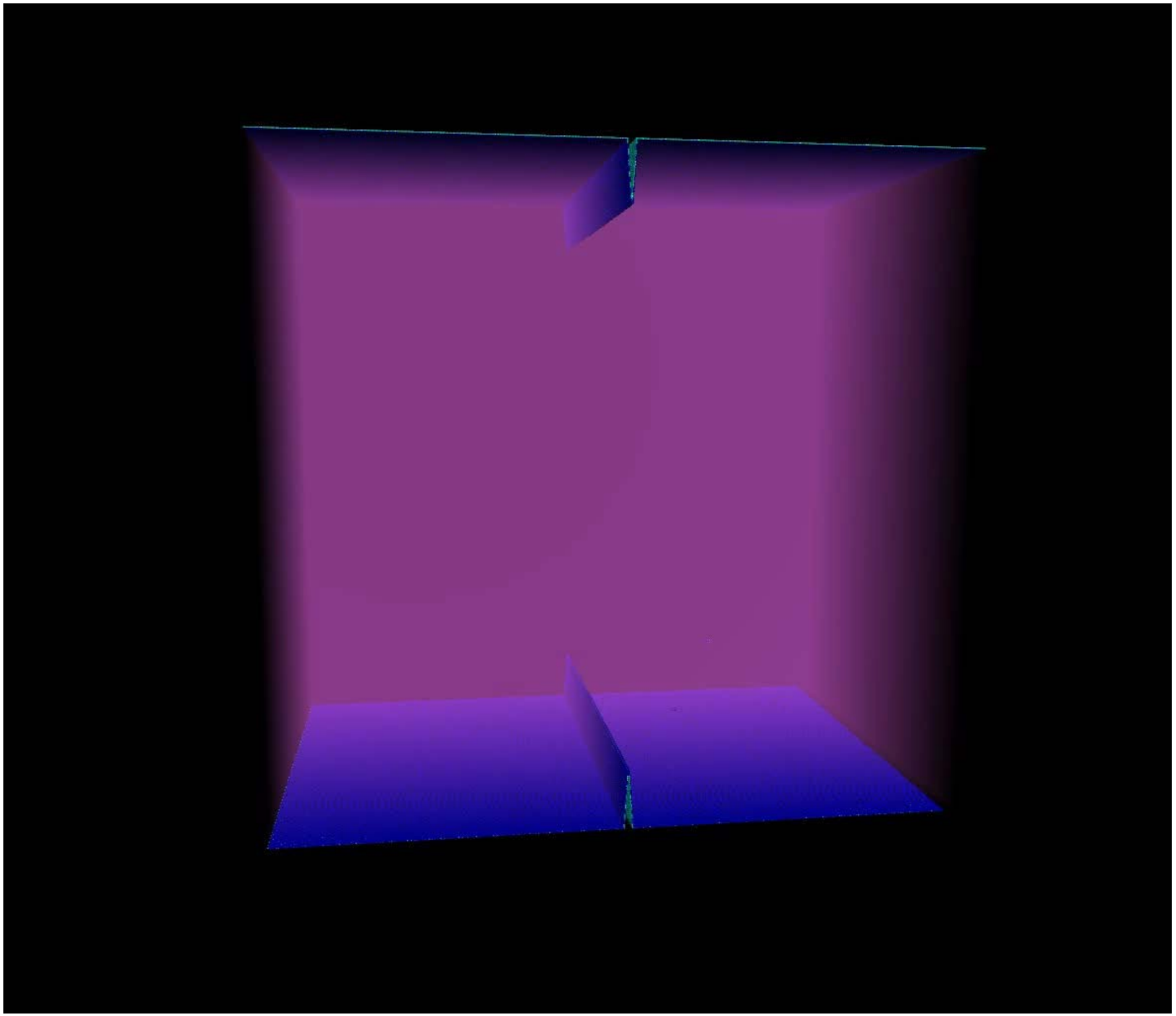
1.2 μm

5 μm



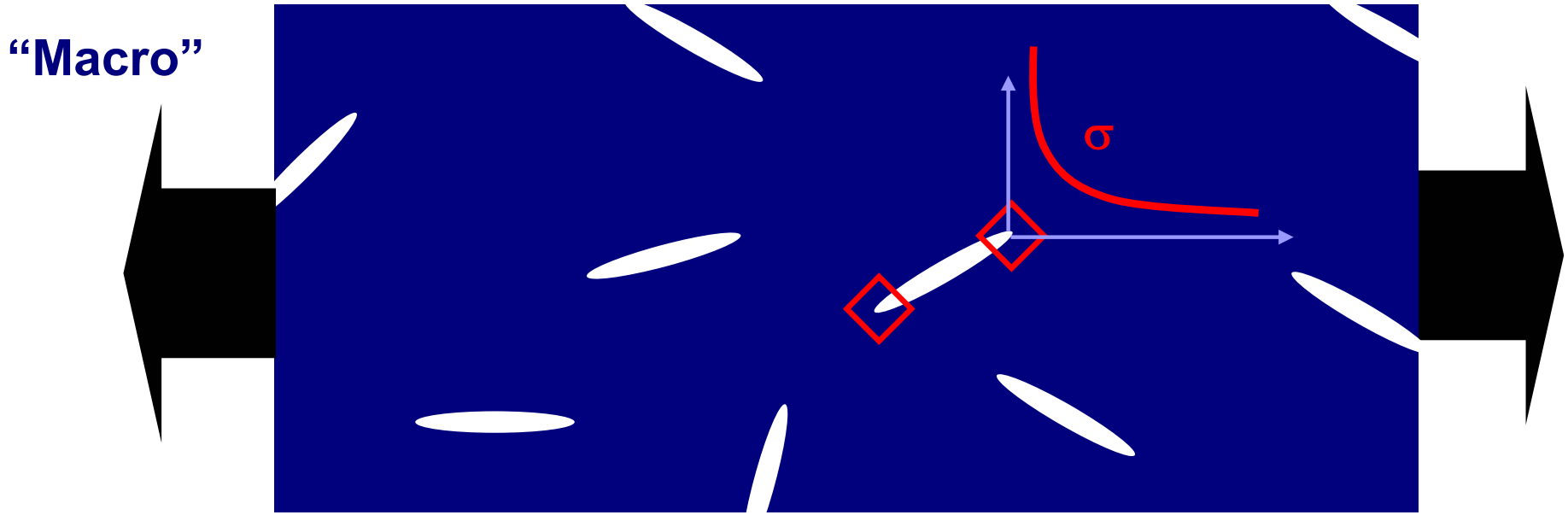
2010
7,000,000,000,000 particles
1,000 TFLOP computers

A simulation with 1,000,000,000 particles



(Abraham, Buehler, Gao, Hartmaier *et al*.)

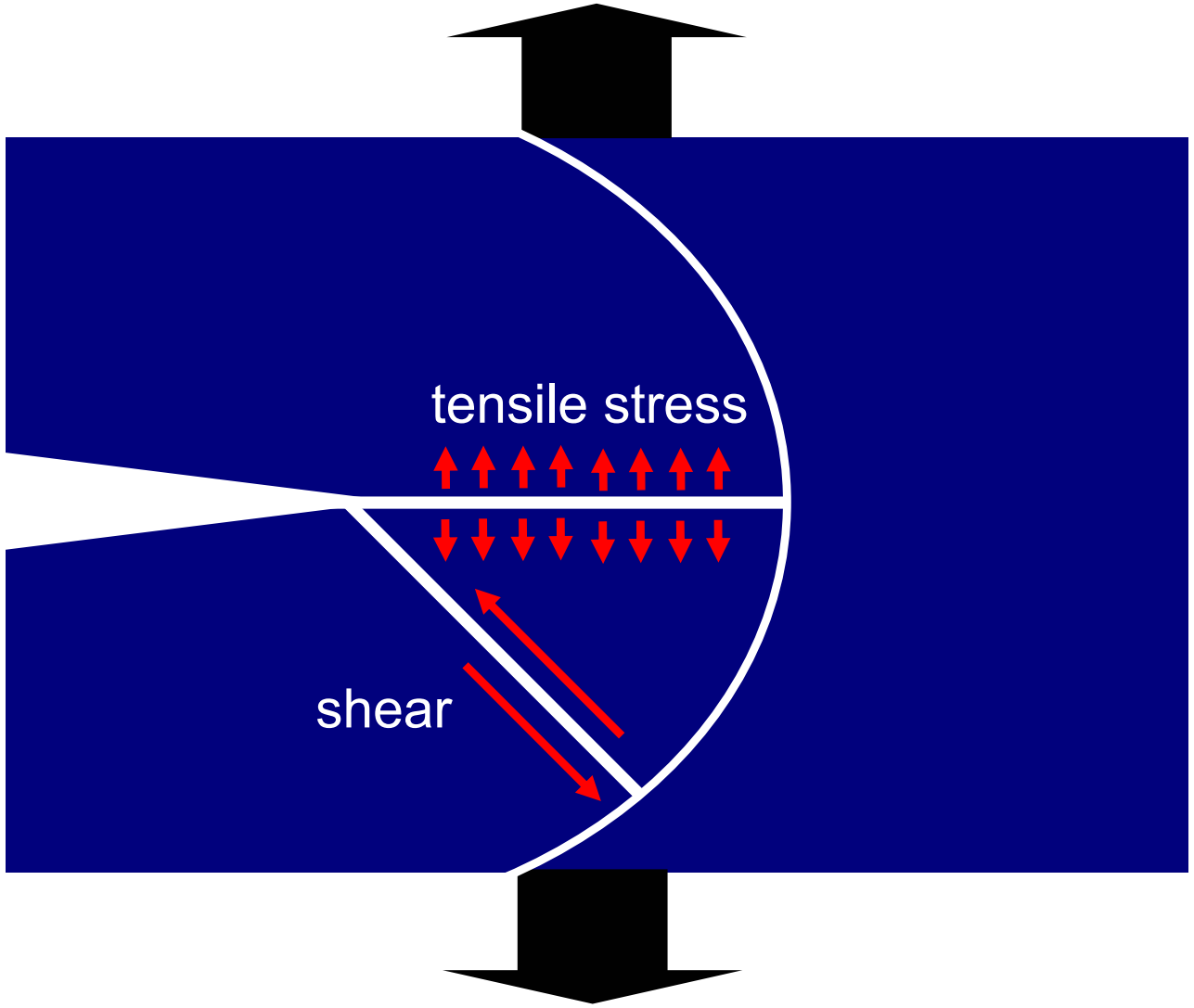
Deformation of materials: Flaws or cracks matter



Failure of materials initiates at cracks

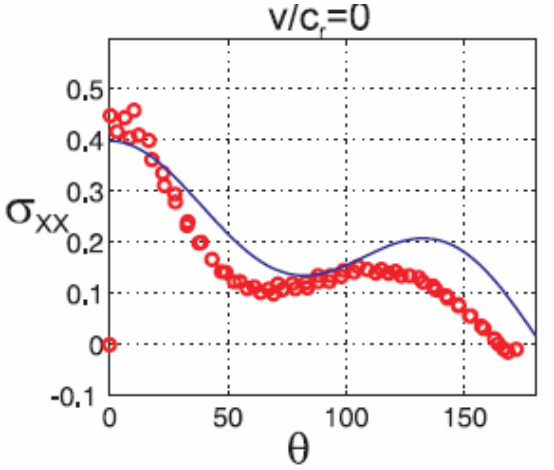
Griffith, Irwine and others: Failure initiates at defects, such as cracks, or grain boundaries with reduced traction, nano-voids

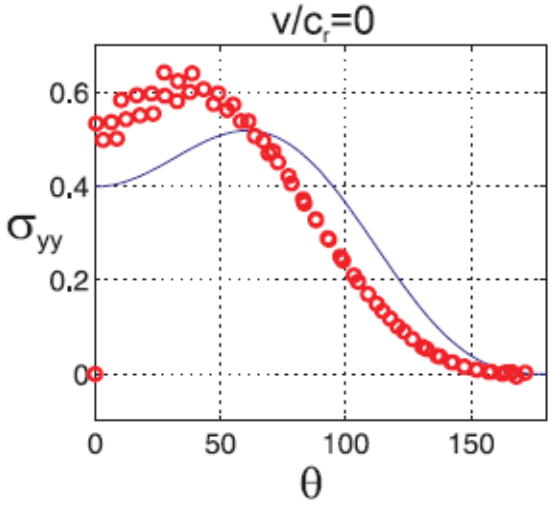
Schematic of stress field around a single (static) crack

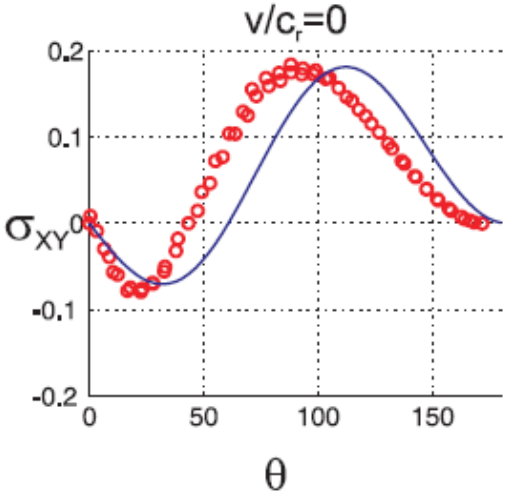


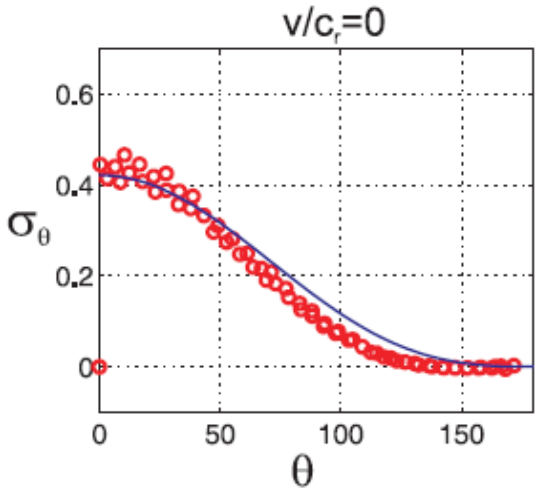
➢ The stress field around a crack is complex, with regions of dominating tensile stress (crack opening) and shear stress (dislocation nucleation)

Stress field around a (static) crack



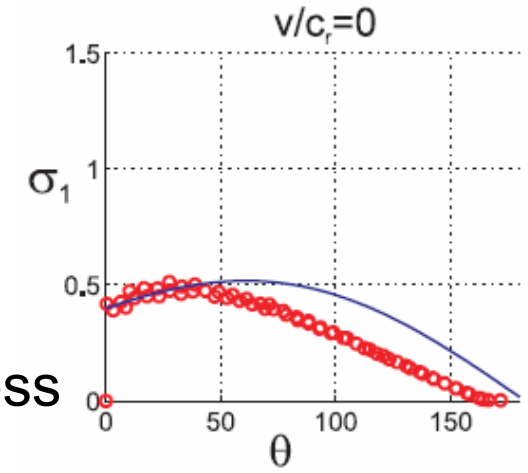






Hoop or opening stress

Maximum principal stress

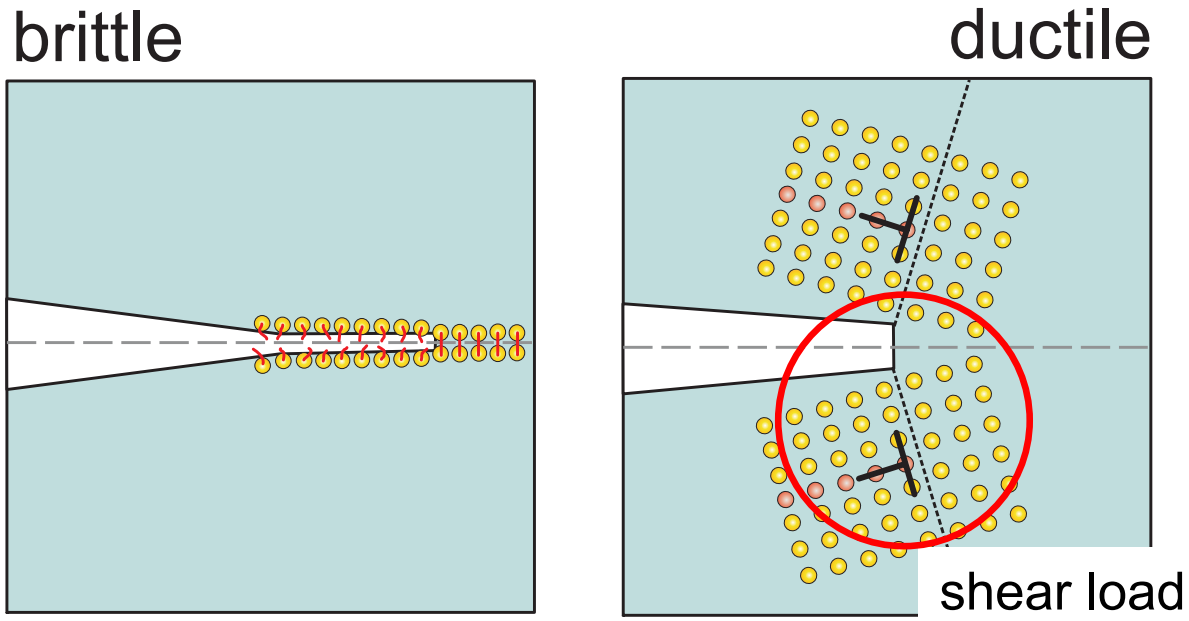


Continuum theory

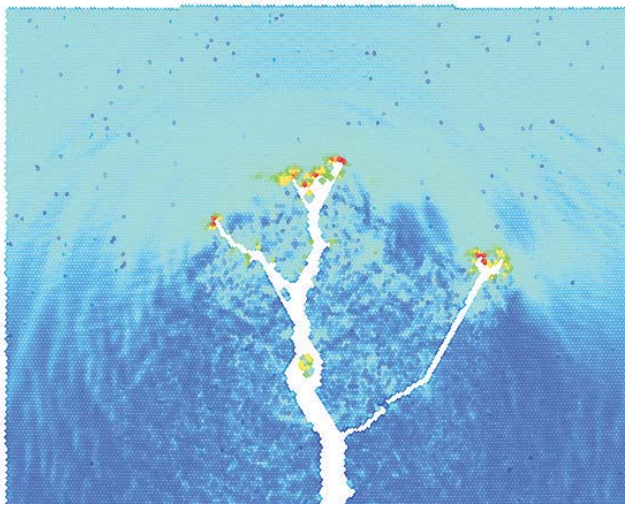
MD modeling

Ductile versus brittle materials

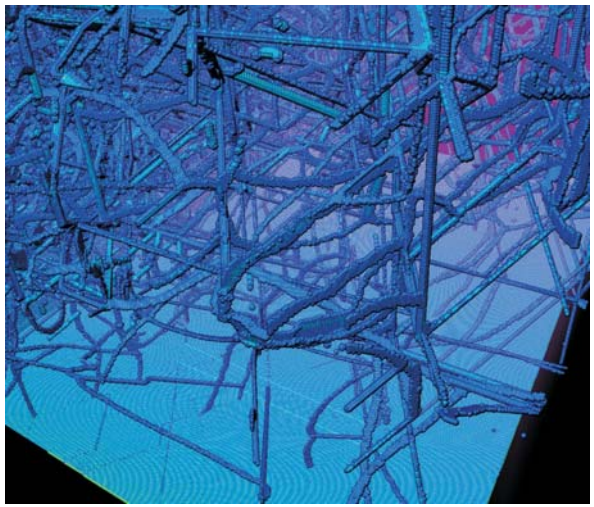
Glass,
Polymers,
Ice…



Copper,
Gold,
…

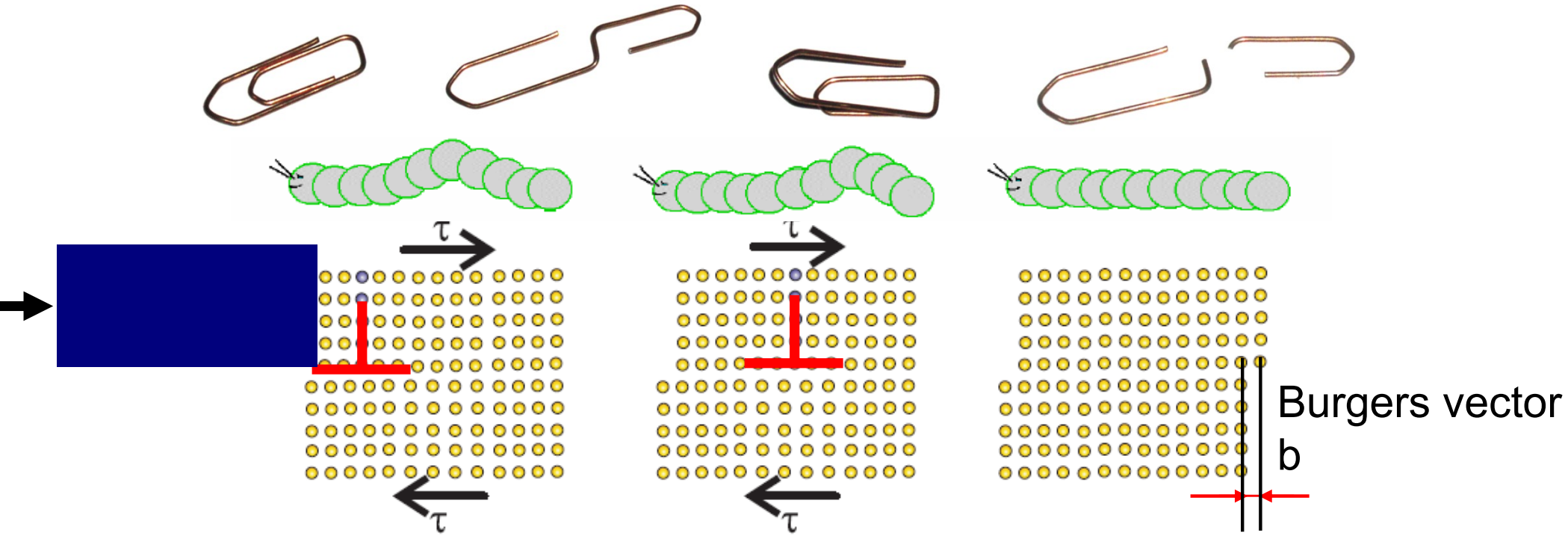


(a)

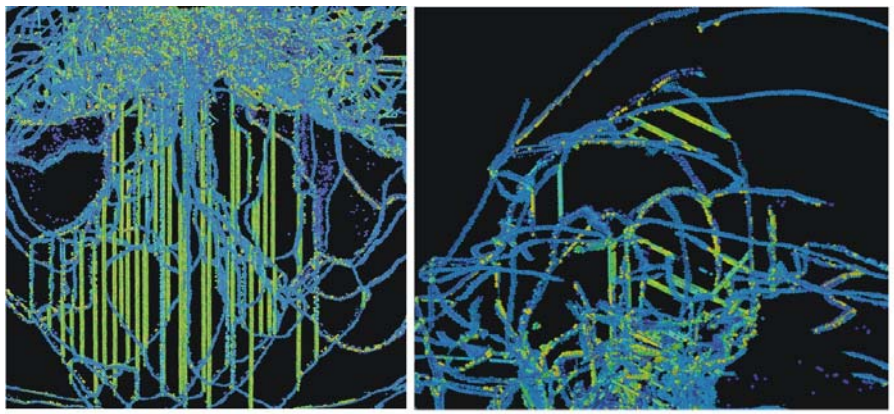


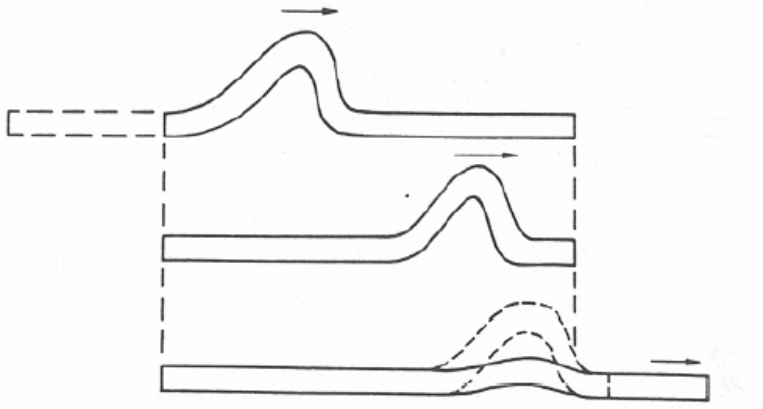
(b)

Ductile materials are governed by the motion of dislocations: Introduction



Dislocations are the <u>discrete</u> entities that carry plastic (permanent) deformation

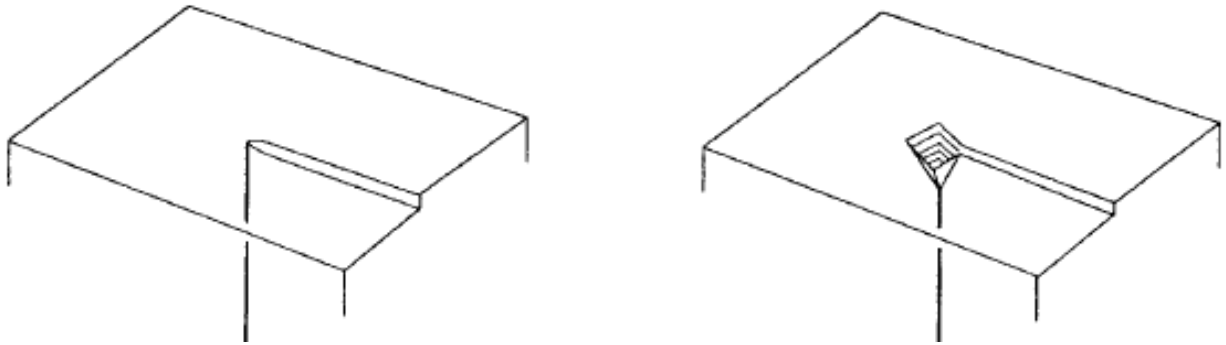




http://www.people.virginia.edu/~lz2n/mse209/Chapter7.pdf

Dislocations: Introduction

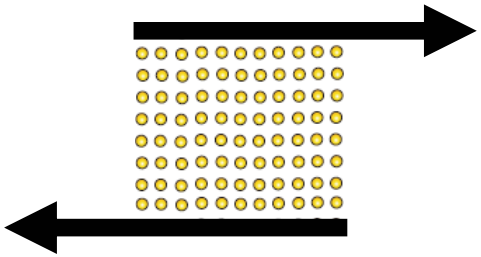
- A dislocation is a linear crystallographic defect, or irregularity, in crystal structure. The presence of dislocations strongly influences many of the properties of real materials. The theory was originally developed by Vito Volterra in 1905.
- Some types of dislocations can be visualized as being caused by the termination of a plane of atoms in the middle of a crystal.
- In such a case, the surrounding planes are not straight, but instead bend around the edge of the terminating plane so that the crystal structure is perfectly ordered on either side.
- The analogy with a stack of paper is apt: if a half a piece of paper is inserted in a stack of paper, the defect in the stack is only noticeable at the edge of the half sheet.



Theoretical shear strength

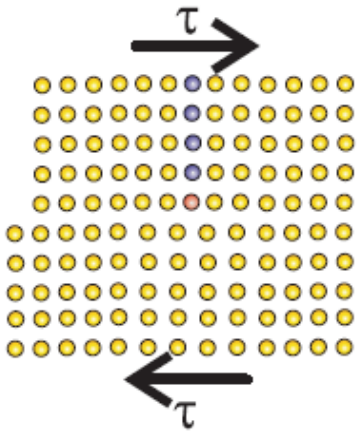
- Dislocations play an important role in reducing the critical applied shear stress to plastically deform a material compared to the theoretical shear strength
- Perfect crystal: Deformation needs to be cooperative movement of all atoms; the critical shear stress for this mechanism was calculated by Frenkel (1926):

$$\tau_{th} = \frac{b}{a}\frac{G}{2\pi} \approx \frac{G}{30}$$



- Although this is an approximation, the shear strength measured in experiment is much lower:

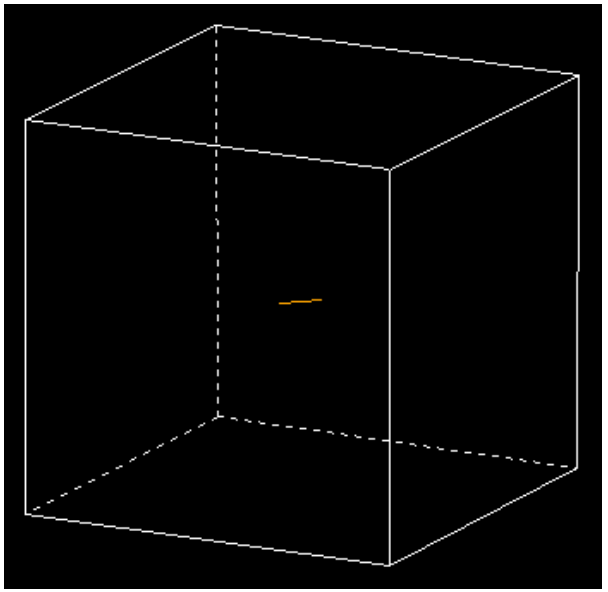
$$\tau_{\exp} = \frac{G}{10{,}000...100{,}000{,}000}$$

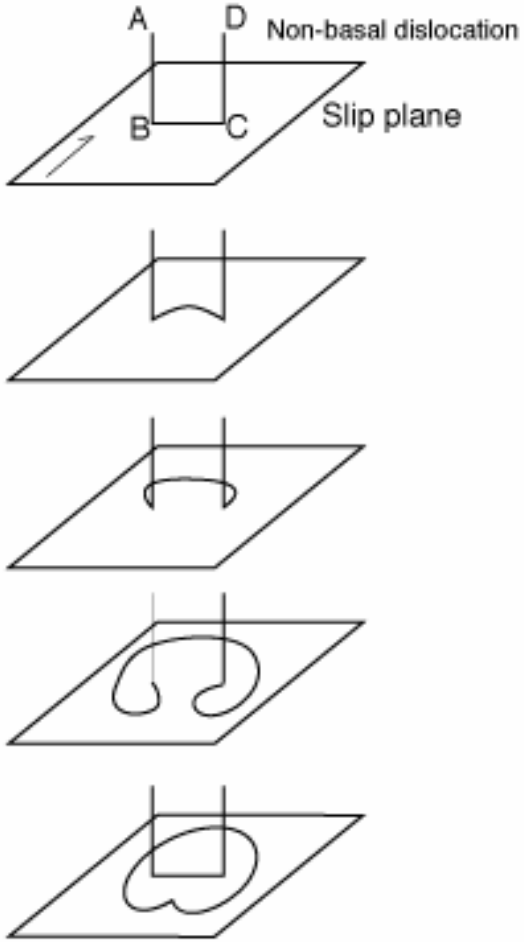


- Difference explained by existence of dislocations by Orowan, Polanyi and Taylor in 1934
- Confirmed by experiments with whiskers (dislocation free crystals)

Sources of dislocations

- Dislocation densities can vary from 10^5 cm^{-2} in carefully solidified metal crystals to 10^{12} cm^{-2} in heavily deformed metals
- Most metals have dislocations intrinsically present (statistical dislocations), e.g. due to deformation or manufacturing history
- During deformation, dislocations are nucleated from cracks (see earlier slides), grain boundaries, other dislocations, or surface defects/surfaces
- Frank-Read sources

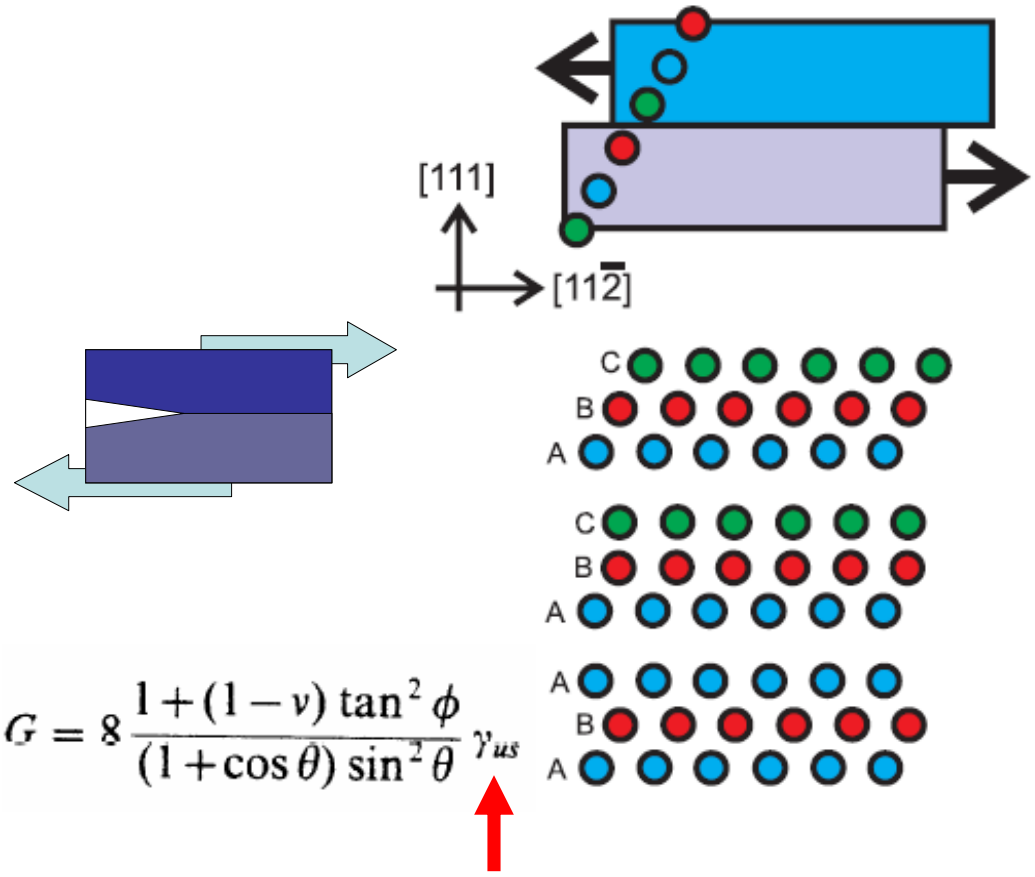




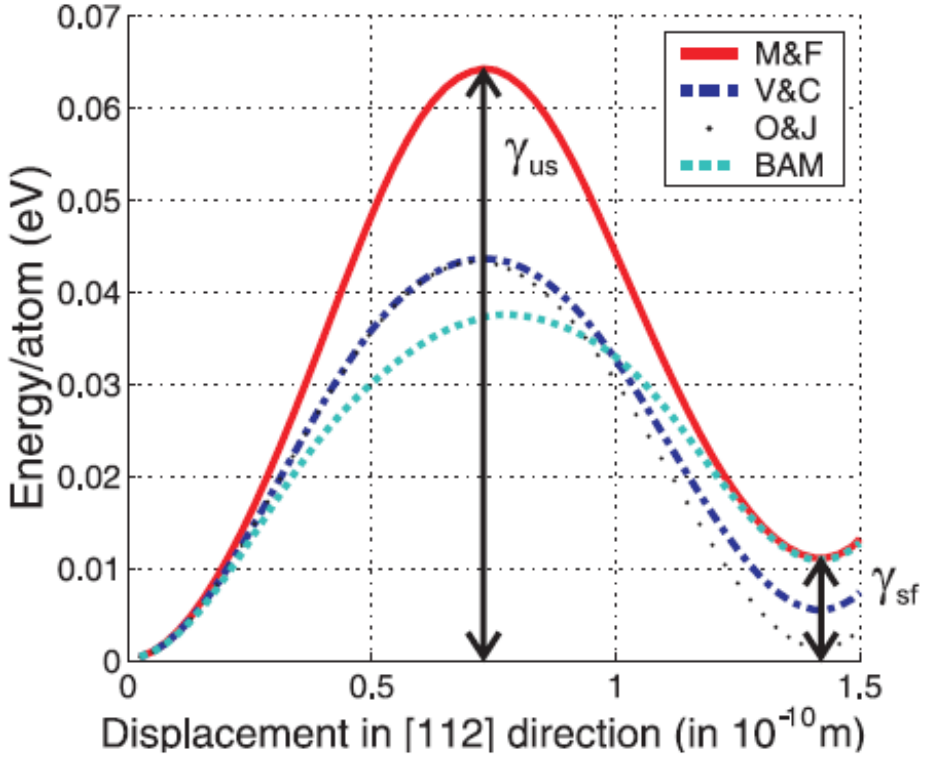
http://web.earthsci.unimelb.edu.au/wilson/ice1/generations.html
http://www.tf.uni-kiel.de/matwis/amat/def_en/kap_5/backbone/r5_3_2.html

Stacking fault energy

Difficulty of creating a dislocation (γ_{us}) and moving a dislocation through the crystal (γ_{sf})



$$G = 8\frac{1+(1-\nu)\tan^2\phi}{(1+\cos\theta)\sin^2\theta}\gamma_{us}$$



(Buehler, 2006)

Calculation of stacking fault energy for different interatomic potentials

Partial dislocations

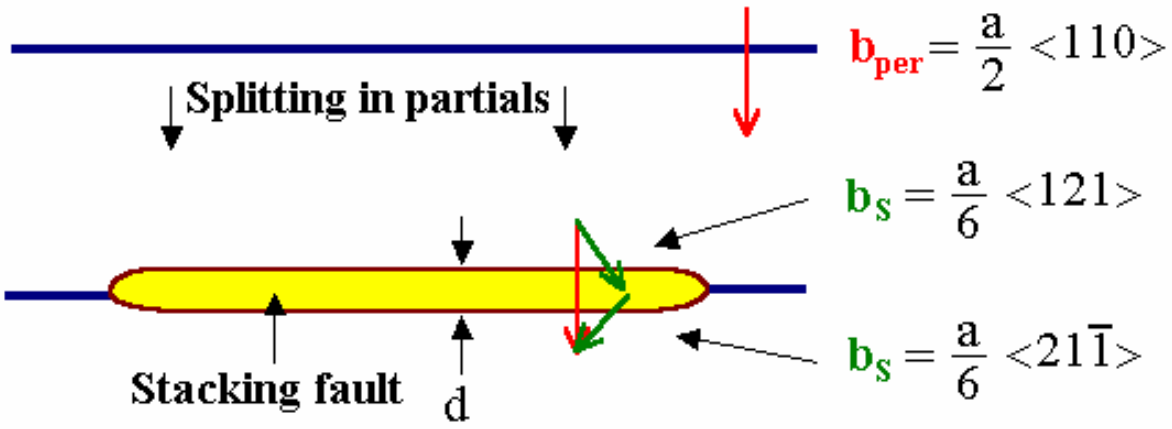
- In FCC, dislocations with Burgers vector [110] split up into two “partial dislocations” with Burgers vector 1/6[112]

Energy of the perfect dislocation

$$= G \cdot b^2 = G \cdot (a/2\langle 110\rangle)^2 = \frac{G \cdot a^2}{2}$$

Energy of the two partial dislocations

$$= 2G \cdot (a/6\langle 112\rangle)^2 = 2G \cdot a^2/36 \cdot (1^2 + 1^2 + 2^2) = \frac{G \cdot a^2}{3}$$



Metals with low SFE and materials under geometric confinement have large stacking faults

http://www.tf.uni-kiel.de/matwis/amat/def_en/kap_5/backbone/r5_4_2.html

Ductile versus brittle materials

- Ductile failure: Nucleation of dislocations at crack tip (γ_{us})
- Brittle fracture: Creation of two new surfaces (γ_s)
- Rice and others (1990s) have quantified this transition from brittle to ductile for various materials, by investigating the relative ease of either crack propagation or shear and dislocation nucleation:

  Use energy argument

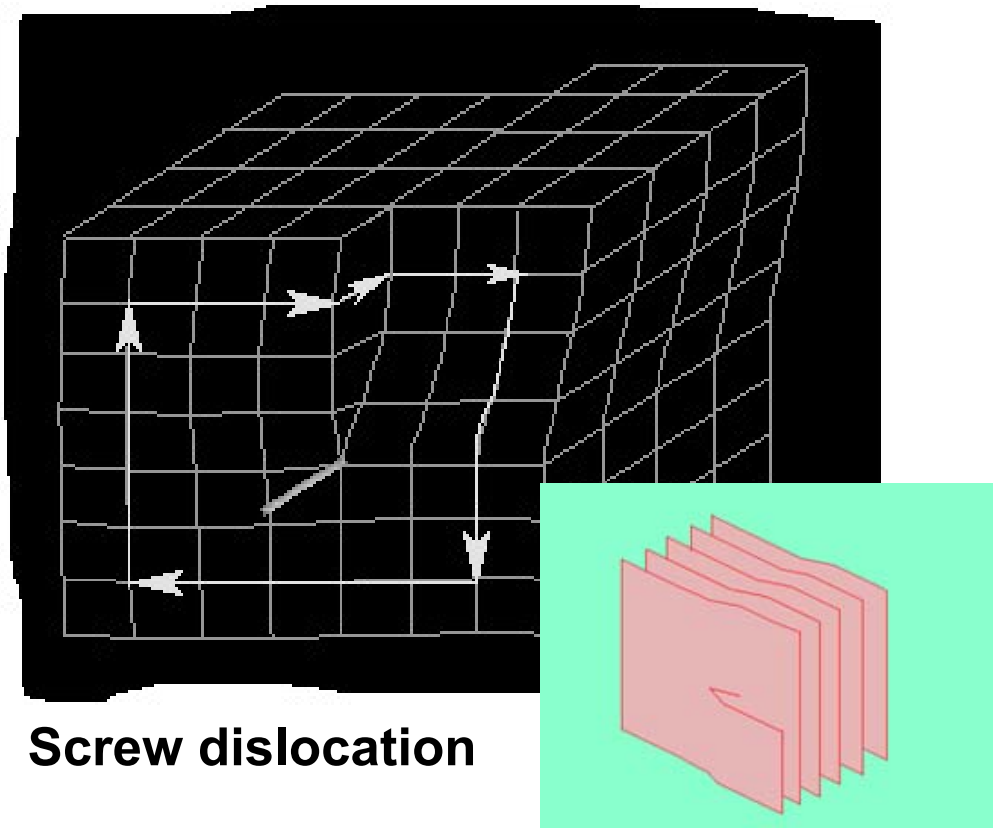
$$G = 8\frac{1+(1-\nu)\tan^2\phi}{(1+\cos\theta)\sin^2\theta}\gamma_{us}$$ "ductile"

$$G = 2\gamma_s$$ "brittle"

$$\frac{\gamma_s}{\gamma_{us}} > 4\frac{1+(1-\nu)\tan^2\phi}{(1+\cos\theta)\sin^2\theta}$$

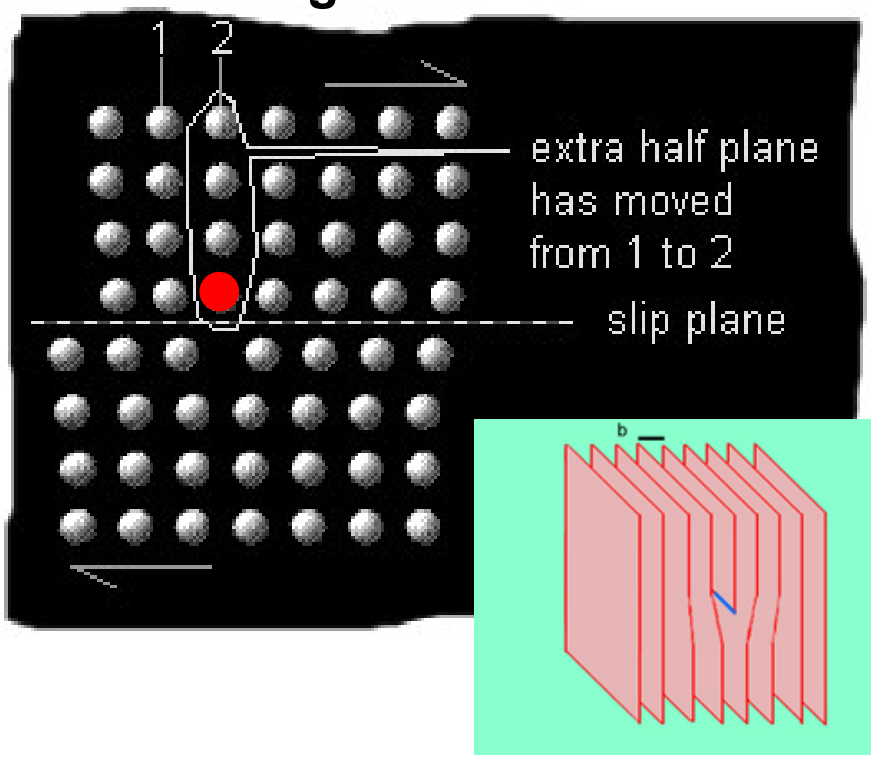
- These early results already suggested the great importance of the atomic interaction in determining the materials behavior.
- This was later verified in many studies, including for cases of brittle fracture

Edge and screw dislocations



Screw dislocation

Edge dislocation



Dislocation line || Burgers vector

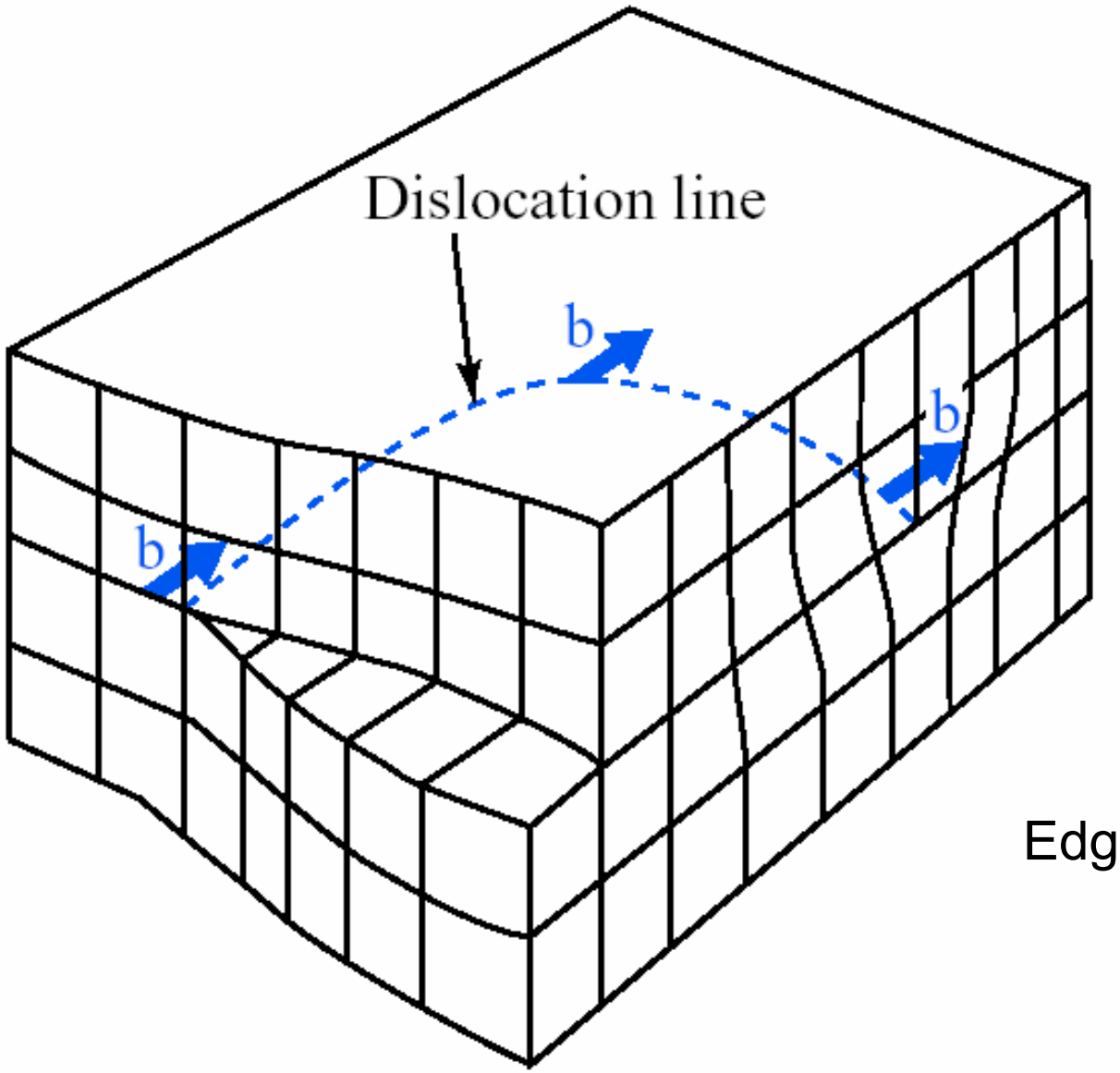
Screw dislocation

Dislocation line ⊥ Burgers vector

Other crystal defects

Grain boundaries, vacancies, interstitials

Edge and screw dislocations

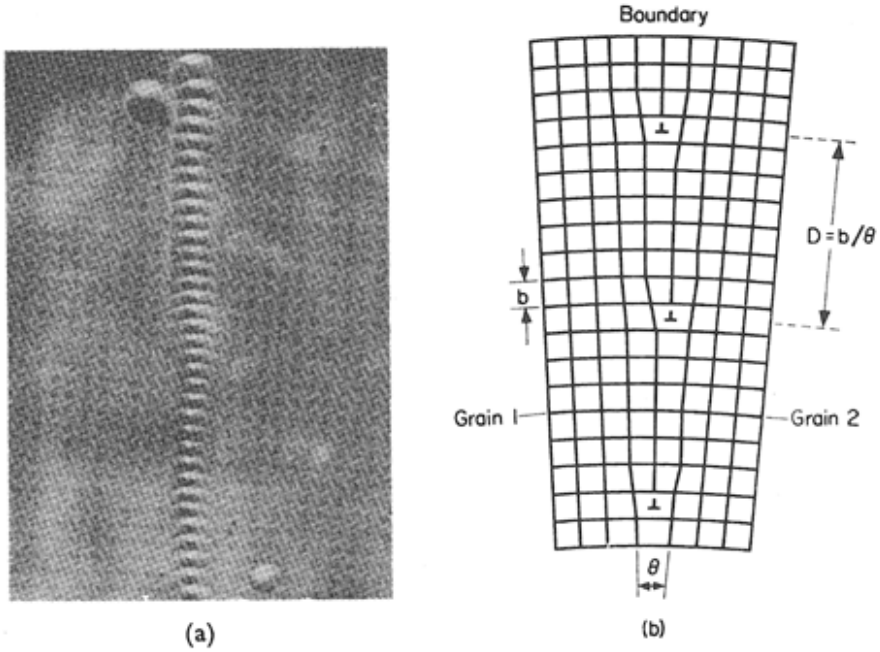


Screw

Edge

Experimental observation

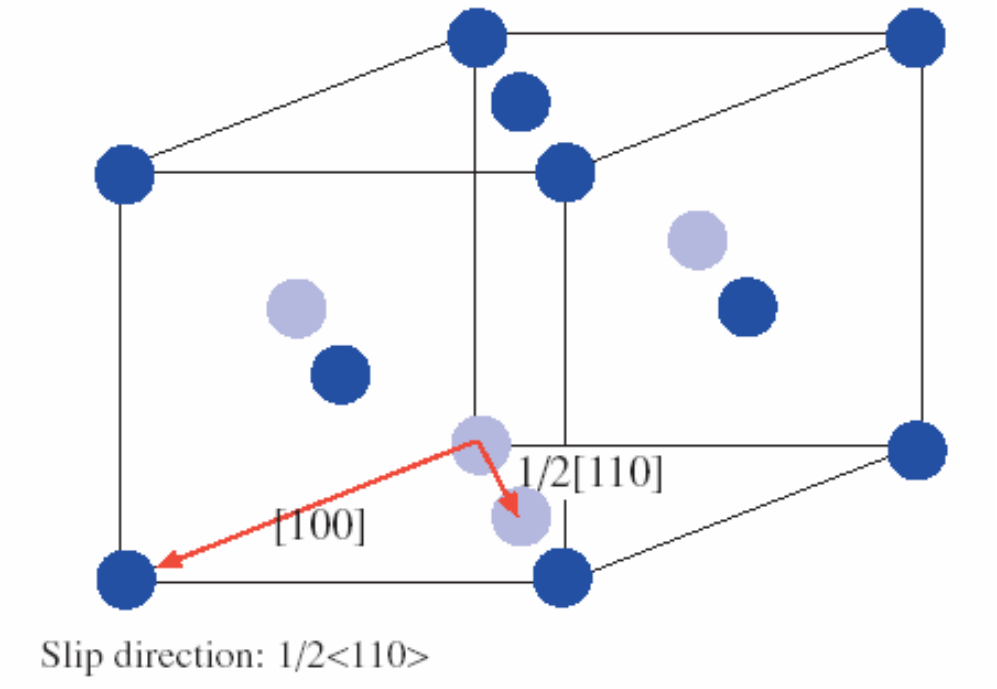
Transmission Electron Micrograph of Dislocations



Grain boundary misfit dislocations

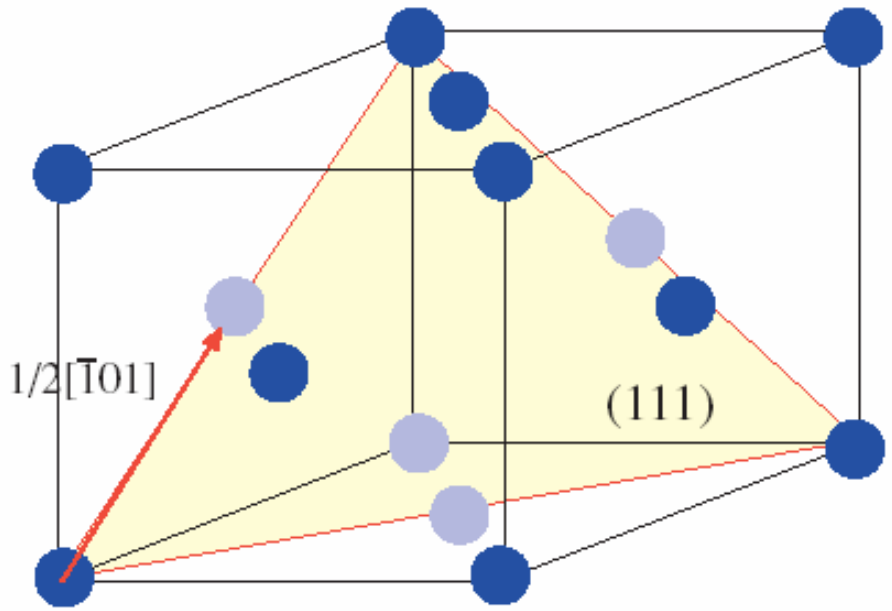
Dieter, G. E. (1988) *Mechanical Metallurgy* ISBN 0071004068
Honeycombe, R.W.K. (1984) *The Plastic Deformation of Metals* ISBN 0713121815
Hull, D. & Bacon, D. J. (1984) *Introduction to Dislocations* ISBN 0080287204
Read, W. T. Jr. (1953) *Dislocations in Crystals* ISBN 1114490660

Slip direction and plane in FCC



Slip direction: 1/2<110>

For specific crystals, there are certain directions of Burgers vectors and slip planes that are energetically favored



Slip plane: {111}

FCC:

Slip directions are ½<110>

Glide planes are {111}

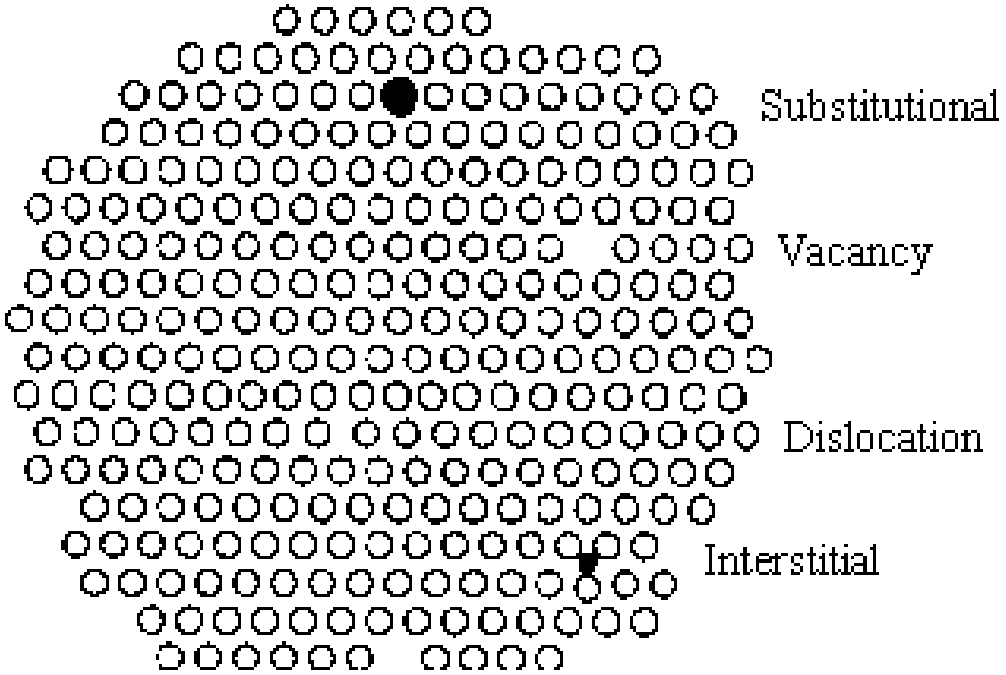
The slip planes and directions are those of highest packing density

Other crystallographic defects

- Point defects: Vacancies and interstitials
- Can be produced by plastic deformation

• Vacancy formation energy ca. E_v~1-3 eV/atom, scale with melting temperature T_m: $E_v \sim 8kT_m$

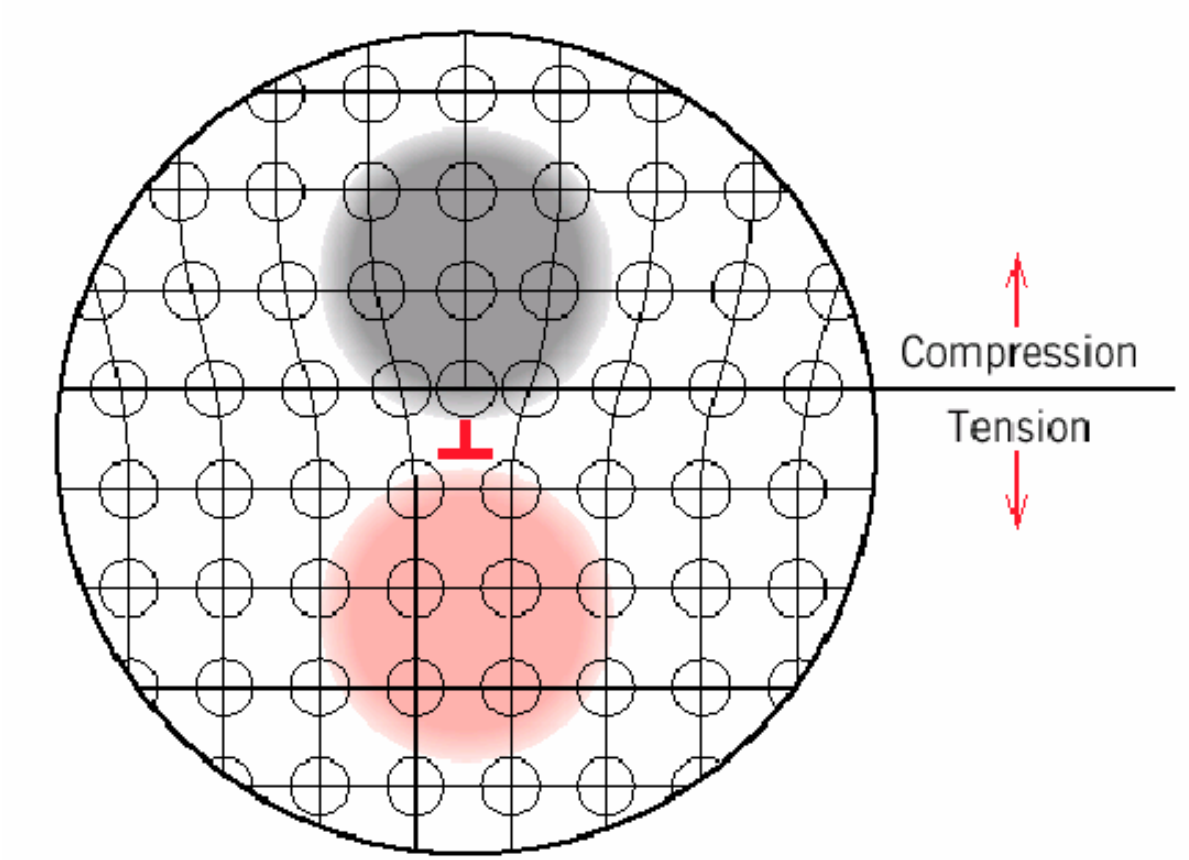
• Impurity either substitutional (other atom species on lattice site) or interstitial (non-lattice site)



http://chemed.chem.purdue.edu/genchem/topicreview/bp/materials/defects3.html

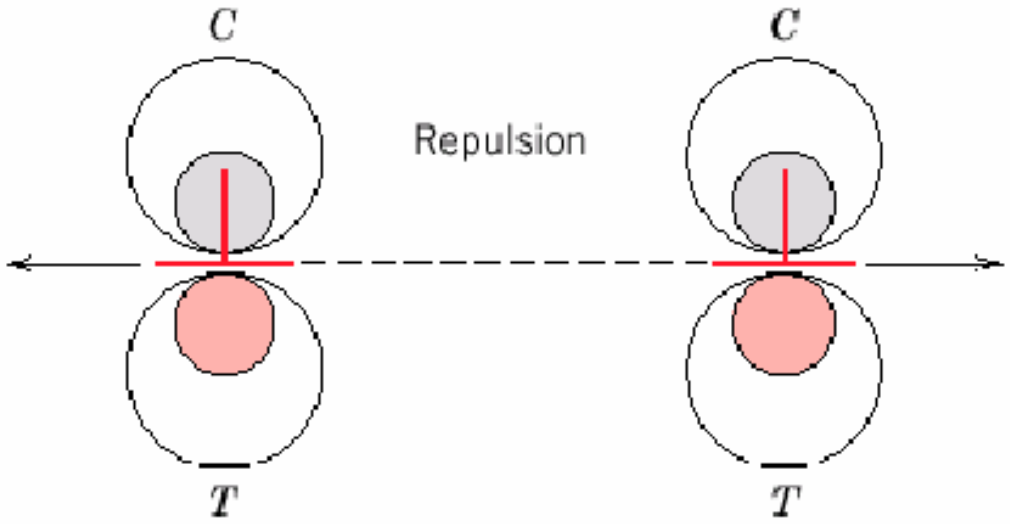
Dislocations: Stress field around a dislocation

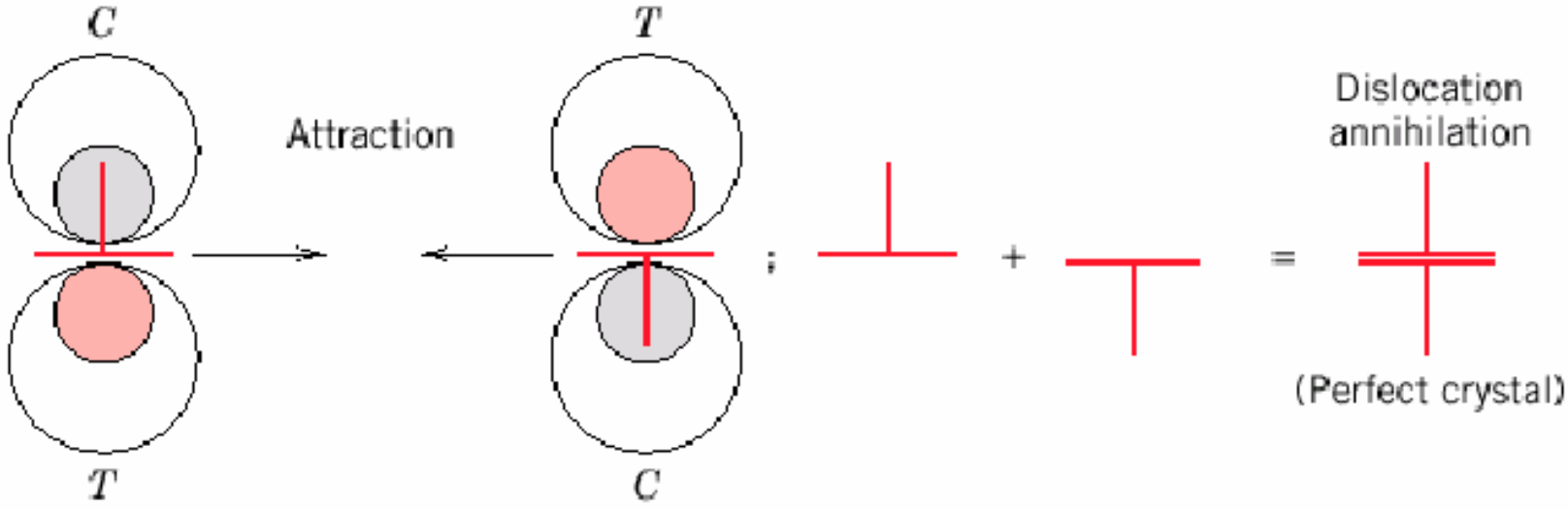
- Each dislocation induces a long-range stress field in the crystal
- Around the dislocation core:



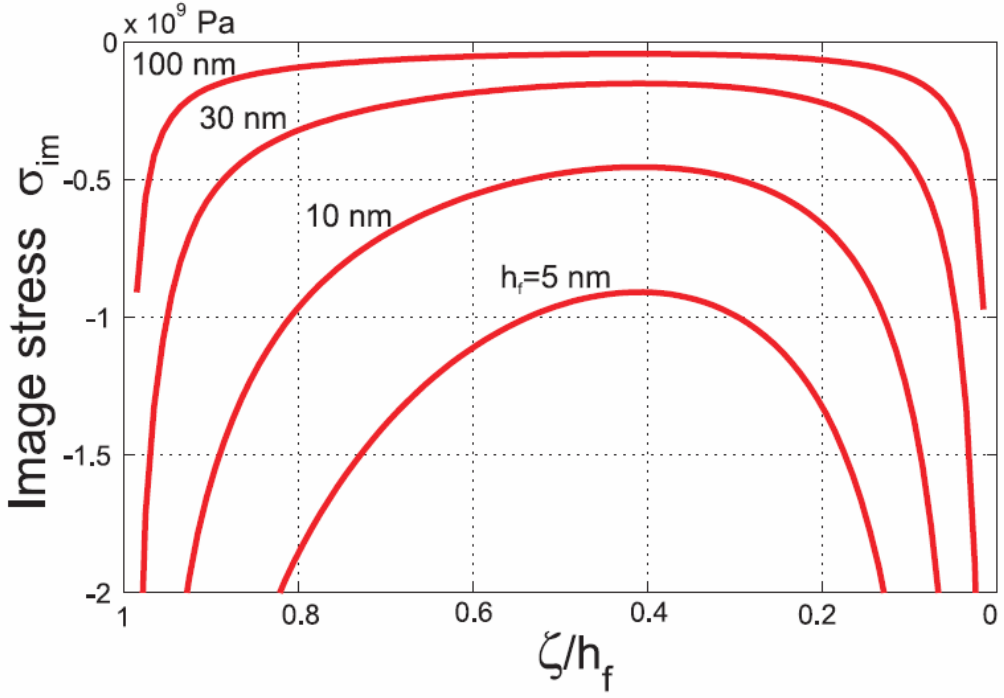
Dislocations: Interaction

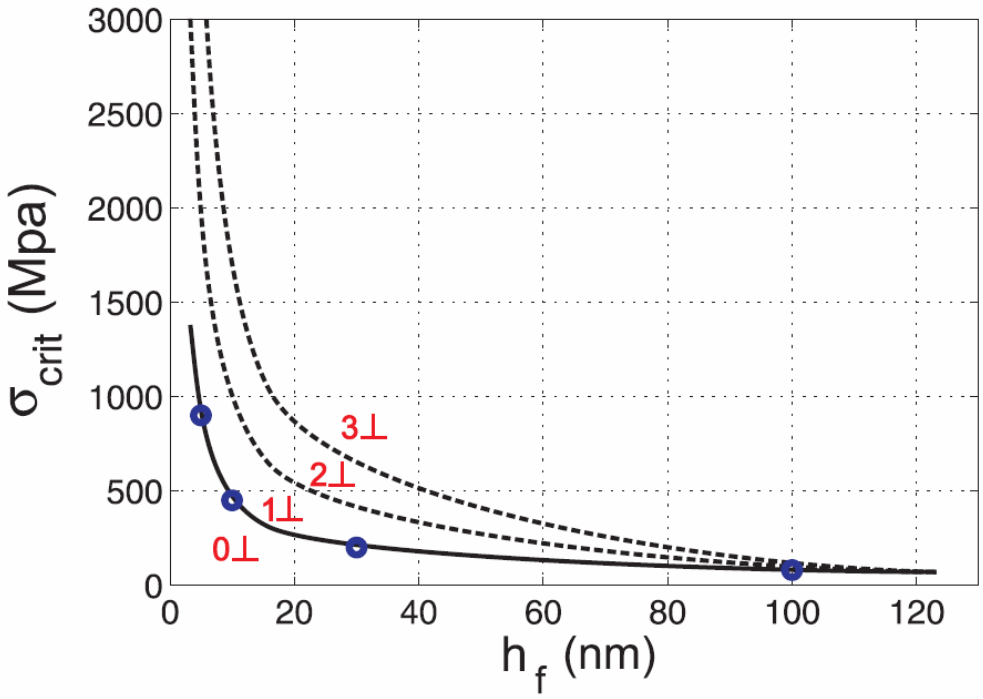
Important to understand how materials deform

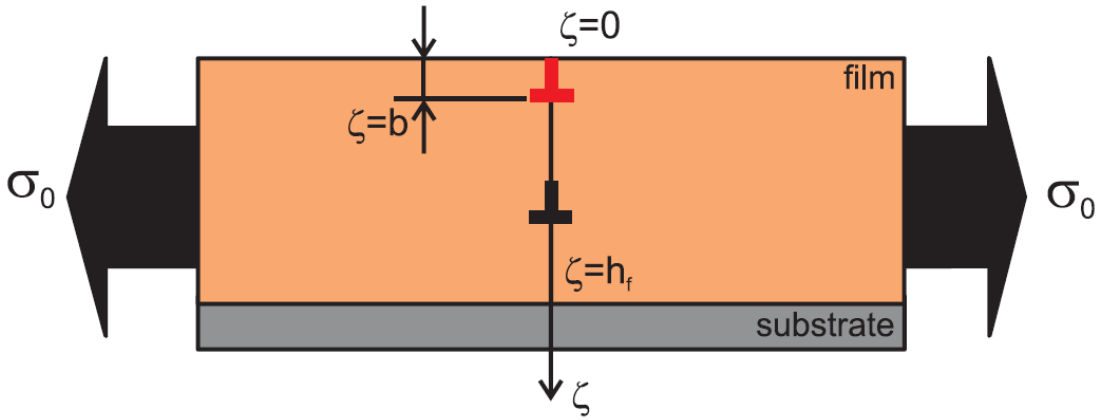




Nano-confinement of dislocations in ultra thin films on substrates



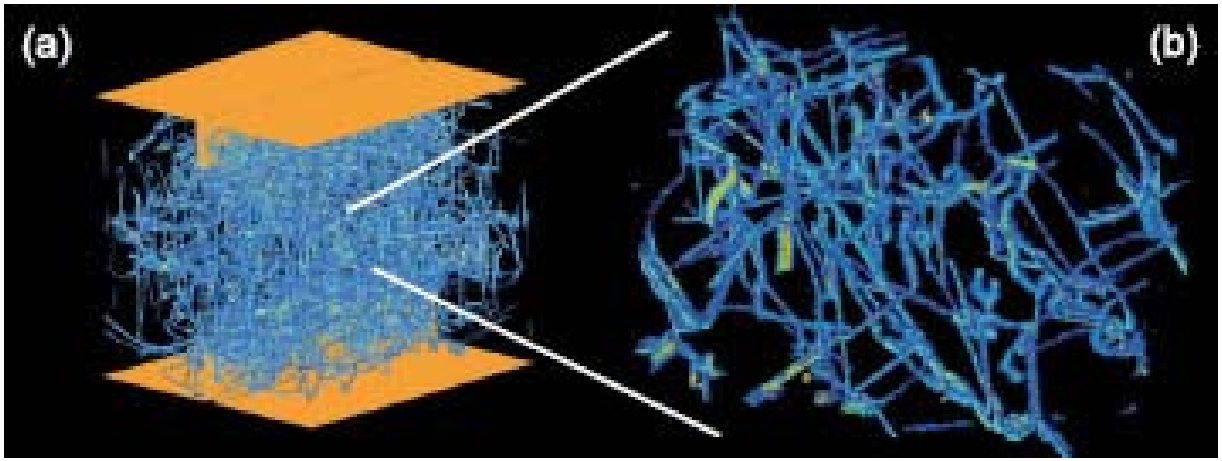




(Buehler *et al*., 2006)

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



Analysis of a one-billion atom simulation of work-hardening

- Can computer simulation be used to study work-hardening ("feasibility study")?

- How can the results of ultra-large scale atomistic computer simulation be analyzed (1,000,000,000 atoms!) – reach cube w/ μm side length

- What are the fundamental, atomistic mechanisms of work-hardening in ductile materials, and how do these mechanisms compare with the classical picture of work-hardening?

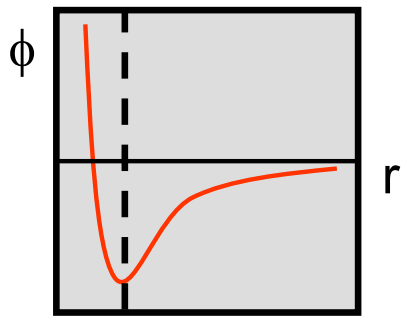
„bending a paper clip until it breaks"

1 2 3 4

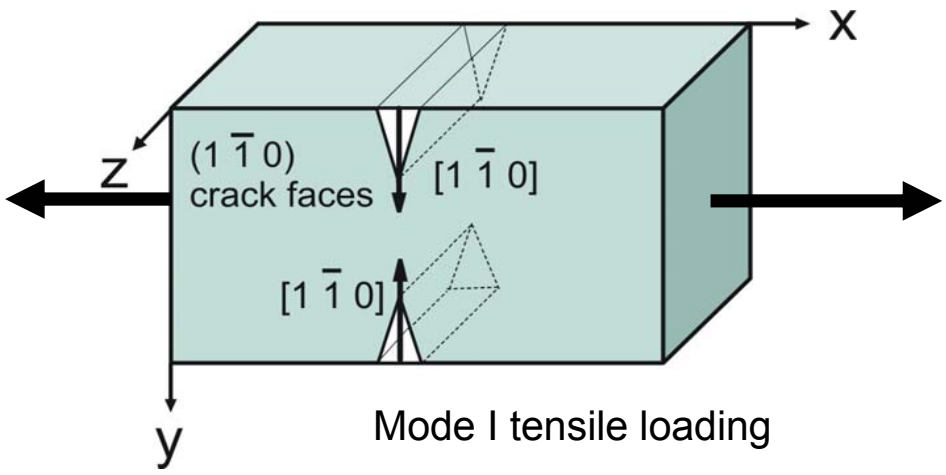
Analysis of a one-billion atom simulation of work-hardening

Simulation details

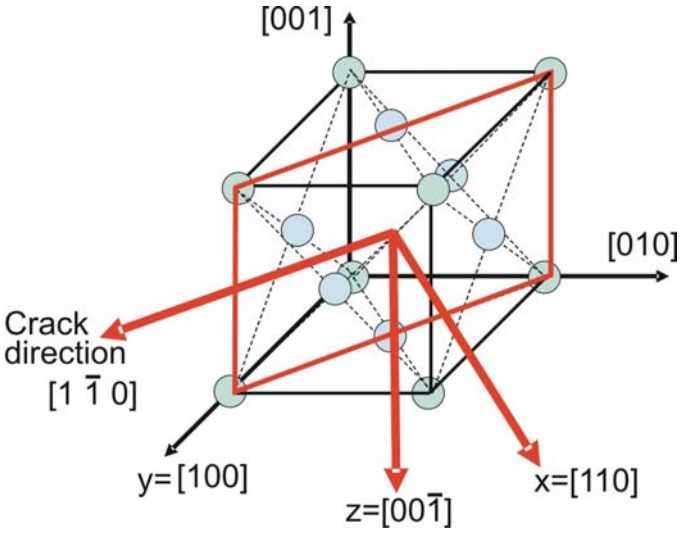
- 1,000,000,000 atom simulation carried out at ASCI WHITE, LLNL (PNAS, 2002)
- Lennard-Jones ductile "model material"



Generic features of atomic bonding: „repulsion vs. attraction"



Mode I tensile loading



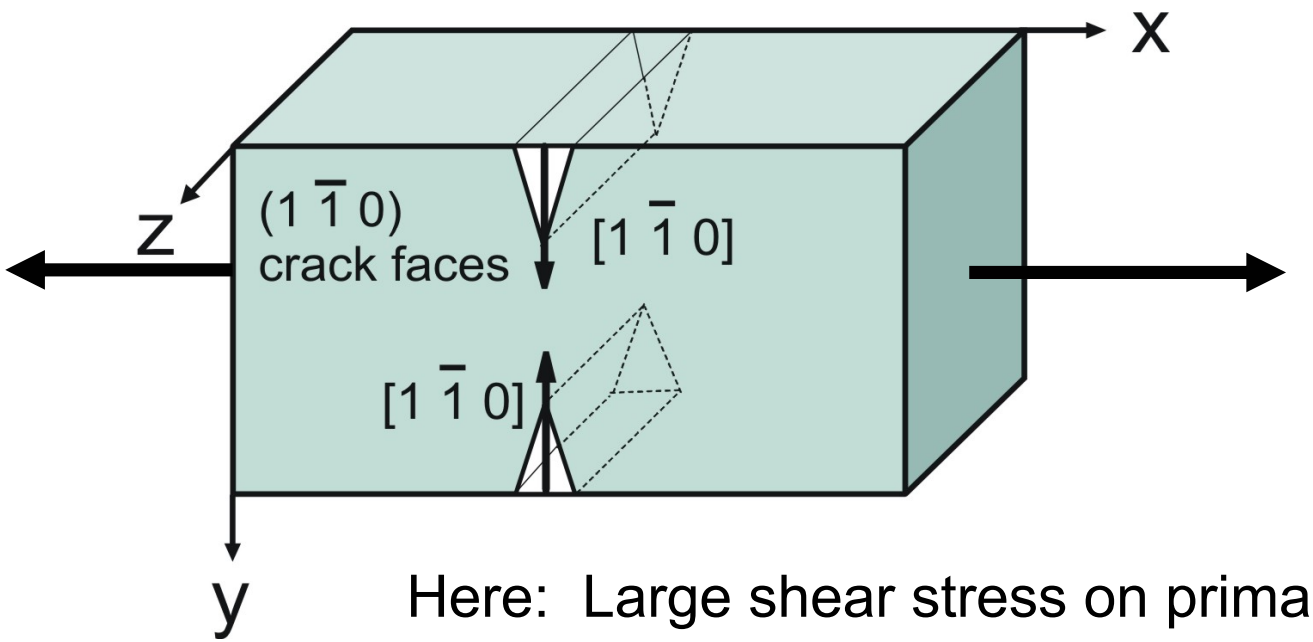
The purpose of scientific computing is insight, not numbers.

(Richard Hamming)

Choosing a “smart” model

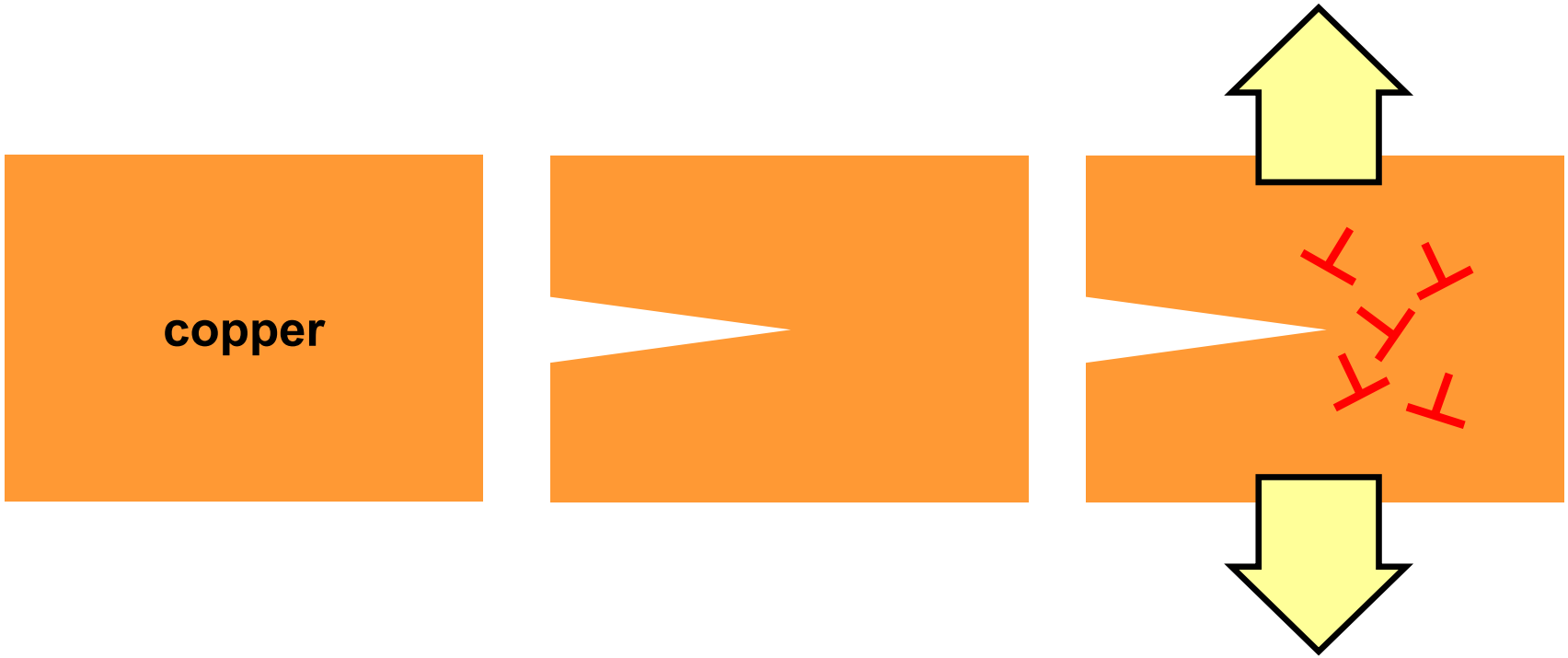
- Choosing the “right” model is the key
- Overly complex models, e.g. “brute force QM” or ultra-large scale models may not lead to insight
- Overly simple models, “harmonic bonds” may lead to irrelevant results, if not interpreted correctly

- Goal: A balance between accuracy and simplicity to achieve maximized insight into the physical problem



Here: Large shear stress on primary glide planes
Obtain many dislocations

Case study:
Cracking of a copper crystal…



- Critical load for cracking
- What happens when the load becomes large?
- How to analyze the complex data?
- Limitations of modeling…

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

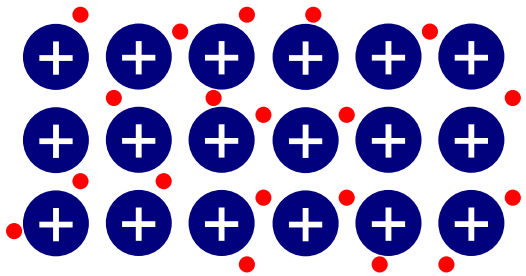
positive ions in a sea of electrons

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)

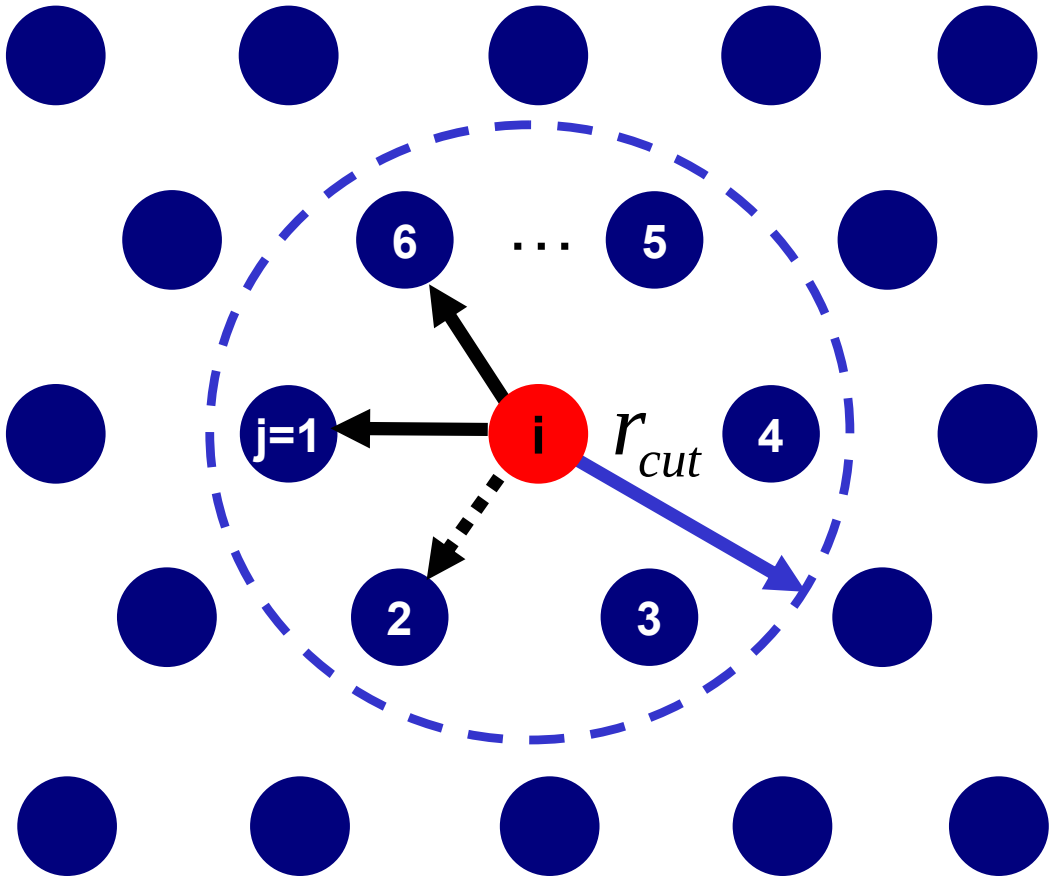


Properties of metals

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

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

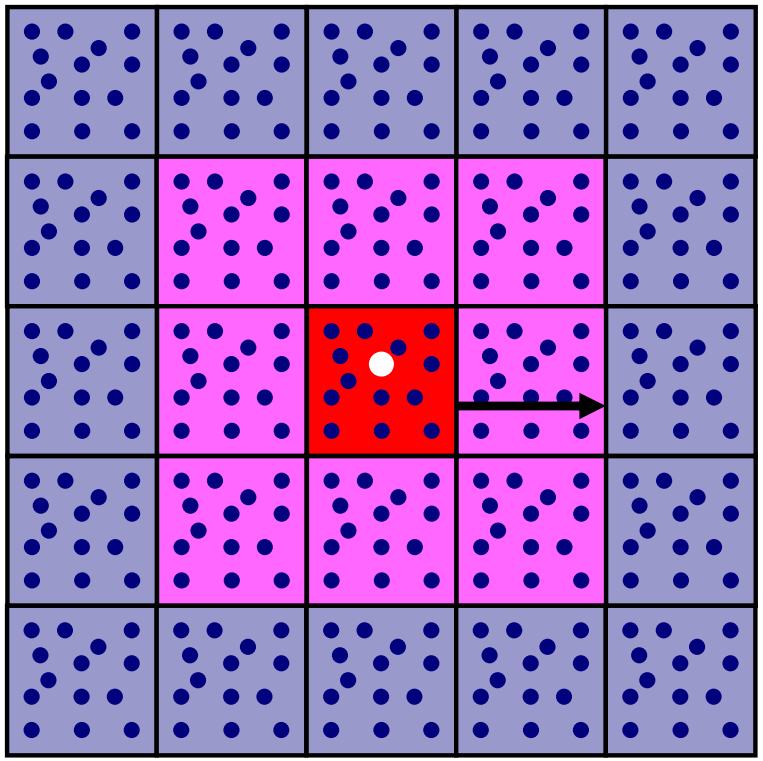
Morse

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

Good for noble gas Ar
(FCC in 3D)

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

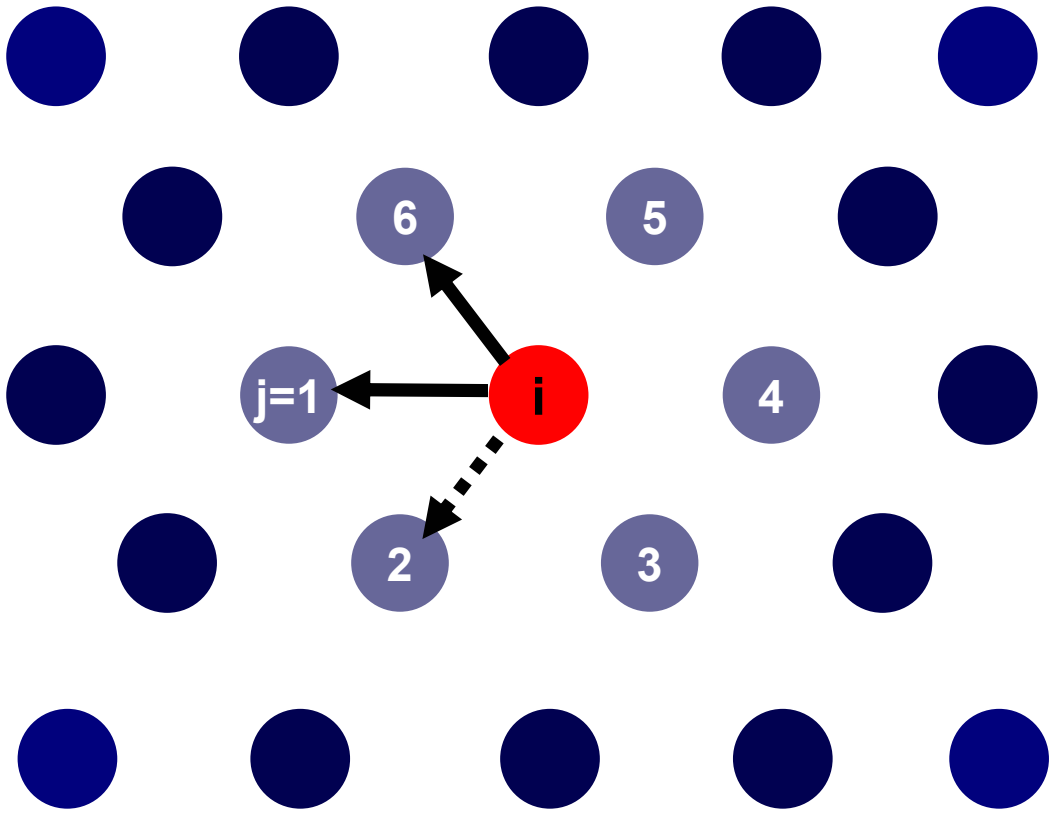
- Need nested loop to search for neighbors of atom *i:* Computational disaster
- Concept: Divide into computational cells ("bins", "containers", etc.)
- Cell radius $R>R_{cut}$ (cutoff)



- 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)

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 existence of “electron gas”



new

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

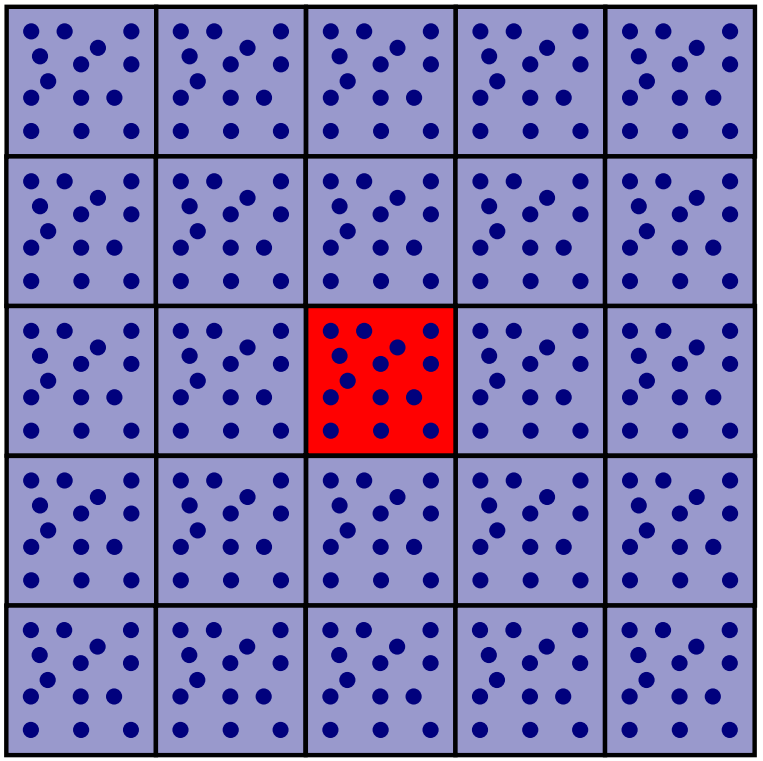
ρ_i Electron density at atom *I* based on a pair potential:

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

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

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

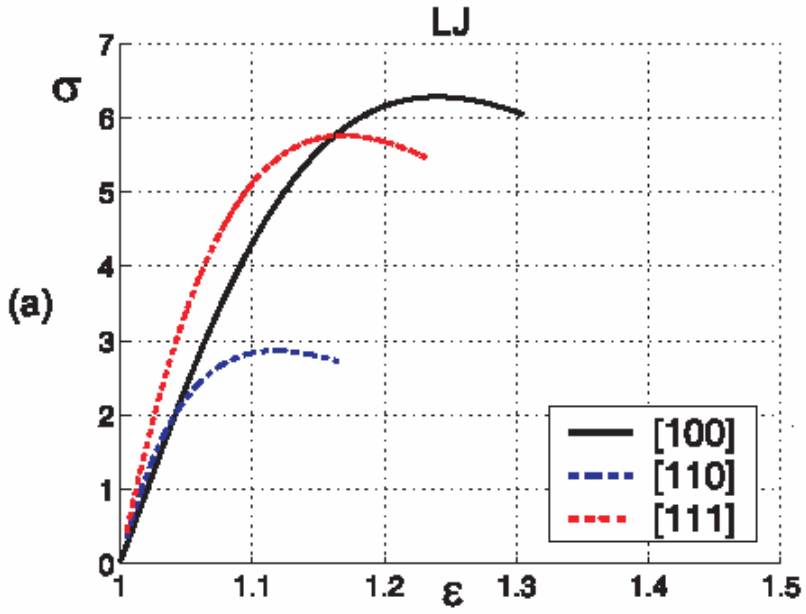
Loop 2:

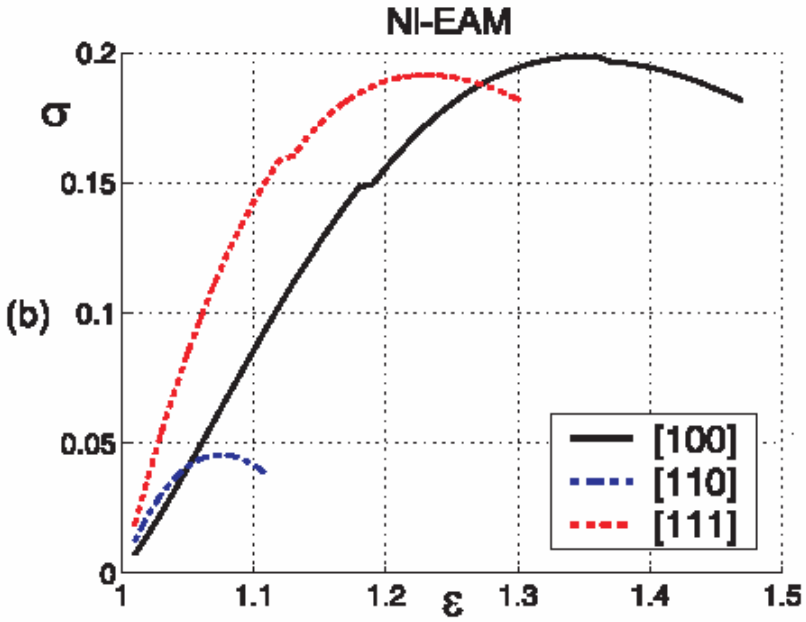
(iii) Calculate embedding function and derivatives

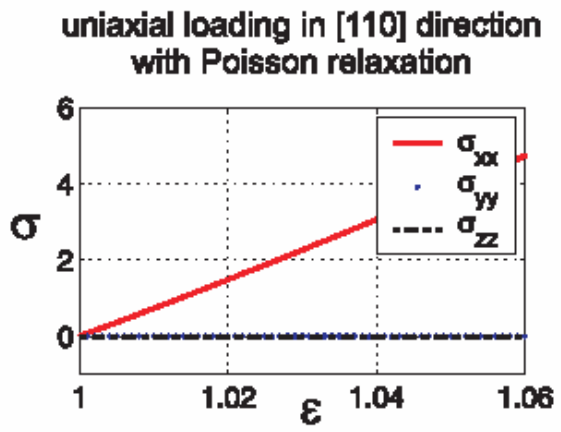
$$\mathbf{F}_i = -\sum_{j \neq i} \left(\phi'(r_{ij}) + [U'(n_i) + U'(n_j)]\rho'(r_{ij}) \right) \frac{\mathbf{r}_{ij}}{r_{ij}}$$

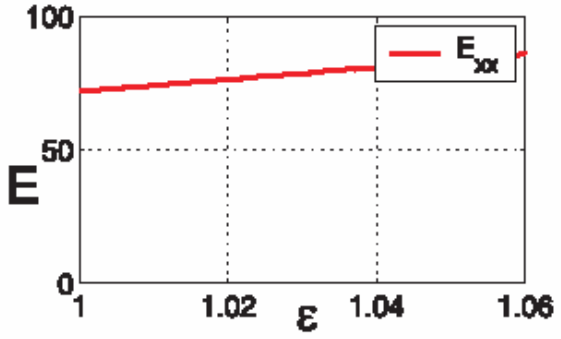
Due to additional (i) calculation of electron density and (ii) embedding contribution EAM potentials are 2-3 times slower than pure pair potentials

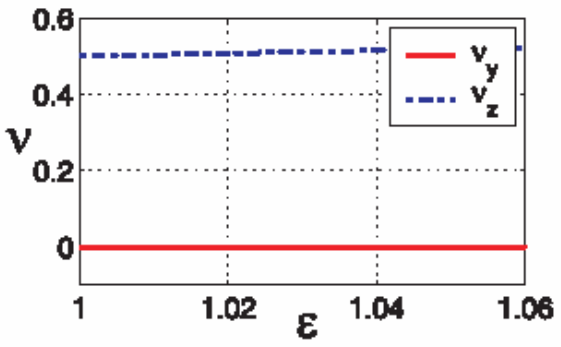
Large-strain elasticity: No dislocations

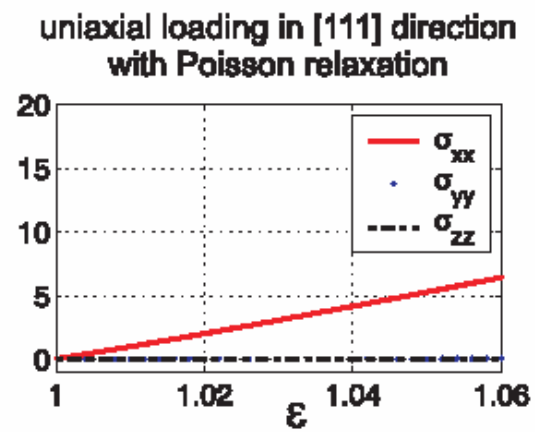


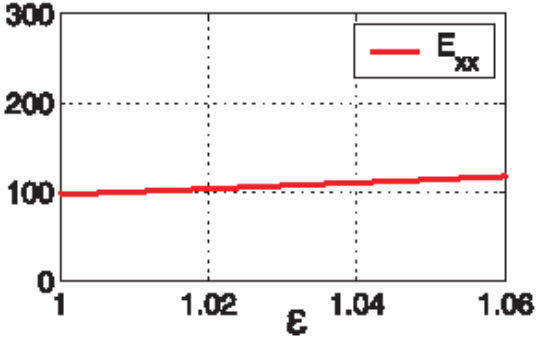


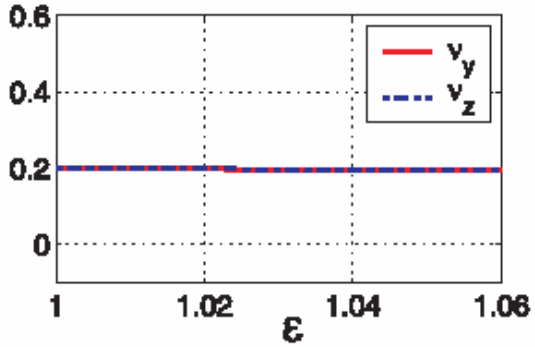






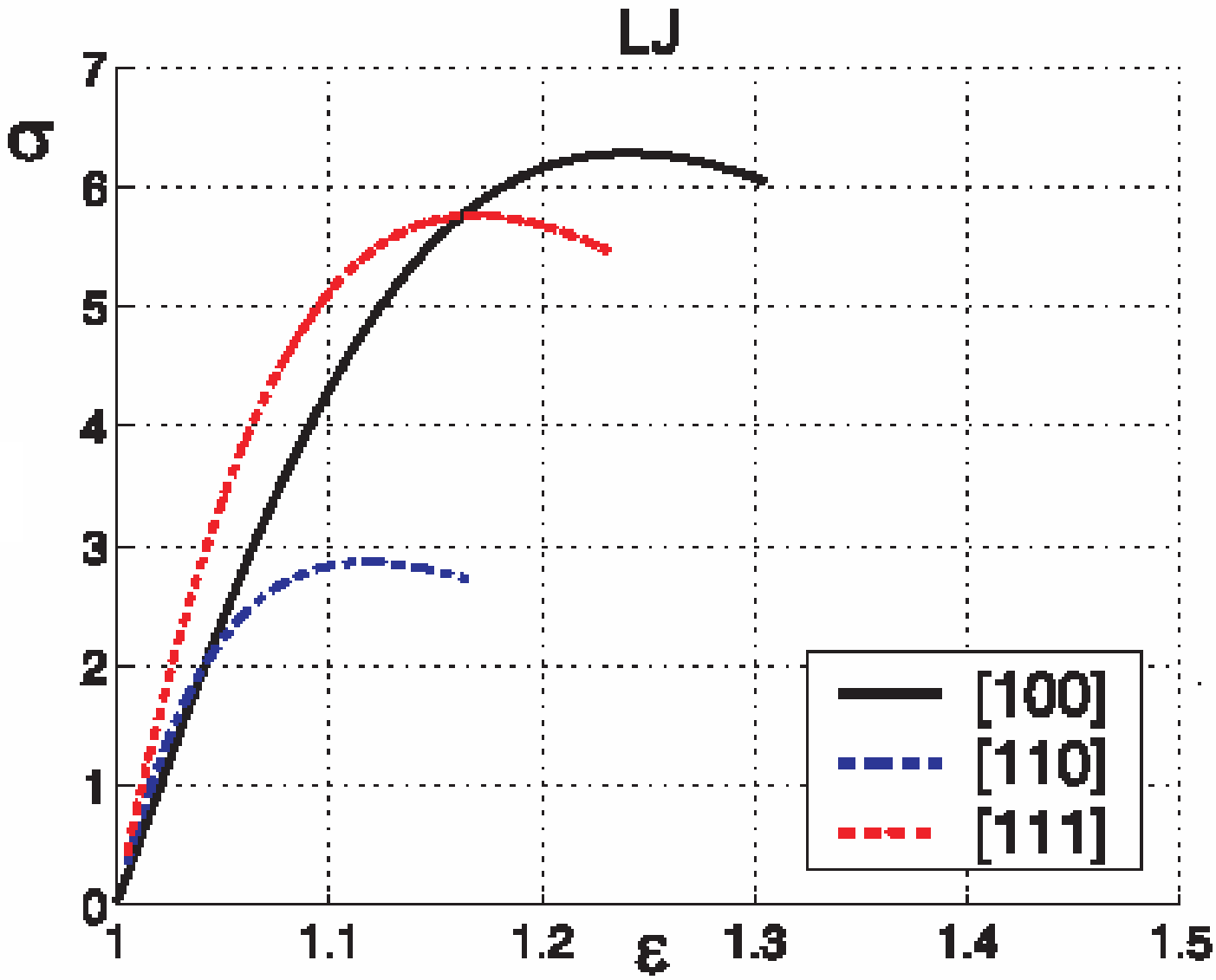




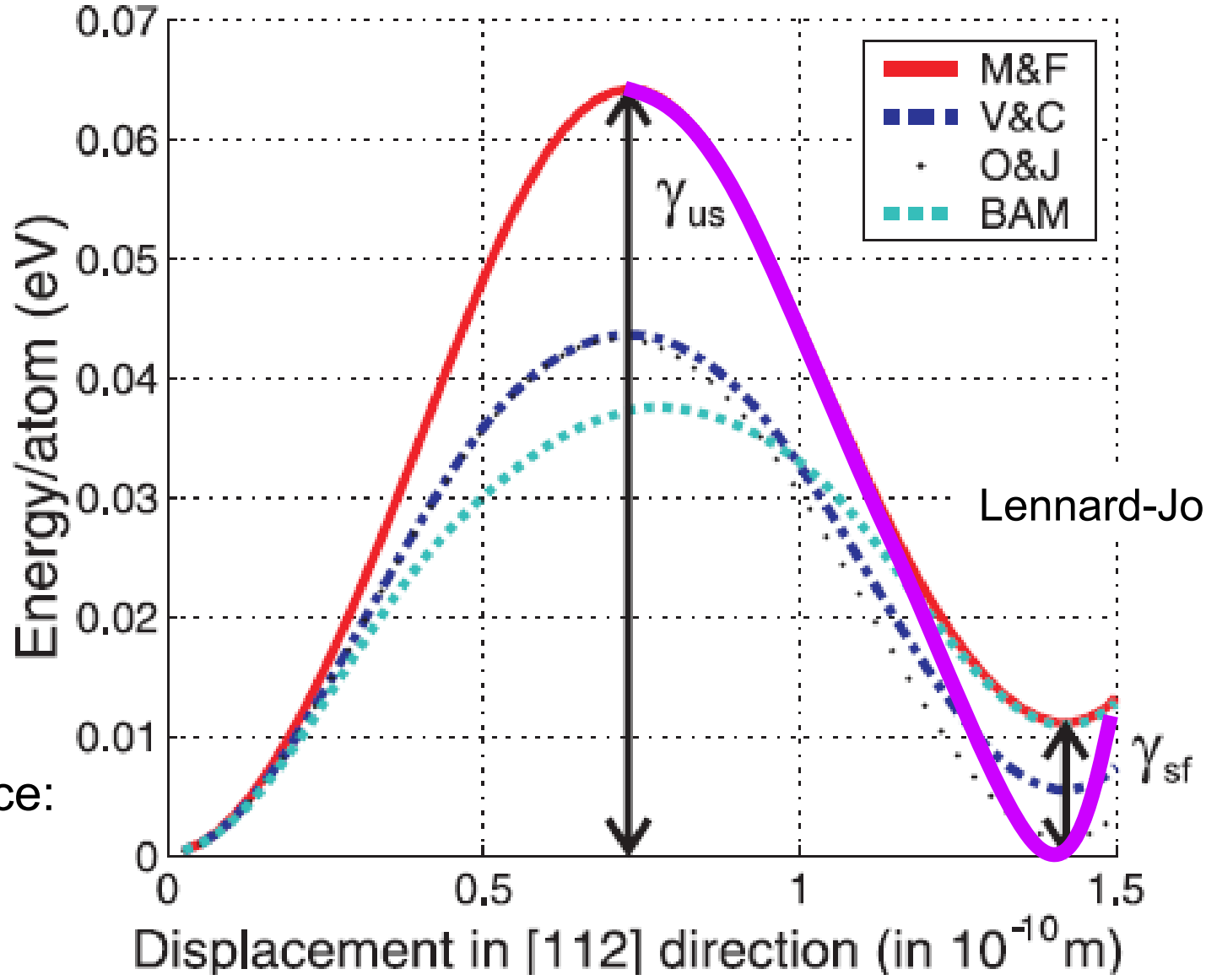


Harmonic potential

Elasticity associated with the LJ potential



Stacking fault energy: LJ potential vs. EAM potential



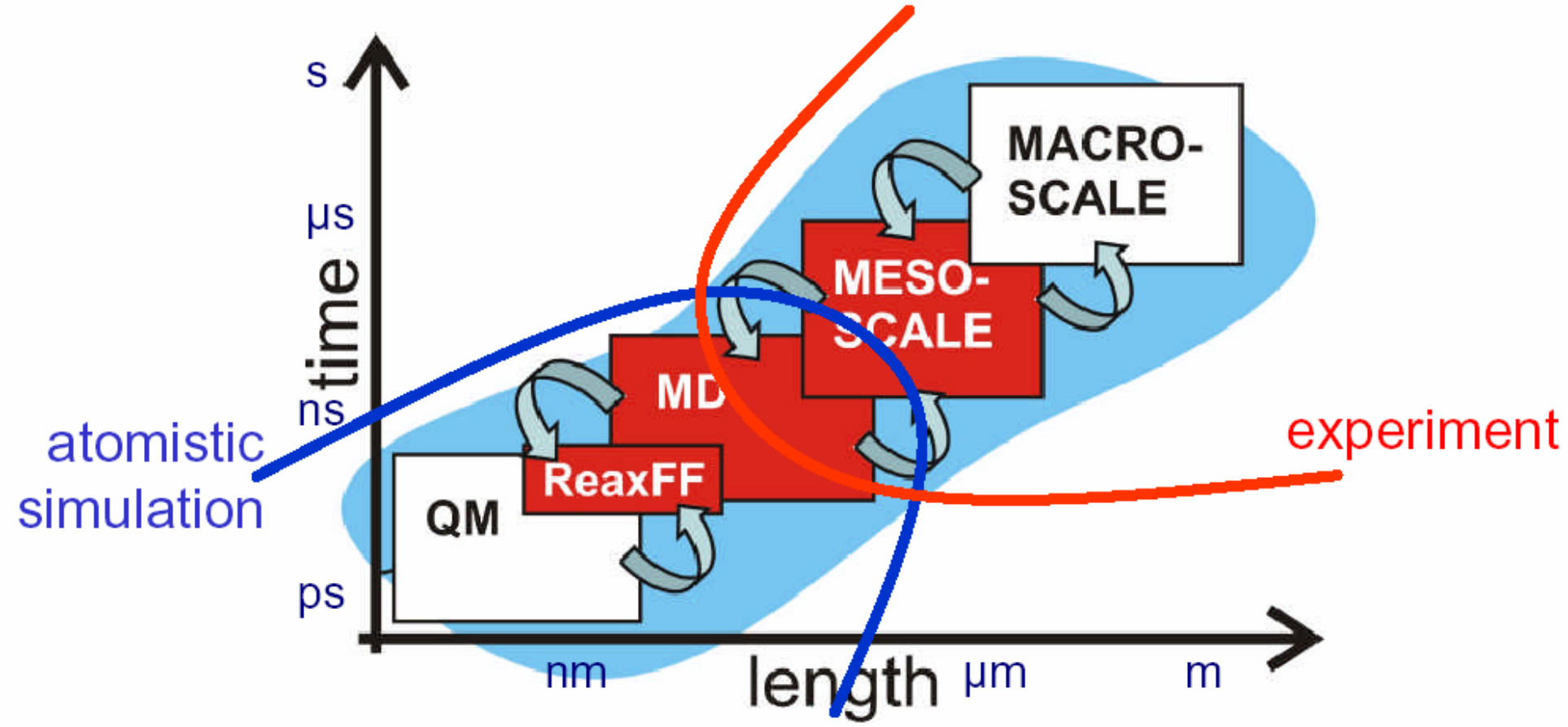
Lennard-Jones potential

Consequence:

Only partial dislocations expected

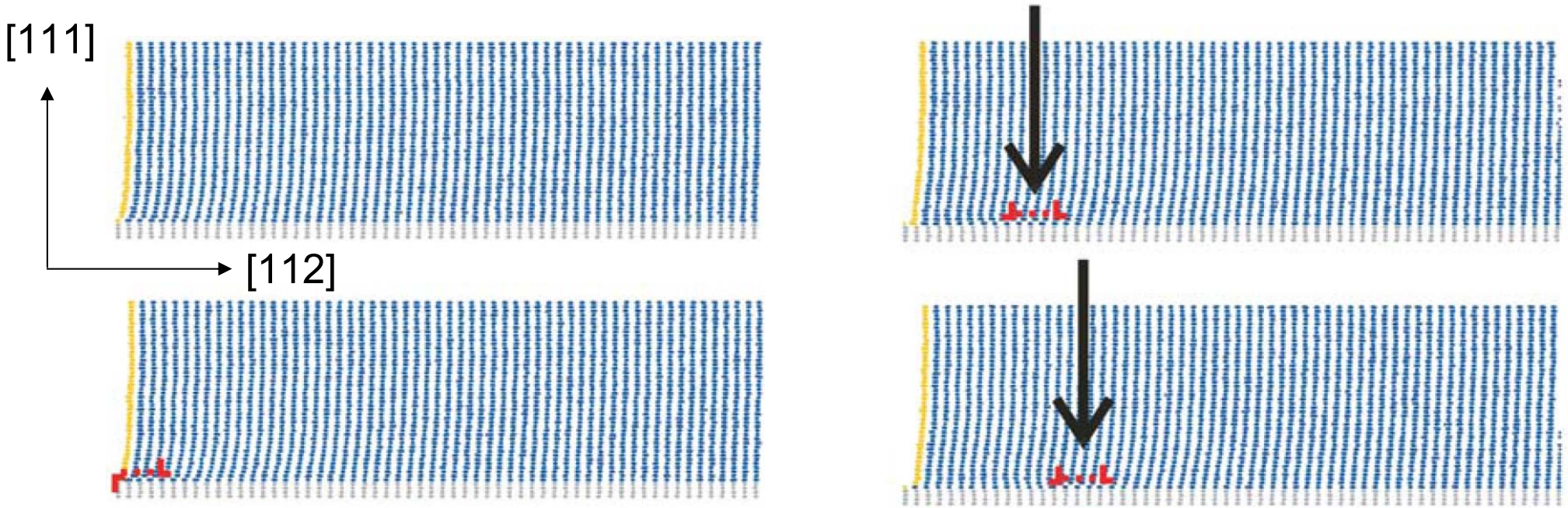
(schematic)

Approach: Overall multi-scale modeling scheme

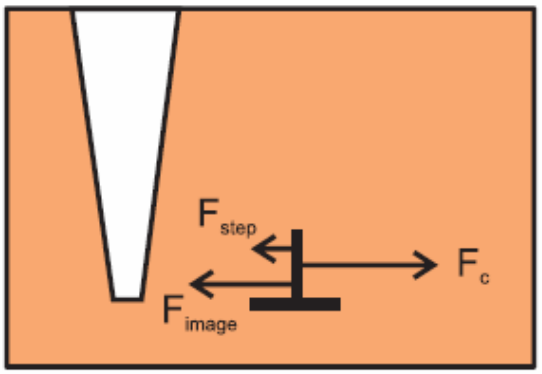


- QM trains ReaxFF, which is used in a hybrid scheme with MD to obtain parameters for mesoscale simulations
- Mesoscale simulations relate to macroscopic scales
- Focus on three methods: **ReaxFF, MD, and mesoscale methods**

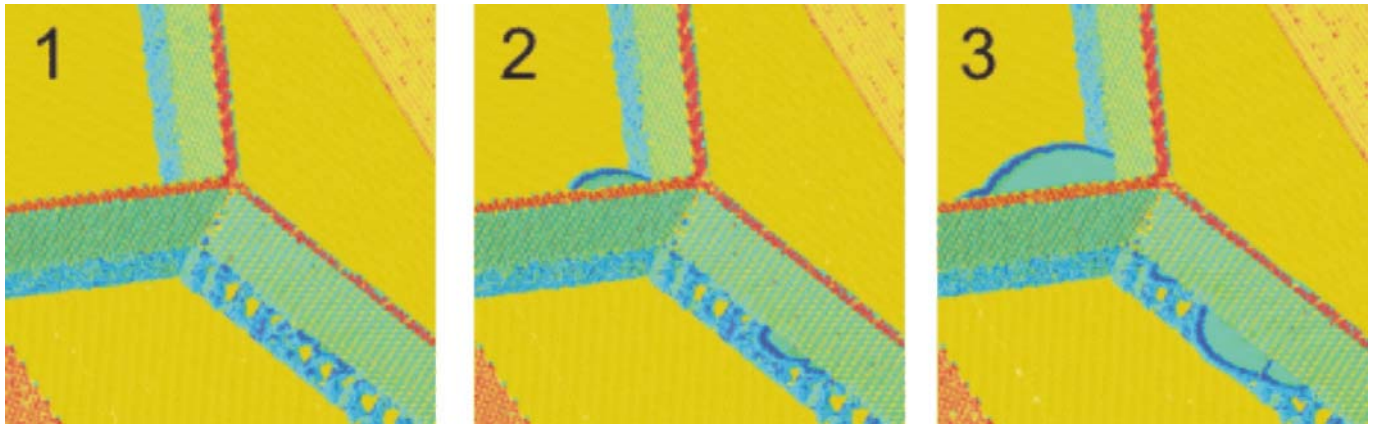
Atomistic details of dislocation nucleation



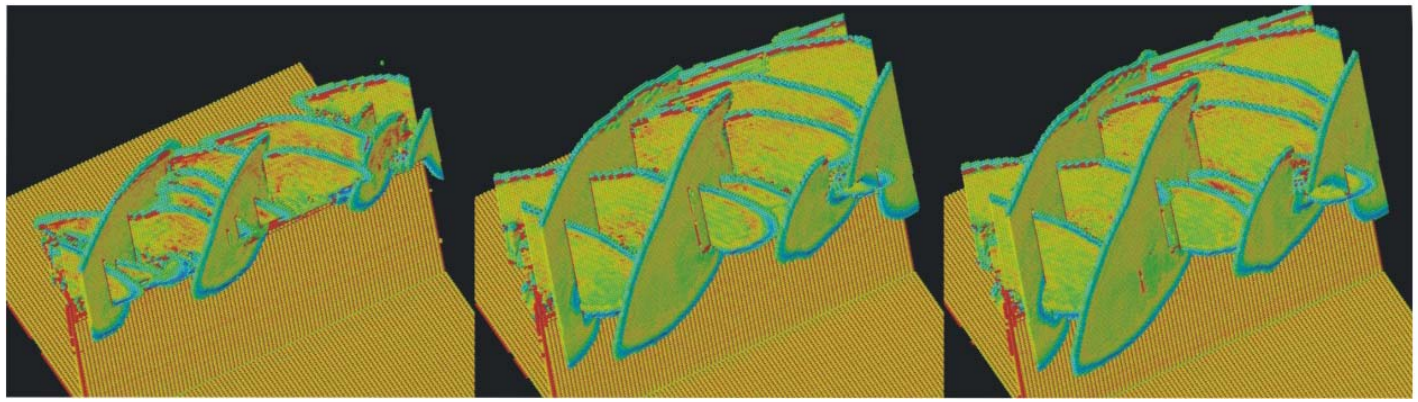
- Dislocation nucleation from a traction-free grain boundary in an ultra thin copper film
- Atomistic results depict mechanism of nucleation of partial dislocation



… more dislocations



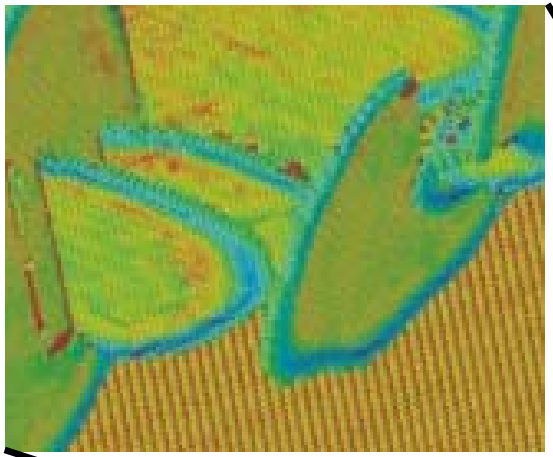
Dislocation nucleation at grain triple junction



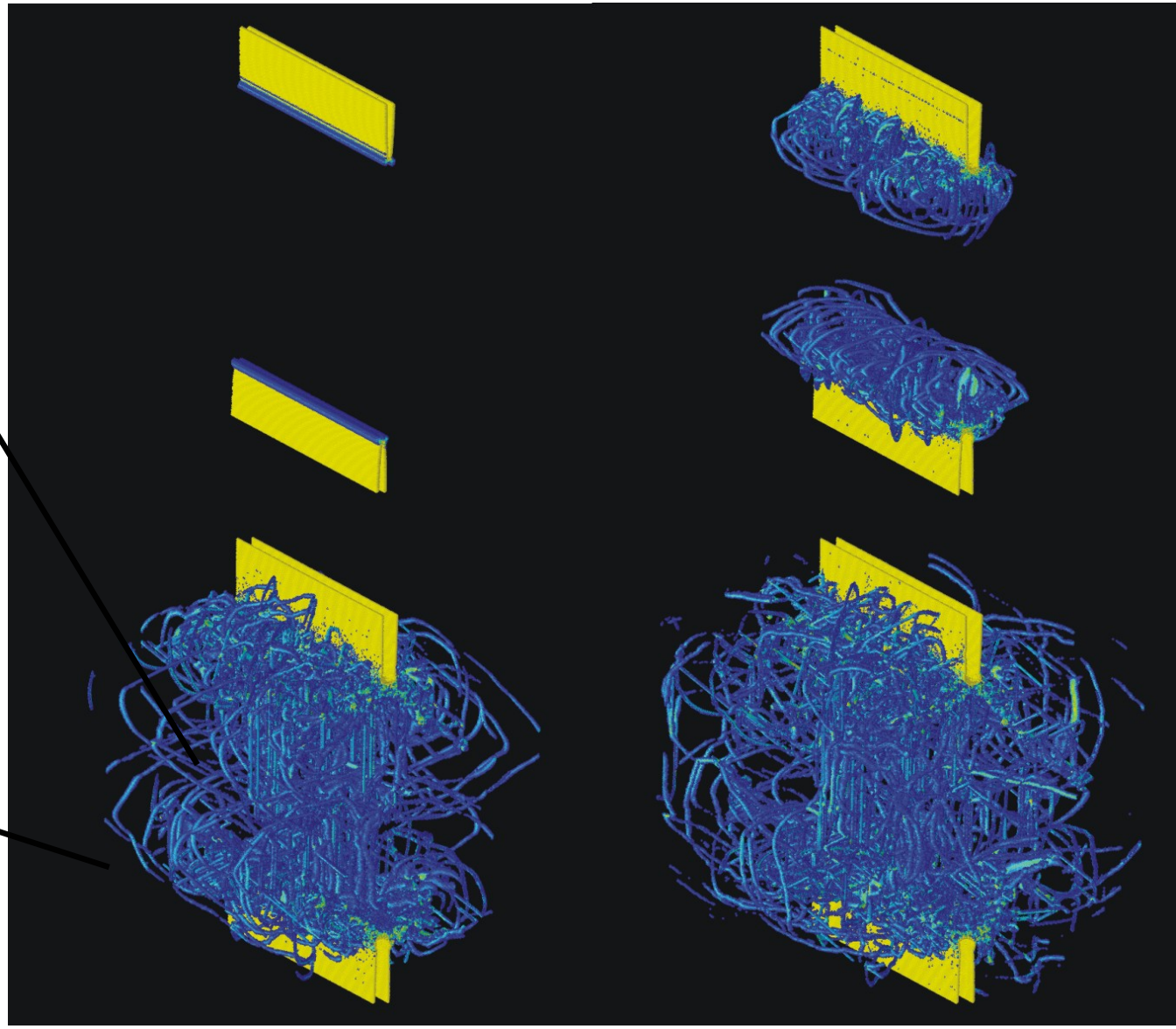
Single crack

(Buehler, 2004)

Cracking of a copper crystal: Thousands of dislocations



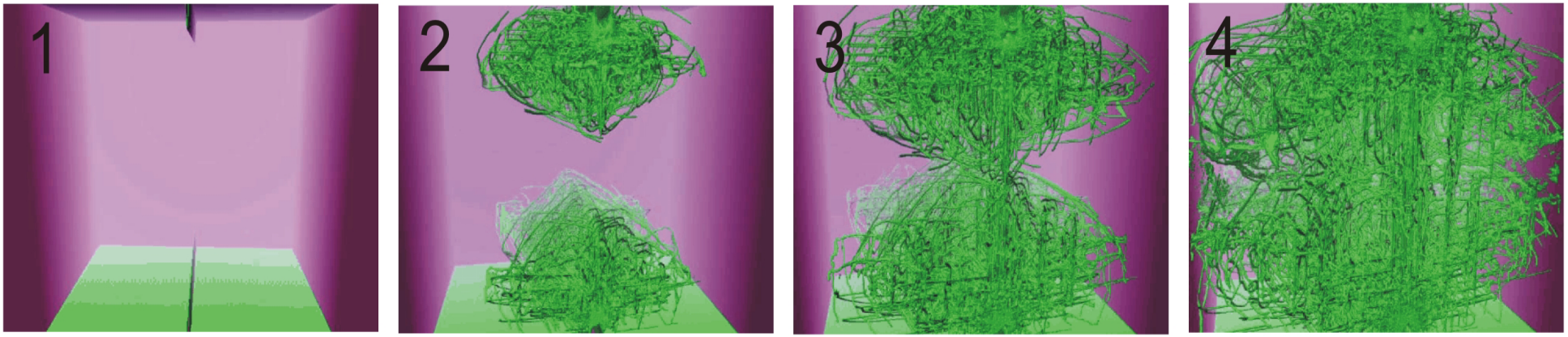
Critical:
Atomic interaction
(potential)



(Buehler, 2006)

Analysis of a one-billion atom simulation of work-hardening

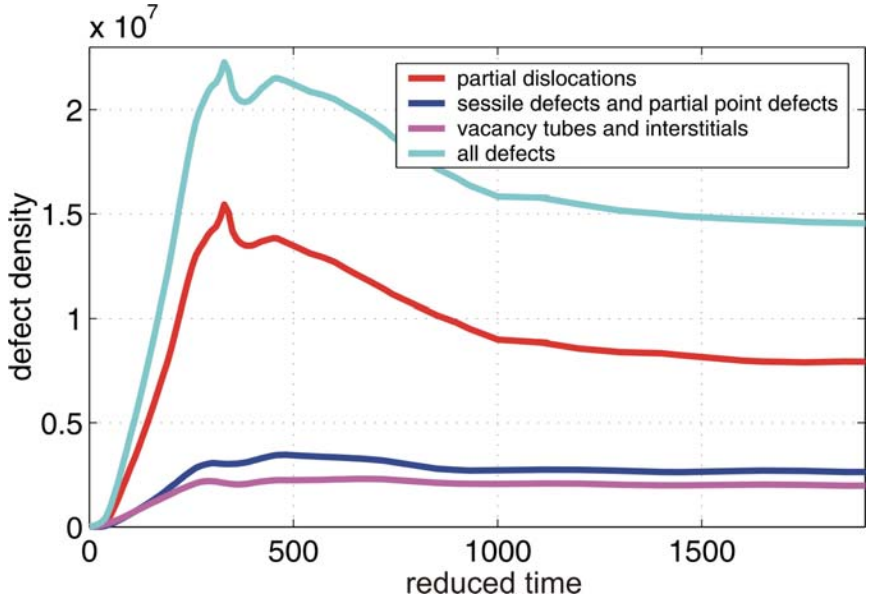
Overview over total simulation time



(Abraham et al., 2002)

Within a few nanoseconds, a rigid, sessile time-independent network develops…

- How can the particular structure be explained?
- What are the atomic mechanisms that lead to the regular structure?

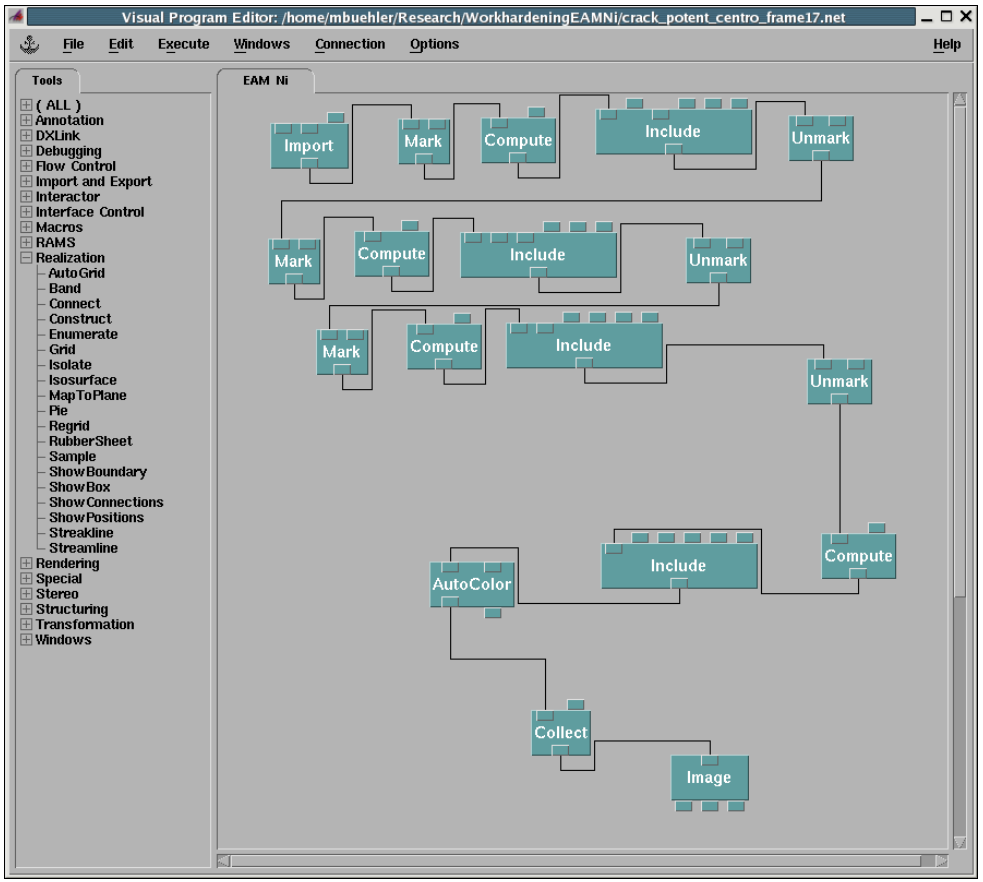


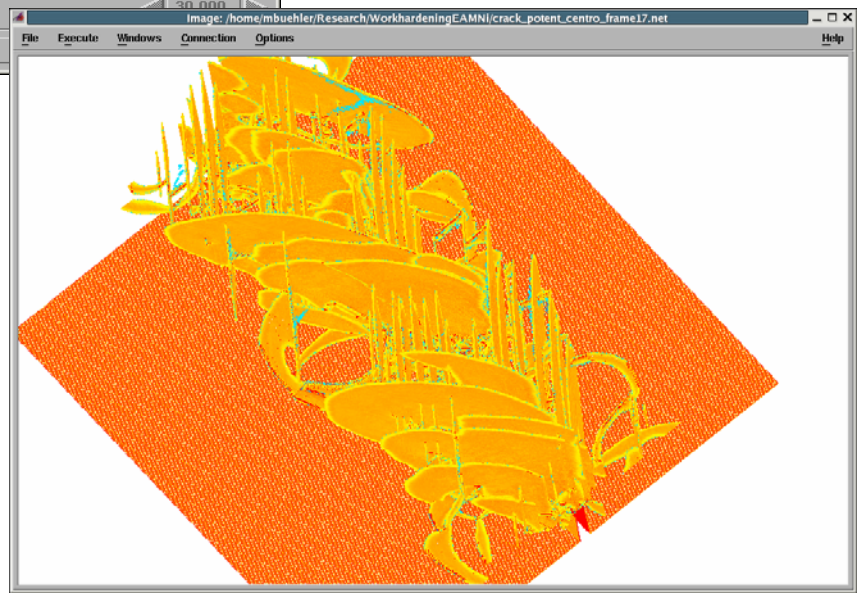
Defect densities

stage I stage II stage III

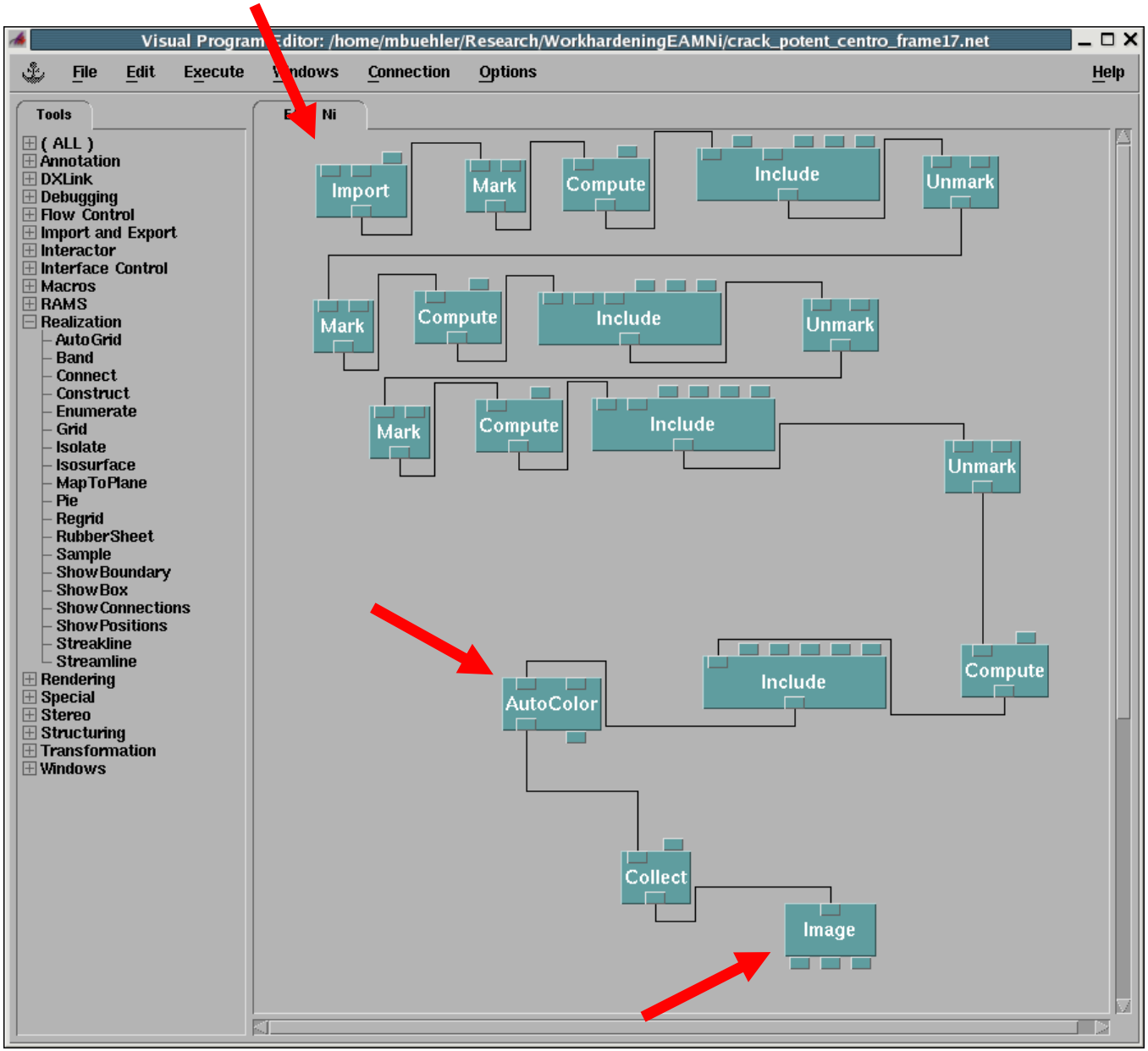
Visualization strategy

- Use IBM OpenDC data explorer to filter and process data
- Very flexible and generally applicable to any kind of data
- Handles several millions of particles
- Open source / freeware: www.opendx.org
- Other programs: AtomEye, Rasmol, VMD…





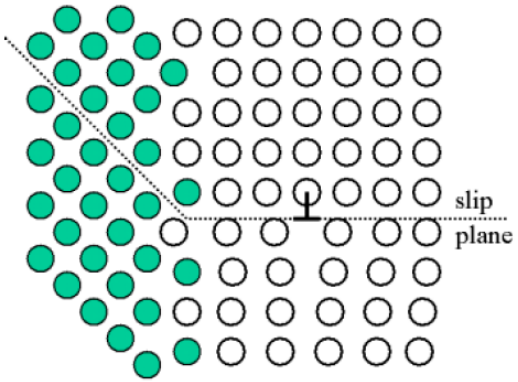
OpenDX – Data Explorer

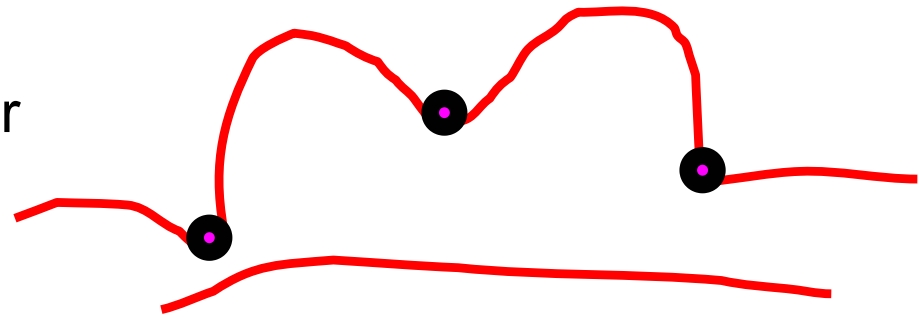


- Different tools for data loading, processing and visualization can be coupled together visually
- Enables efficient development of new visualization programs

Strengthening mechanisms

- Remember: Theoretical shear strength of materials is not reached due to the existence of dislocations
- By hindering the motion or the possibility to create dislocations, the material becomes stronger, approaching the theoretical strength
- Mechanisms:
  - Grain boundary strengthening
  - Grain size reduction (Lecture 4)
  - Introduction of foreign atoms that create strain field (solid-solution strengthening)
  - Introduction of particles that pin/hinder dislocation motion

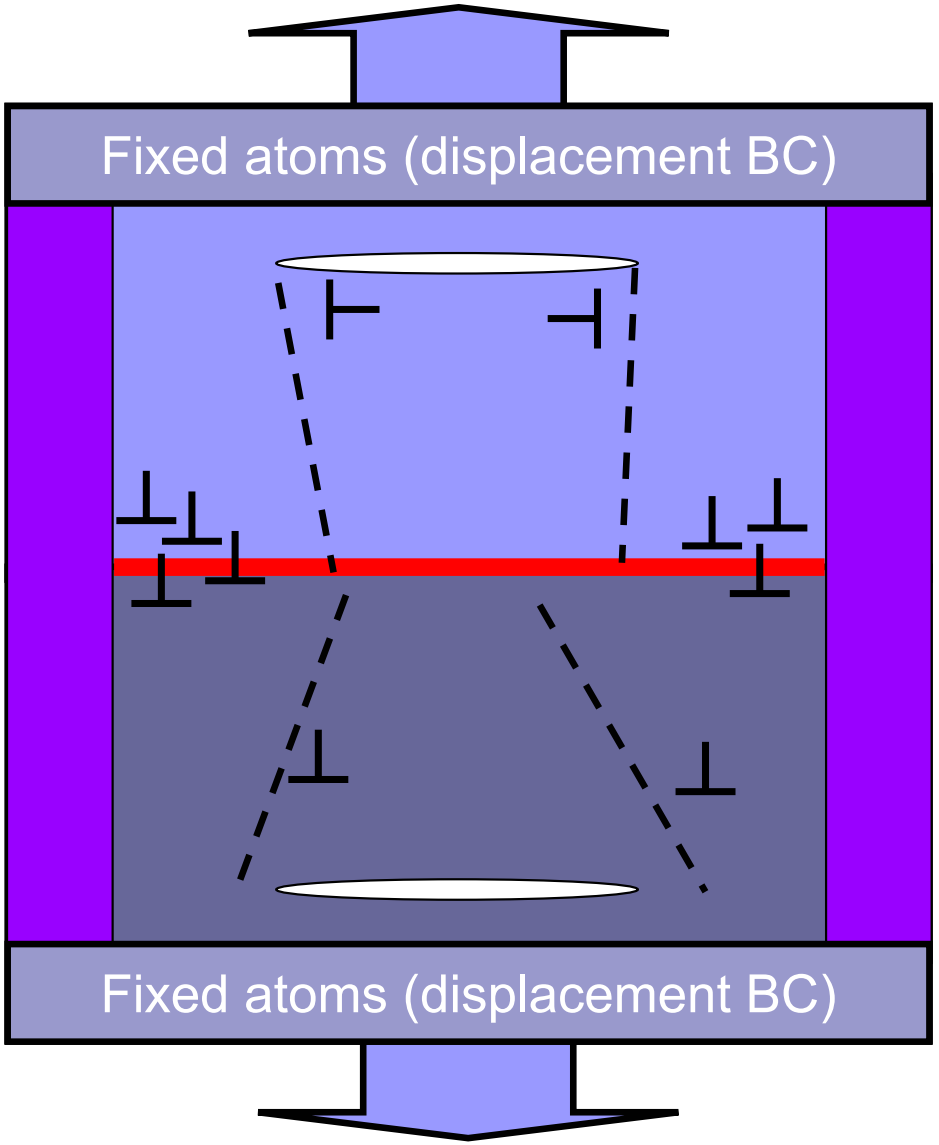




http://www.people.virginia.edu/~lz2n/mse209/Chapter7.pdf

Dislocation pileups at GBs

No displacement in *x*-direction ("substrate" or diffusion barrier)

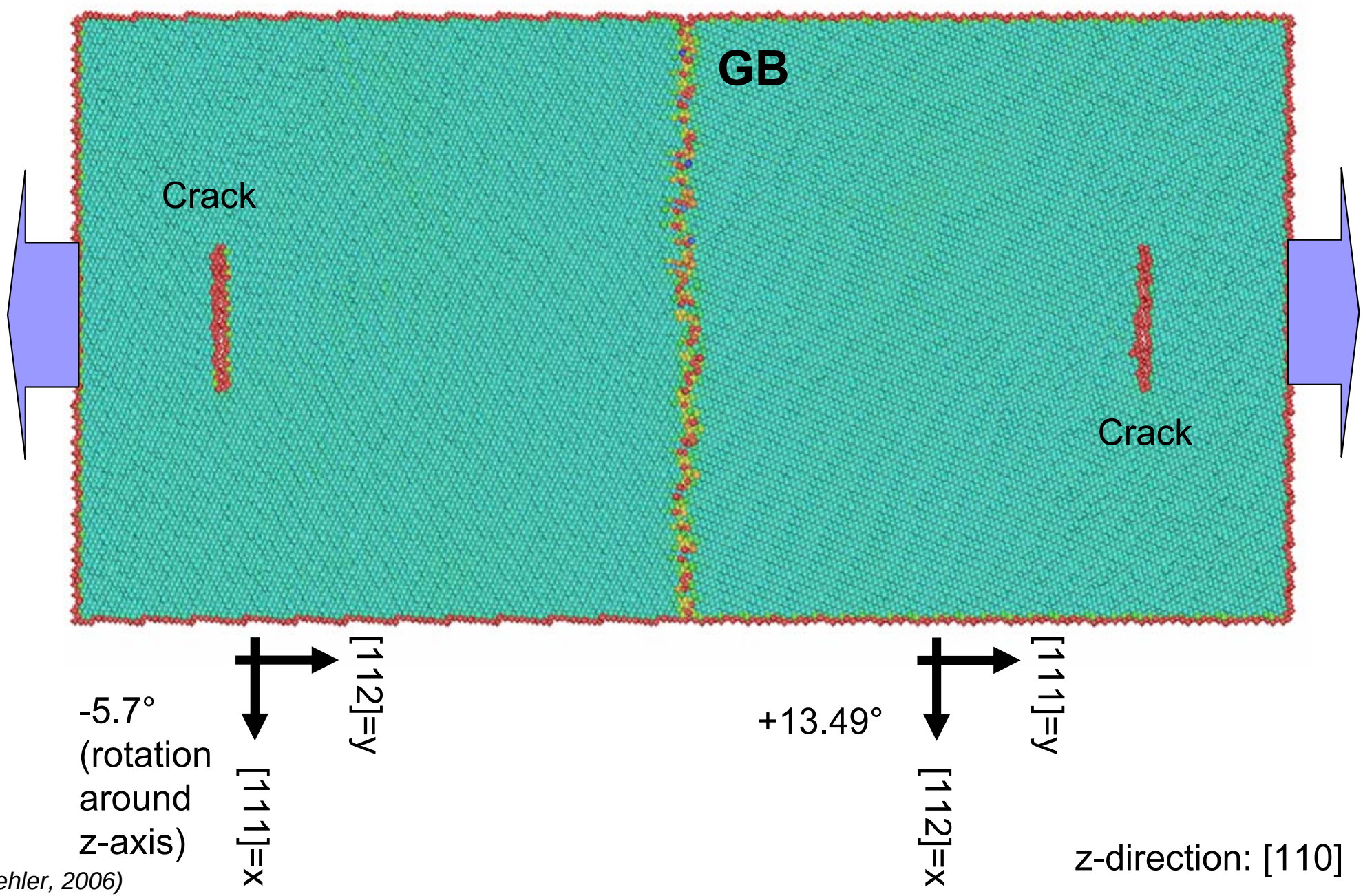


[110]=y

[110]=x

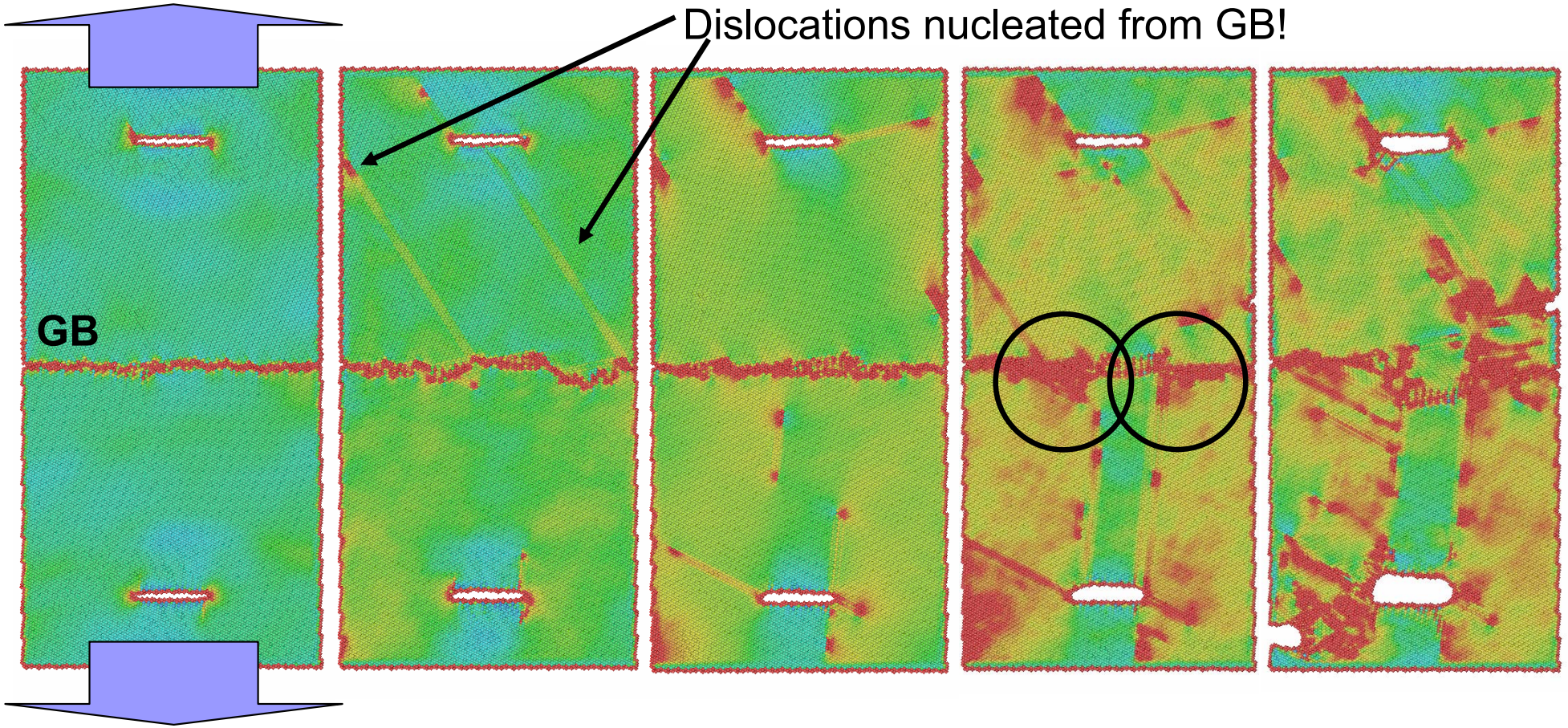
(Buehler, 2006)

Model geometry



(Buehler, 2006)

Dislocation structure as a function of increasing strain

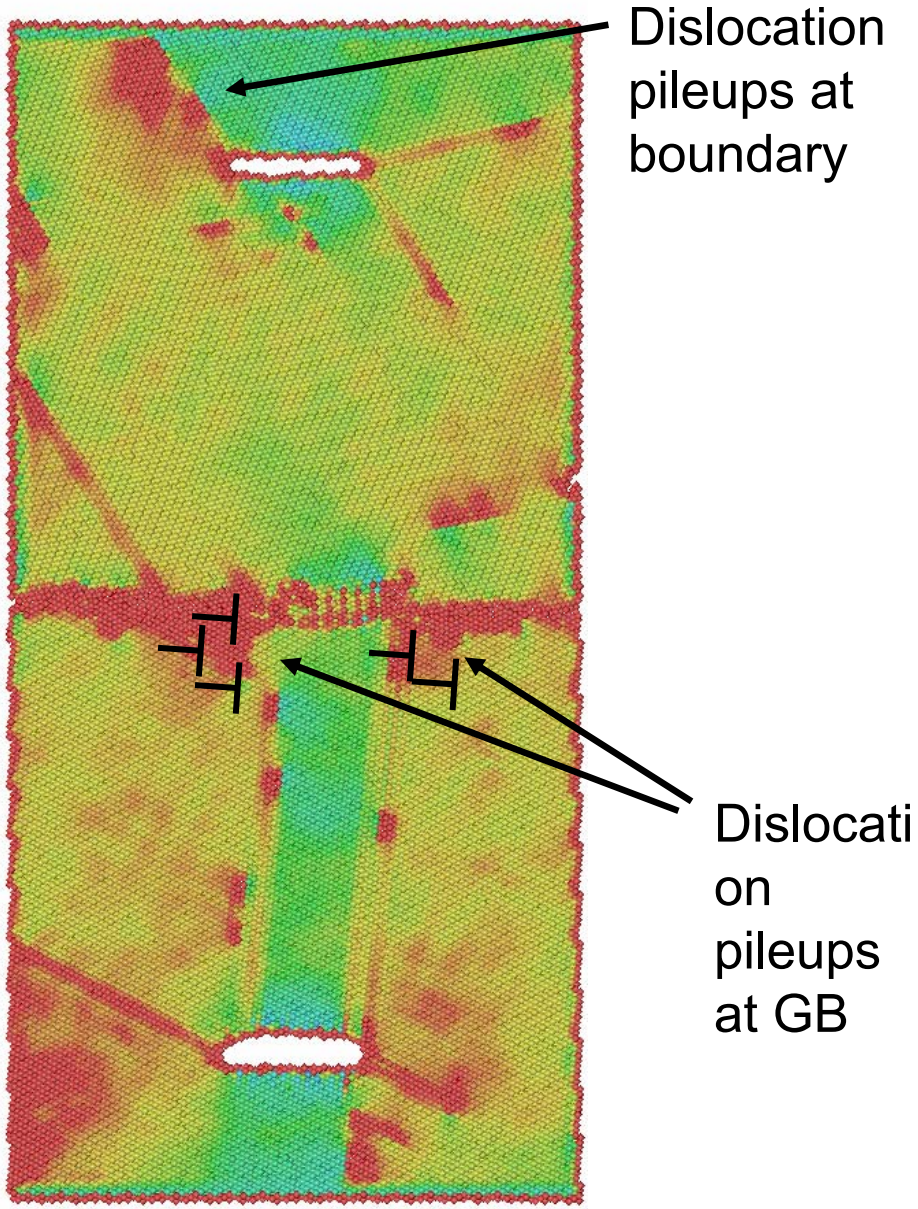


Color scheme: -3.55 eV = blue -3.50 eV = red

Shows stacking fault (as lines) and dislocation core (red), as well as surfaces (also red)

(Buehler, 2006)

Dislocation structure as a function of increasing strain



Zoom into frame #75

Observations

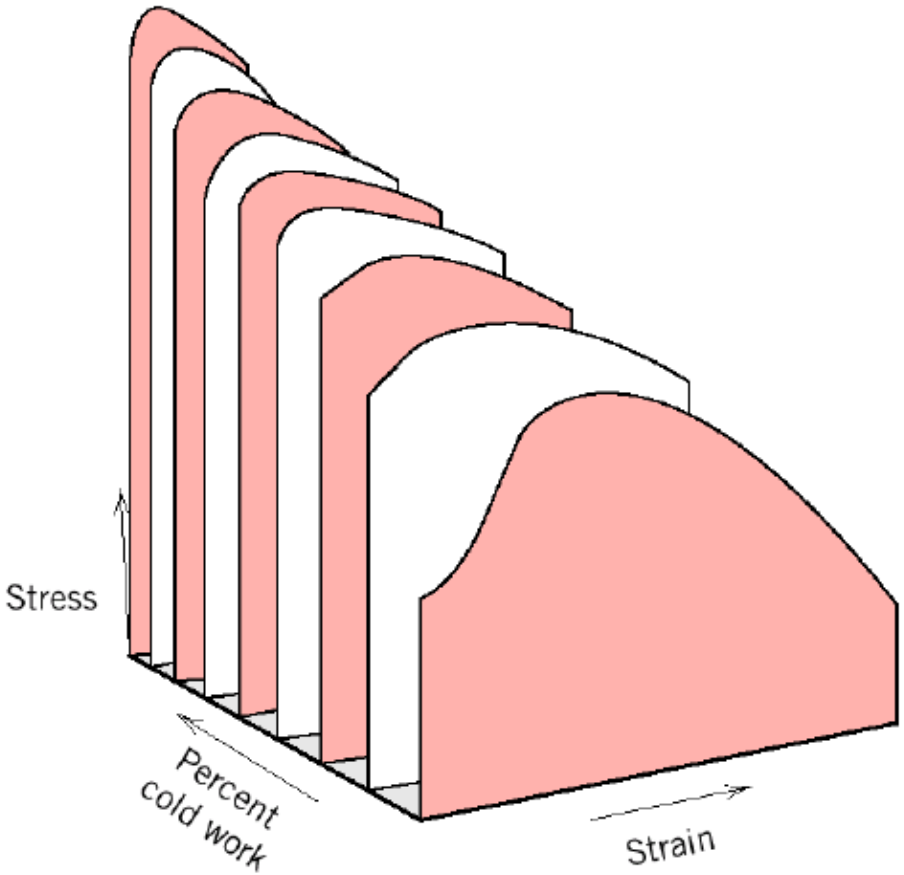
- Dislocations are nucleated from small cracks in the crystal
- As the loading is increased, more dislocations are nucleated, leading to a pileup at the GB
- Also see dislocation nucleation from GB (early, frame #25)
- At large load: Opening of small cracks close at the diffusion barrier surface (frame #100)
- Under high temperature, diffusive processes may relax the dislocation pileups by dislocation climb

(Buehler, 2006)

Strengthening mechanisms and work-hardening

- Work-hardening refers to the phenomenon that occurs in many metals, making them brittle and increasingly hard to deform
- It is often divided into different stages, such as
  - Stage I: Accumulation of defects due to deformation of material
  - Stage II: Beginning interaction of defects
  - Stage III: Approaching steady-state

- **Mechanisms:**
  - Higher dislocation density makes it “harder” for new dislocations to propagate
  - Dislocation-interactions, such as cutting mechanisms or formation of sessile locks hinder motion of dislocations



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

The three hardening mechanisms..

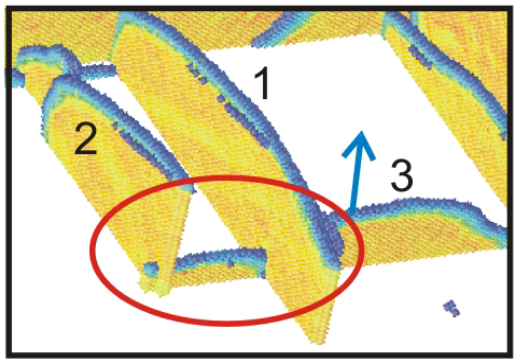
In our MD simulation of copper, we observe three hardening mechanisms:

- Cutting processes of dislocations (point defects, partial point defects,..) – when dislocations cut through each other
- Cross-slip of partial dislocations, to activate secondary slip systems, where no resolved shear stress is present
- Formation of locks (dislocation constructs that can NOT move), provide obstacles for other dislocations

… All contribute to hardening of the material since it becomes more and more difficult for dislocations to glide!!

Then: Tendency towards brittle fracture

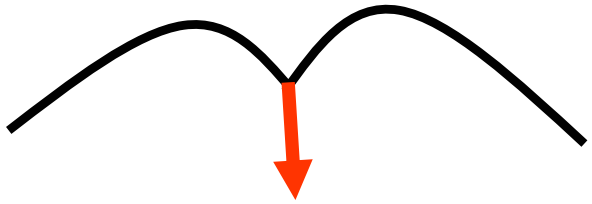
Hardening mechanisms creation of sessile structure

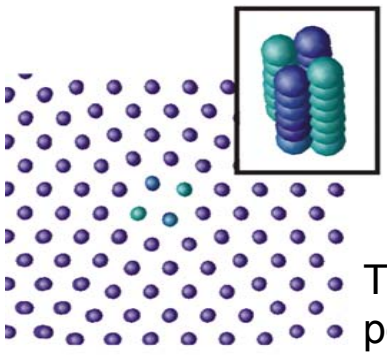


1. Dislocation cutting processes: Intersection of dislocations leads to generation of trails of point defects (trails of partial point defects, vacancy tubes and interstitials):

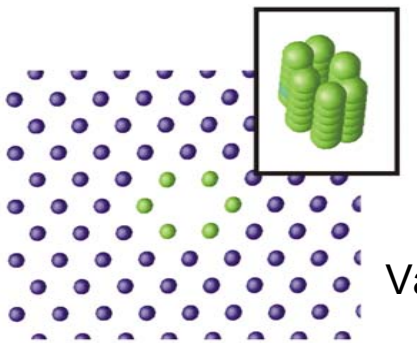
- Energy required to create point defects
- **Therefore**: Pinning of dislocations – dragging force:

Different kinds of point defects

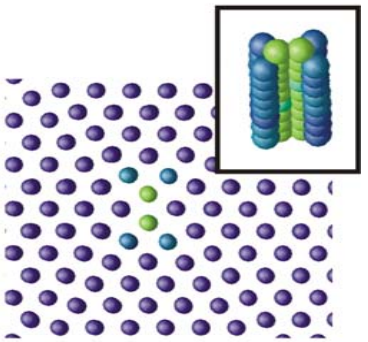




Trail of partial point defects



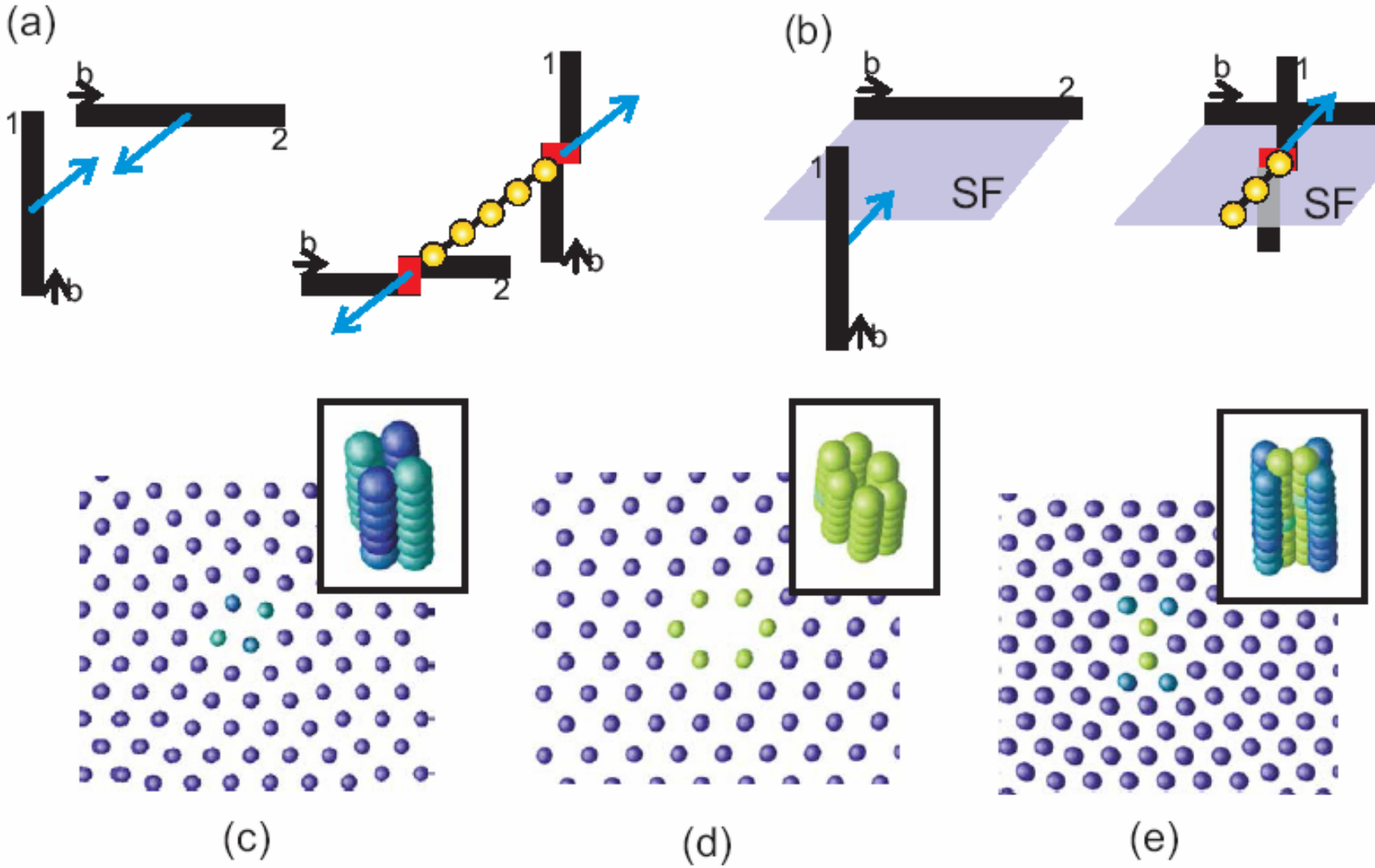
Vacancy tubes



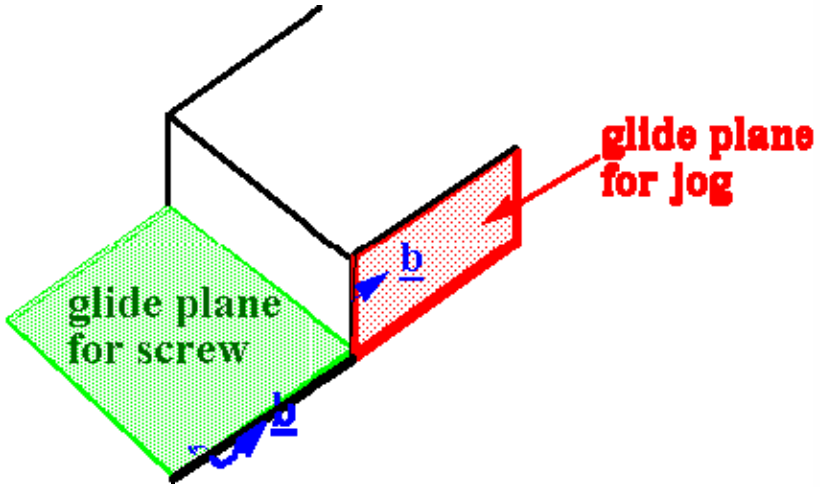
Trail of interstitials

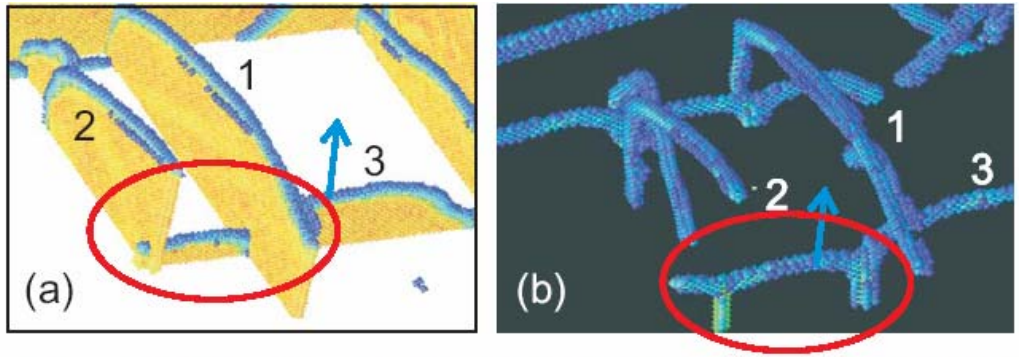
Reduced dragging force (20% of vacancy tube)

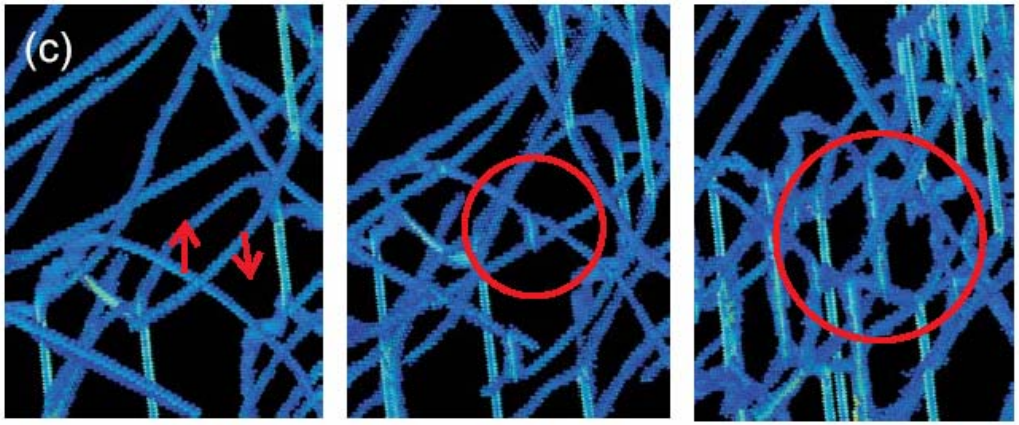
Hardening mechanisms
creation of sessile structure



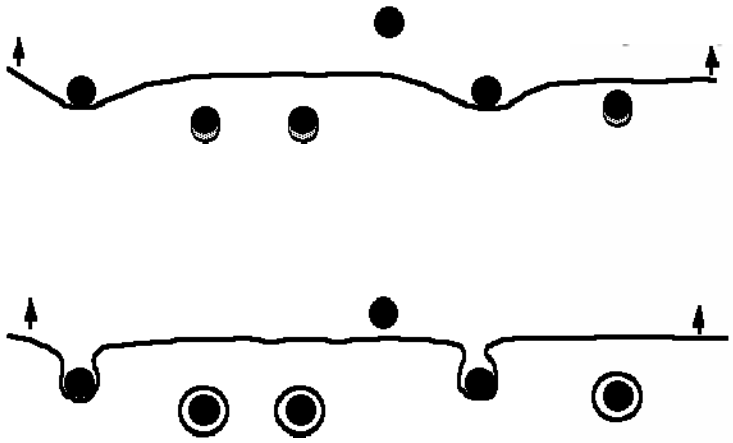
Hardening mechanisms
creation of sessile structure

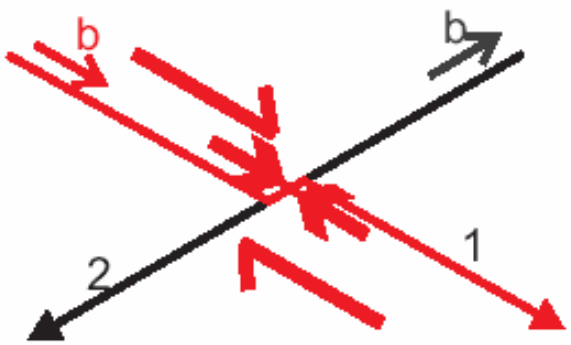




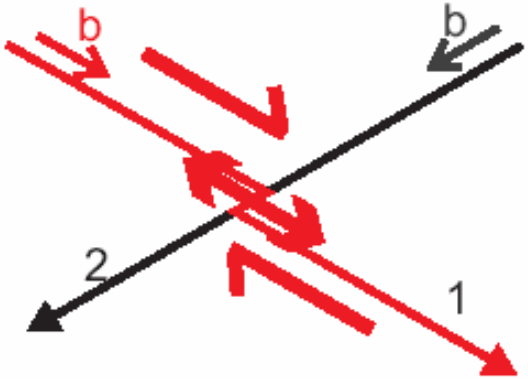


Sessile segment
Pinning



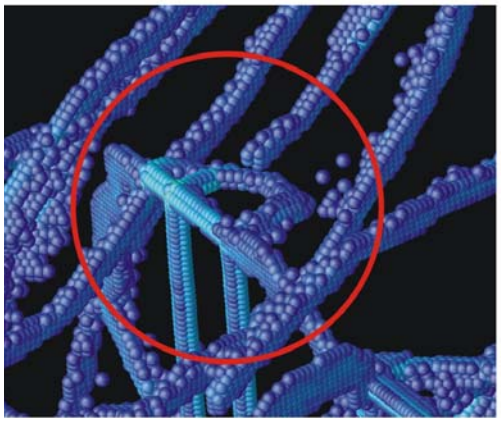


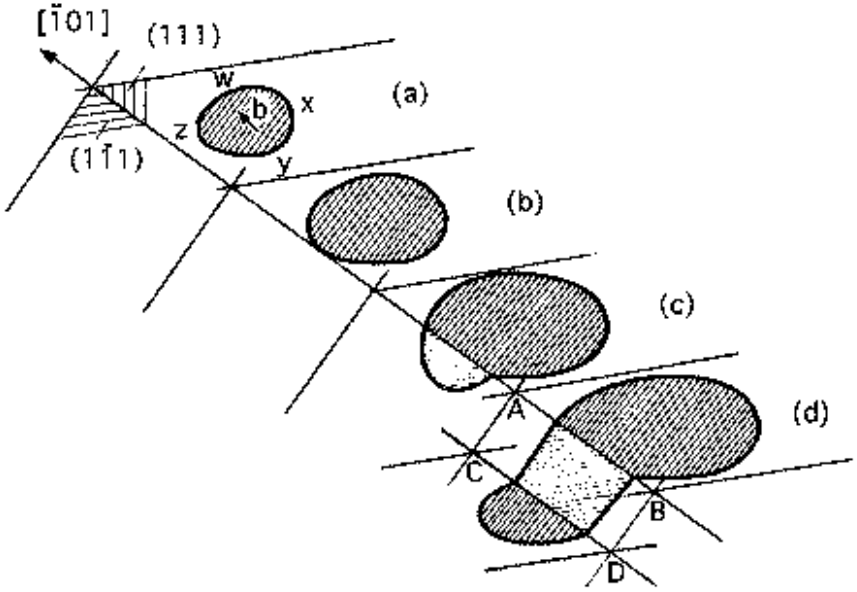
(a)



(b)

Hardening mechanisms creation of sessile structure





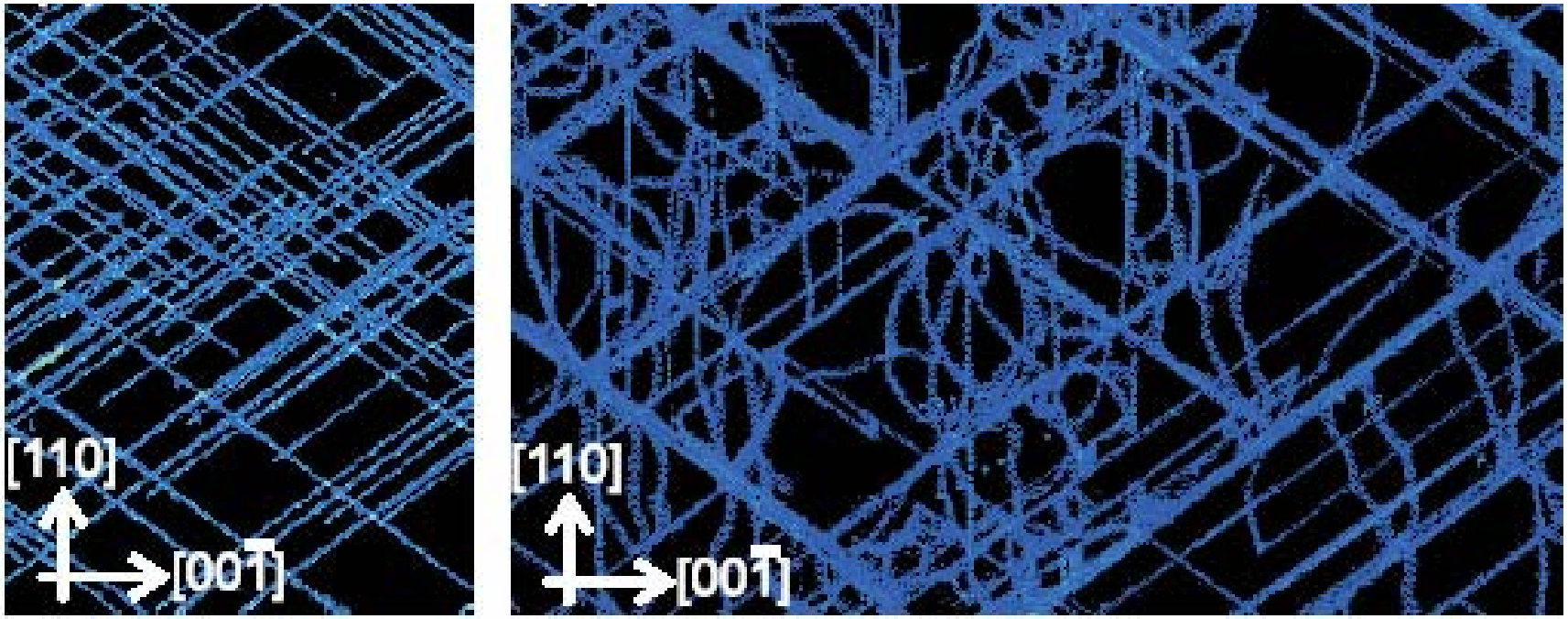
2. Cross-slip

Activation of secondary slip systems by cross-slip and Frank-Read mechanisms: At later stages of the simulation

• After activation of secondary slip systems: More dislocation reactions (e.g. cutting processes).

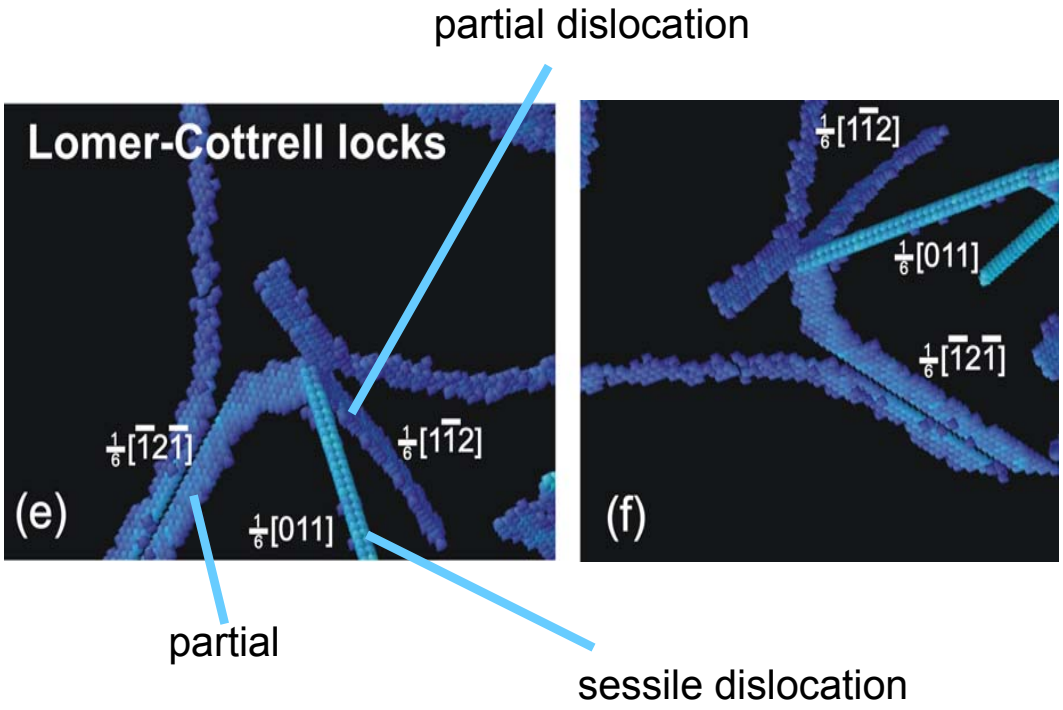
• **"Rediscovered" Fleischer's mechanism of cross-slip of partials that was proposed 1959**

Observation of cross-slip



- At a critical dislocation density, secondary slip systems are activated
- This enables for additional plasticity to occur, but also further contributes to work-hardening as the dislocation density increases making it more difficult for dislocations to move

Hardening mechanisms creation of sessile structure



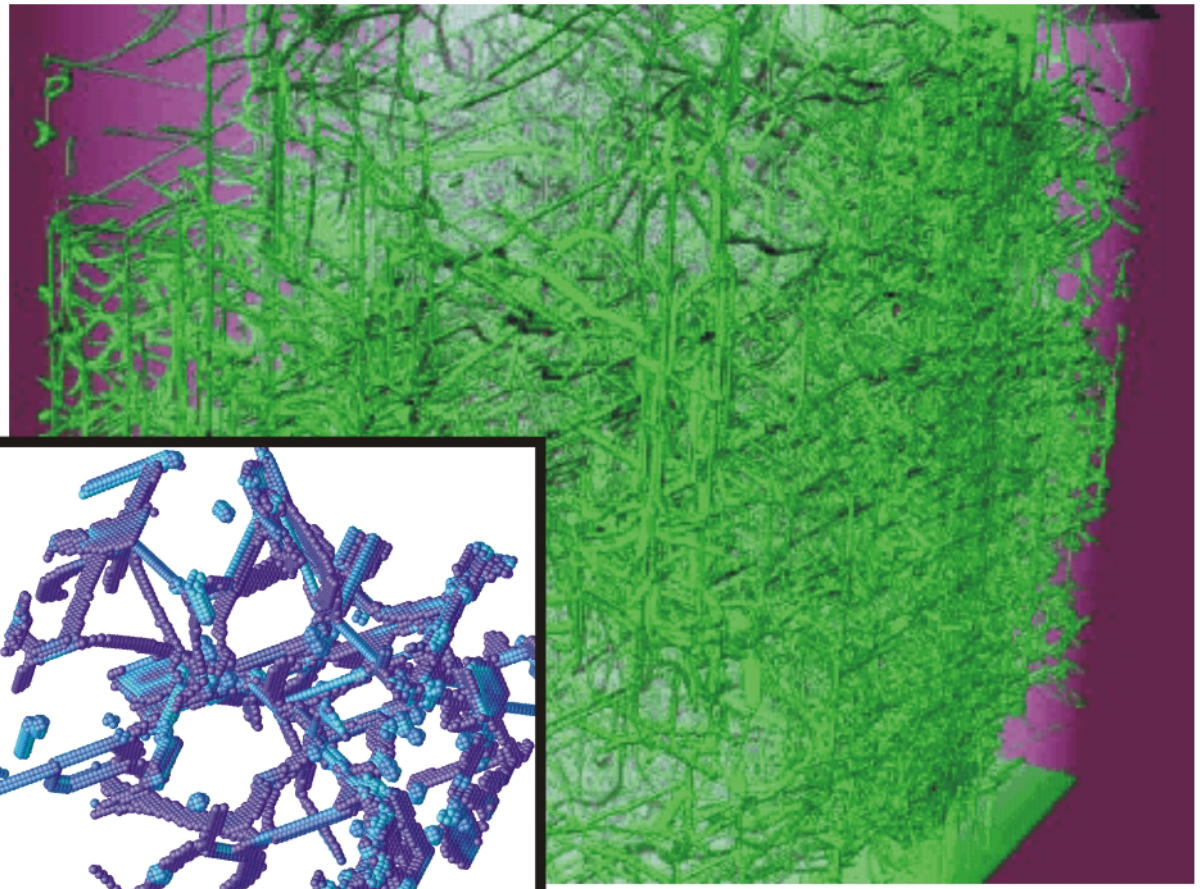
3. Formation of Lomer-Cottrell locks

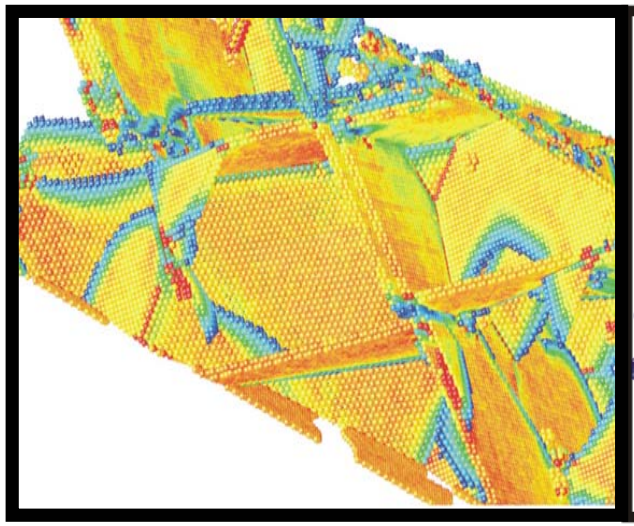
- Formation of sessile Lomer-Cottrell locks, with its typical shape of a straight sessile arm connected to two partial dislocations

- Sessile junctions provide a severe burden for further dislocation glide

Final sessile structure

Consists of…:
Vacancy tubes, interstitials, partial dislocations, and sessile dislocations



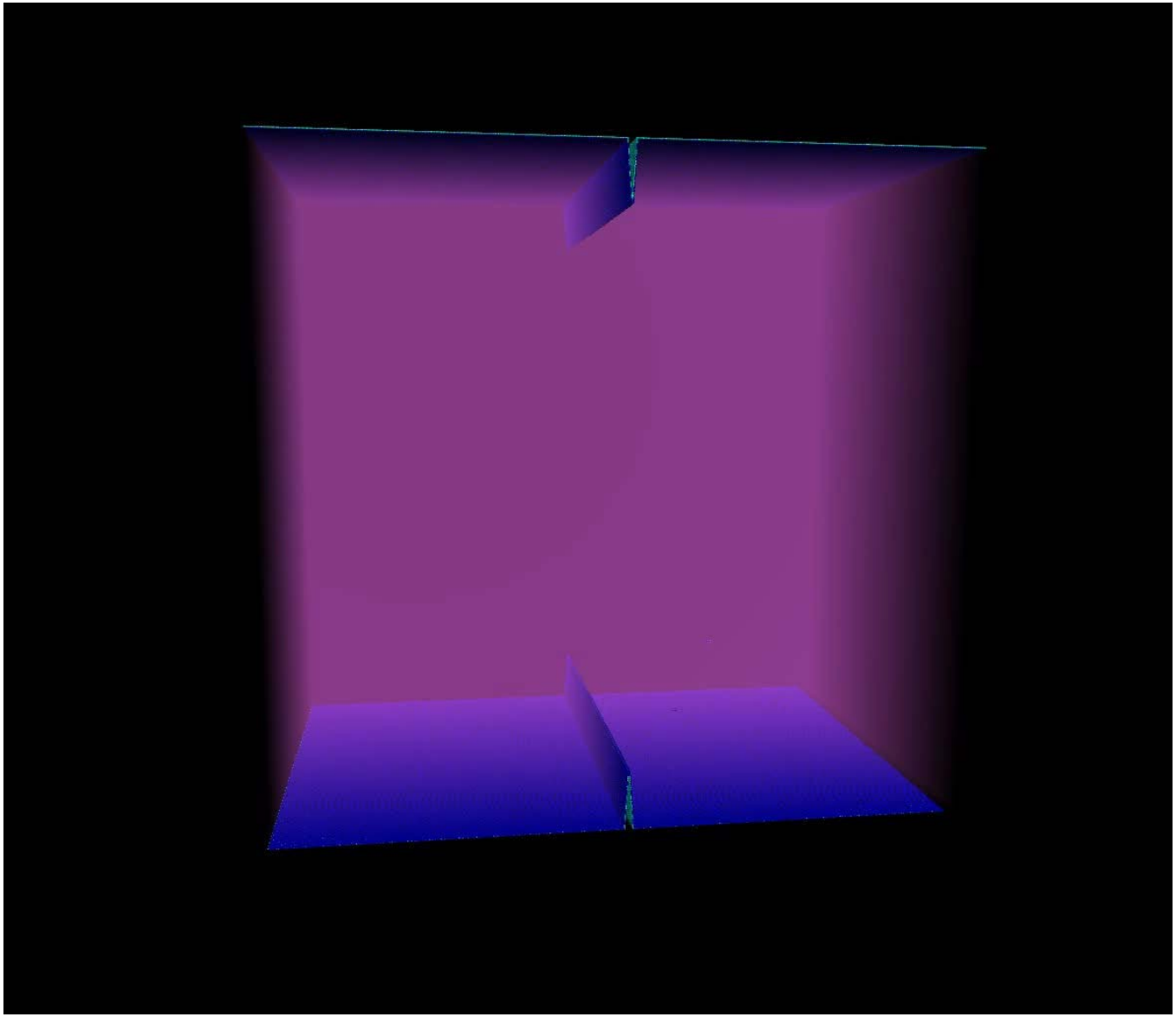


The characteristic structure of the network:

➢ All sessile defects (both trails of partial and complete point defects) as well as sessile dislocations are straight lines that lie on the edges of Thompson's tetrahedron (at intersections of stacking fault planes)

Animation of the work-hardening process

- Movie summarizes creation of dislocations, interaction and reaction leading to formation of the sessile dislocation network



Summary

- Observe classical mechanisms of work hardening in single computer simulation: (1) dislocation cutting processes, (2) cross-slip, (3) formation of sessile dislocation locks.

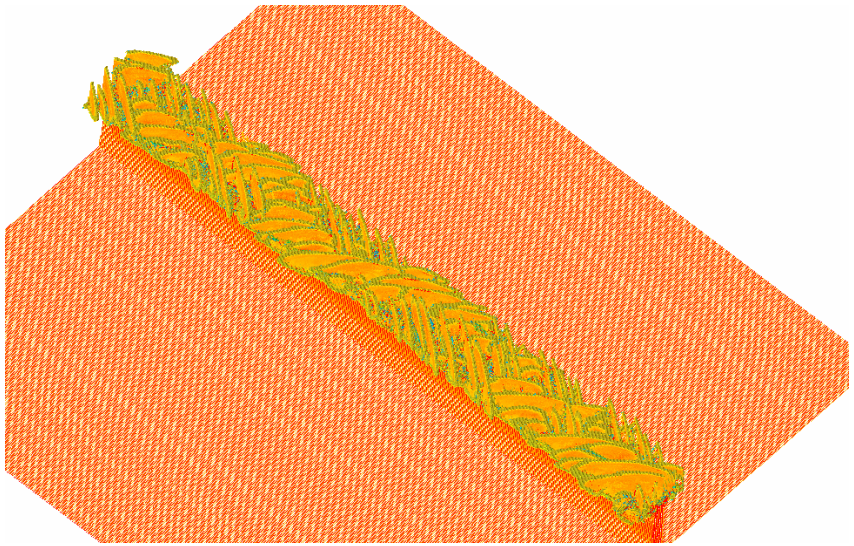
- The collective operation of these mechanisms constricts mobility of dislocations: A large ensemble of defects self-organizes into a complex defect network with a regular structure composed of trails of point defects, sessile dislocations, and partial dislocations.

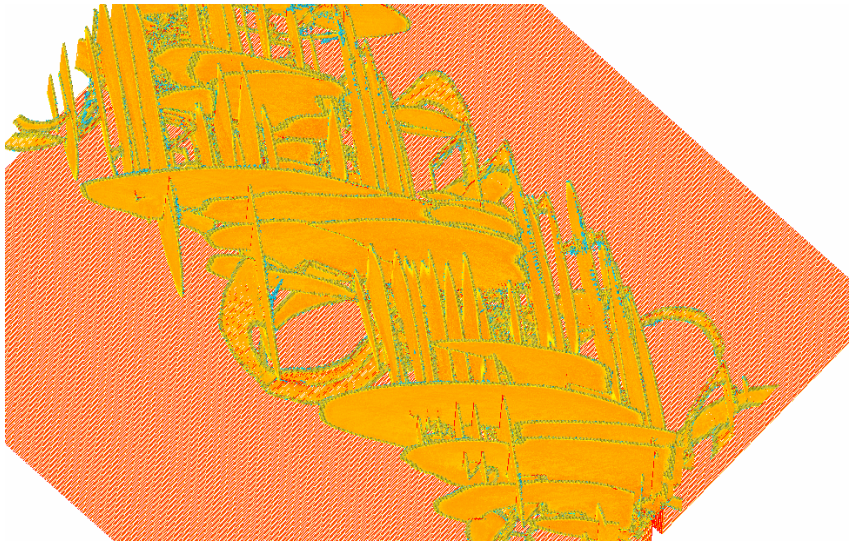
- The characteristic structure of the final network is given by the geometrical condition that the sessile defects are straight lines that lie at the intersection of stacking faults, thus along the sides of Thompson's tetrahedron.

- Even though the LJ potential is a simplistic model for interatomic bonding, it is nevertheless capable of capturing most of the predicted hardening mechanisms: A computer simulation using the LJ potential under extreme conditions reproduces the essential deformation mechanisms of natural crystalline materials such as metals!!

- These results: Not accessible to any other method (experiment or theory)!!

Work-hardening in nickel

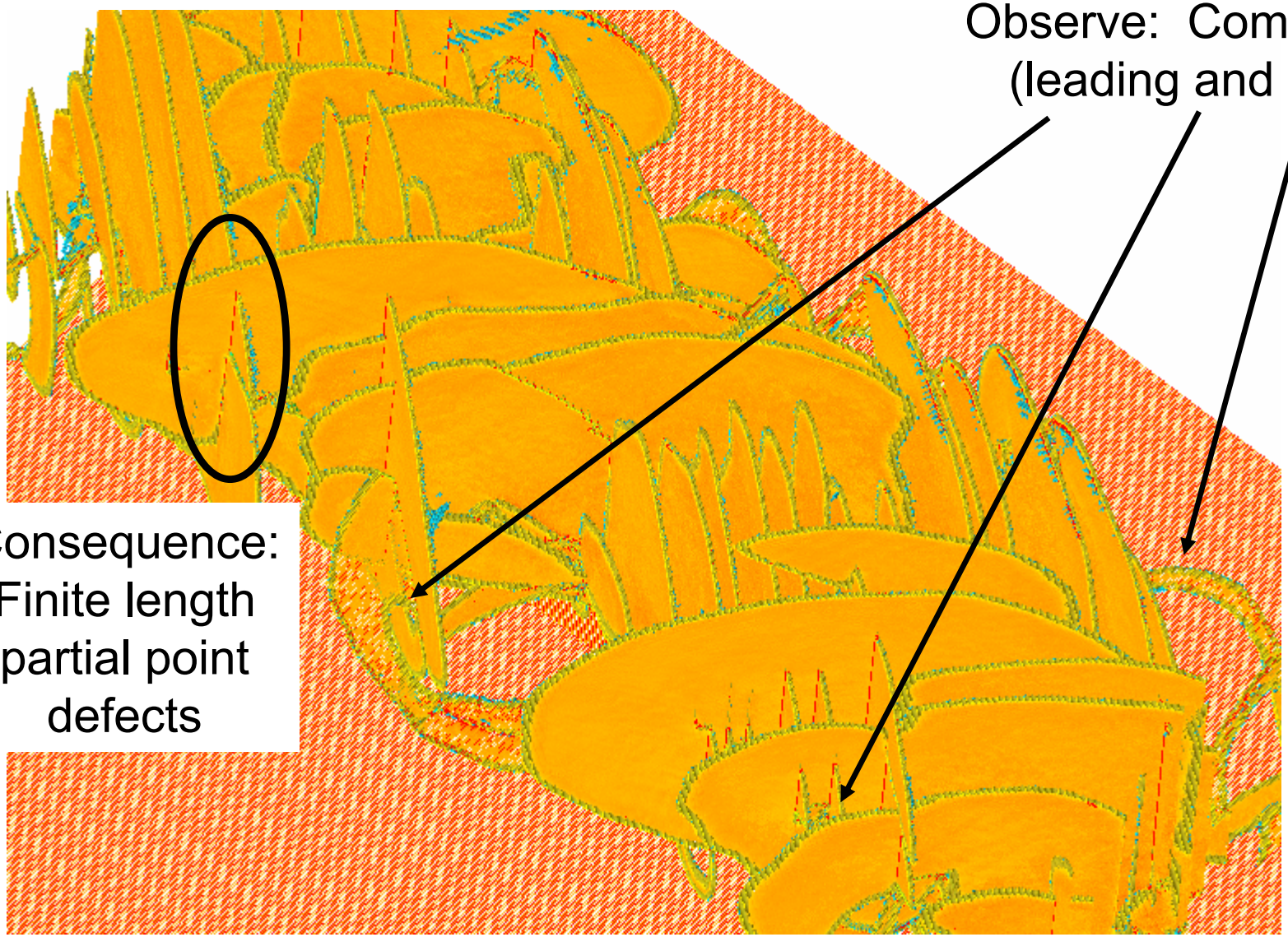




- Same geometry as for LJ copper
- Choose Ni due to higher stacking fault energy and thus, we expect to see complete dislocations rather than only partials

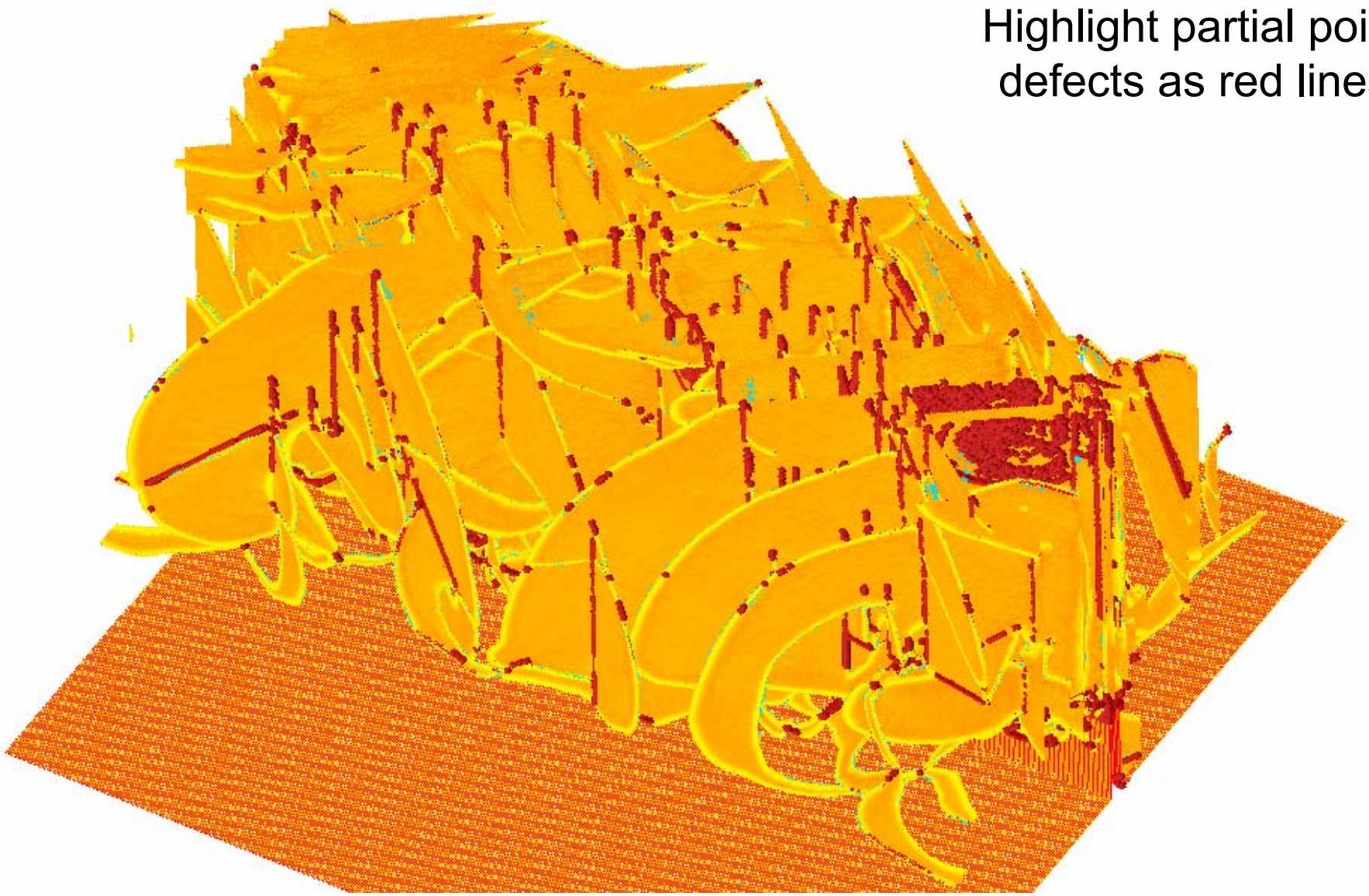
(Buehler, 2006)

Work-hardening in nickel



(Buehler, 2006)

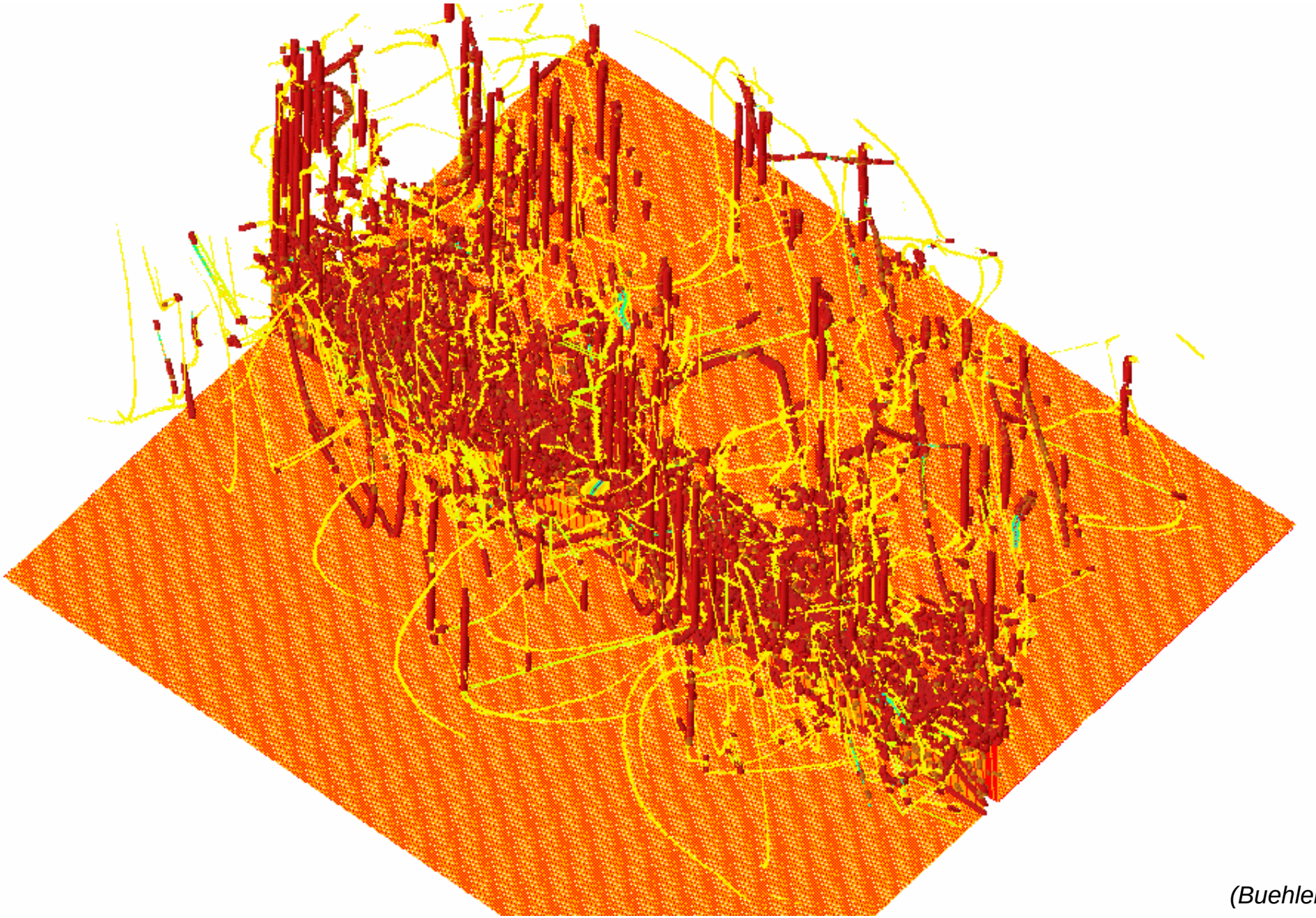
Work-hardening in nickel



Highlight partial point defects as red lines

(Buehler, 2006)

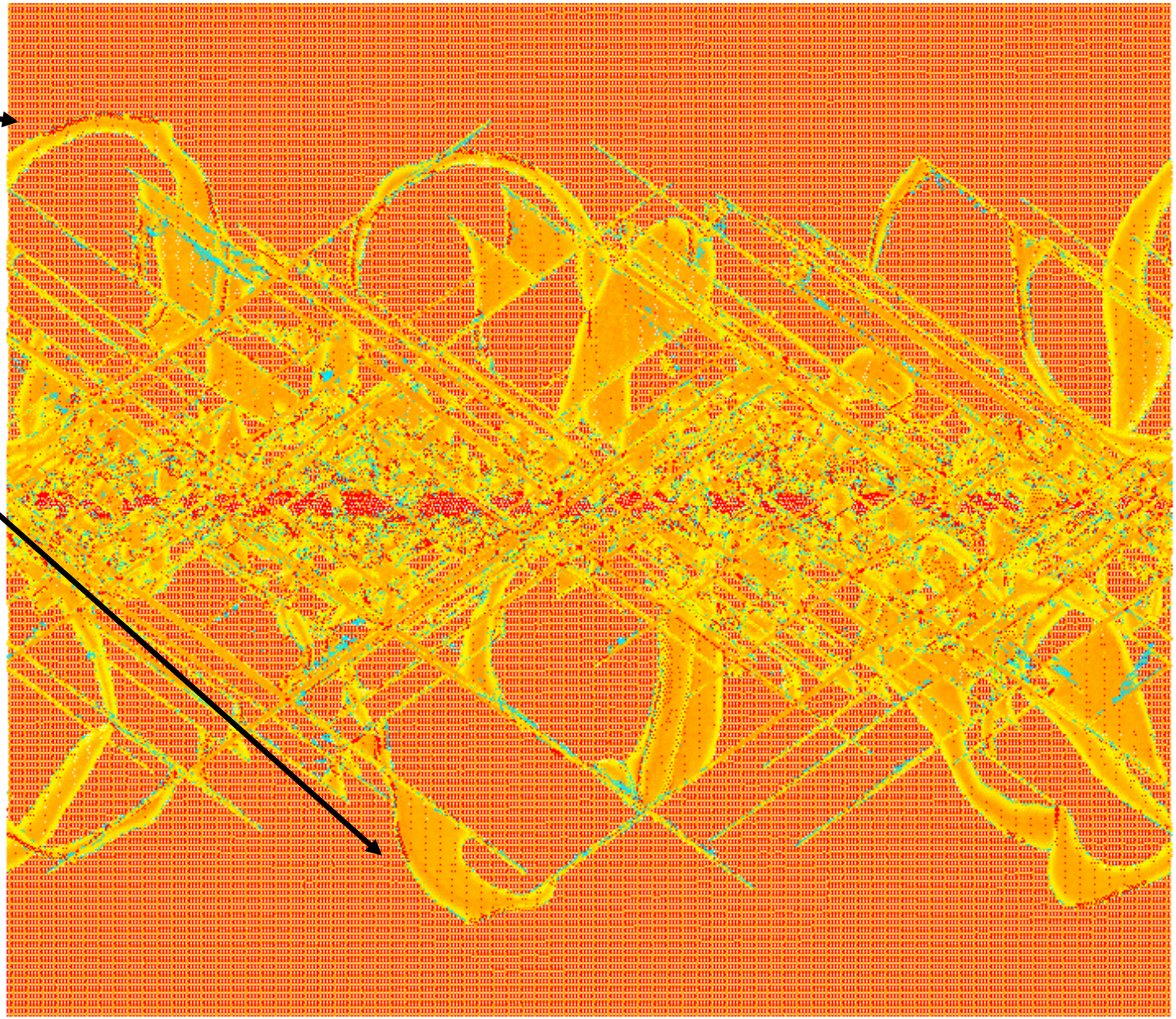
Work-hardening in nickel



(Buehler, 2006)

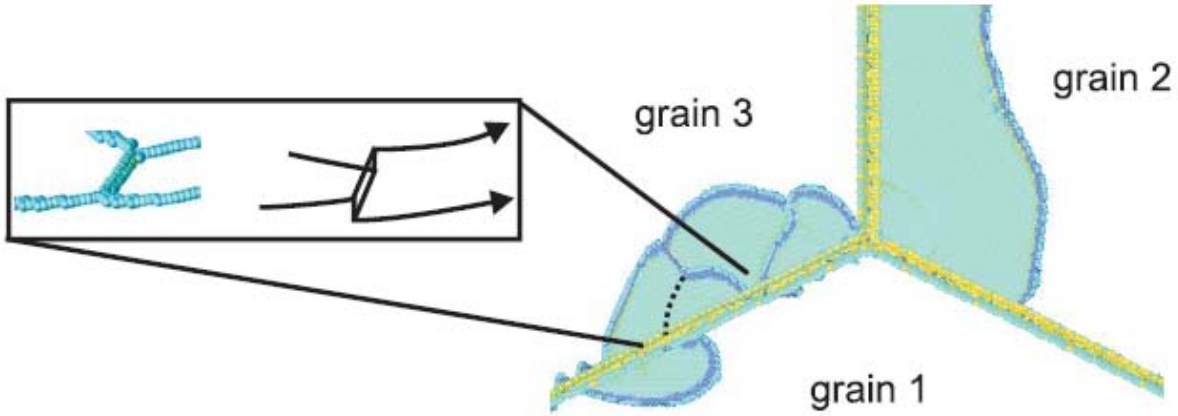
Work-hardening in nickel

Activation of secondary slip systems

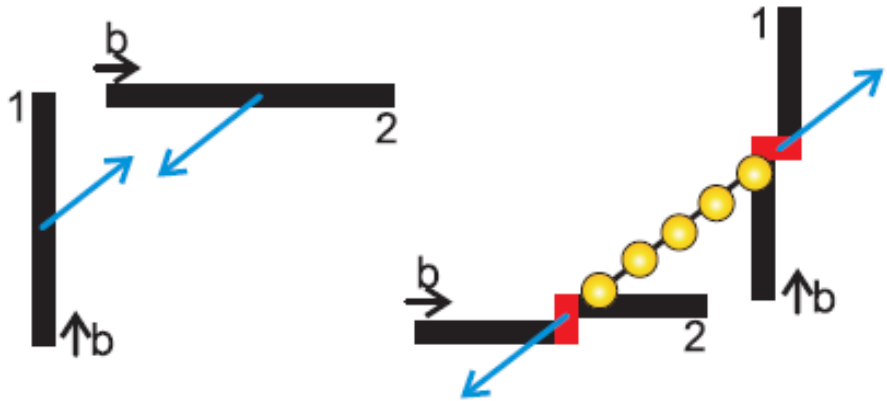


(Buehler, 2006)

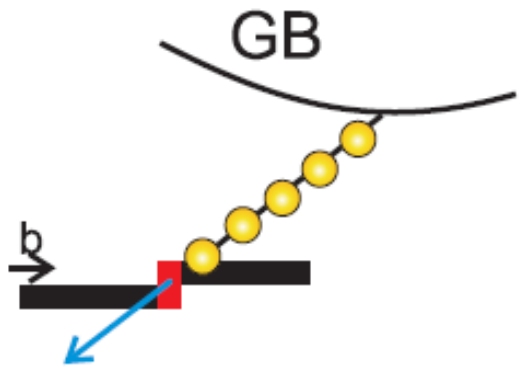
Formation of jogs: Dislocation reactions



- 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)

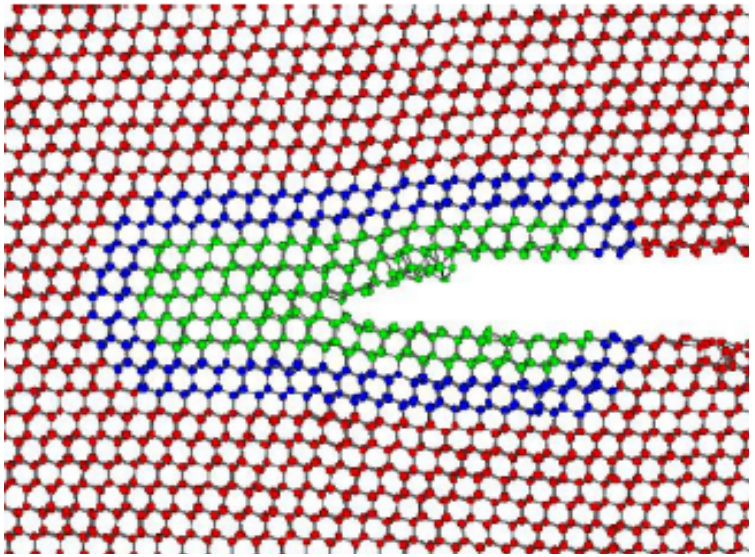


(b)

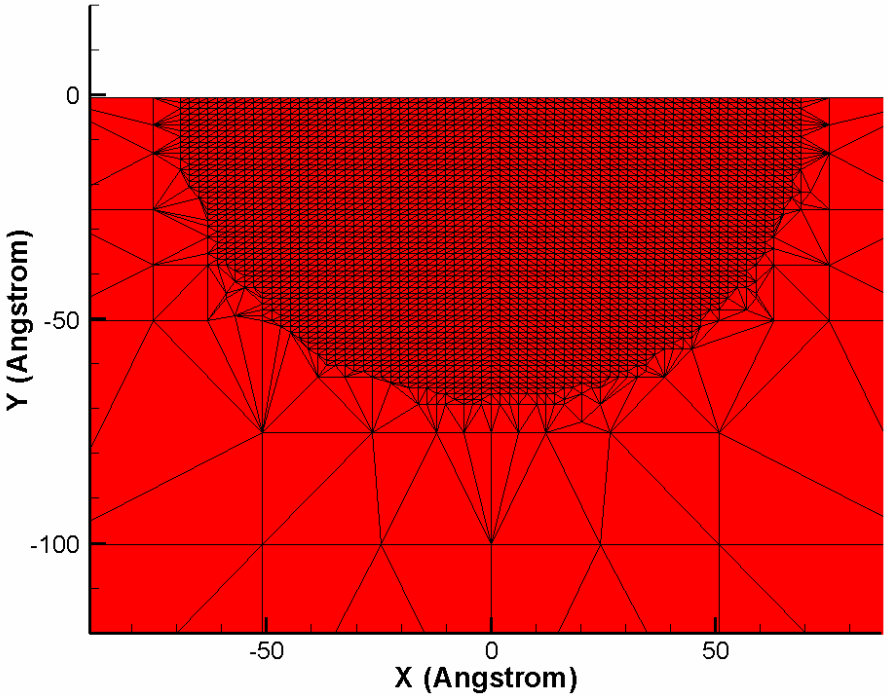
(Buehler, 2004)

Hierarchical versus concurrent multiscale modeling

- Hierarchical multiscale modeling: Pass parameters (paradigm of overlap, FF training,…)
- Concurrent multiscale modeling: Have multiple methods with different resolution in the same domain



Bernstein, Hess, PRL

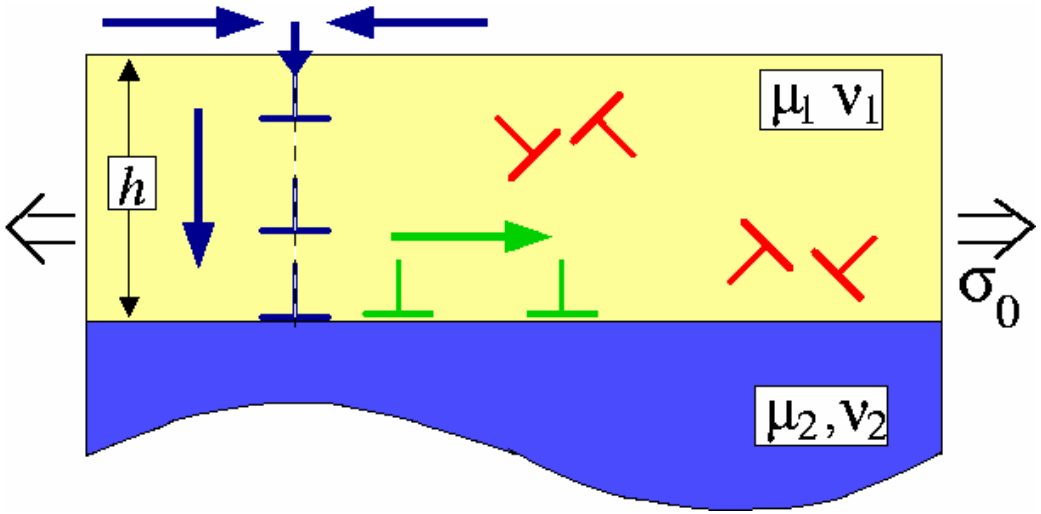


- Quasi-continuum (QC) method dynamically switches from atomistic to continuum method (now extended to finite temperature)

(Ortiz, Phillips et al.)

Mesoscopic model

Dislocations: Sources and sinks of plastic strain

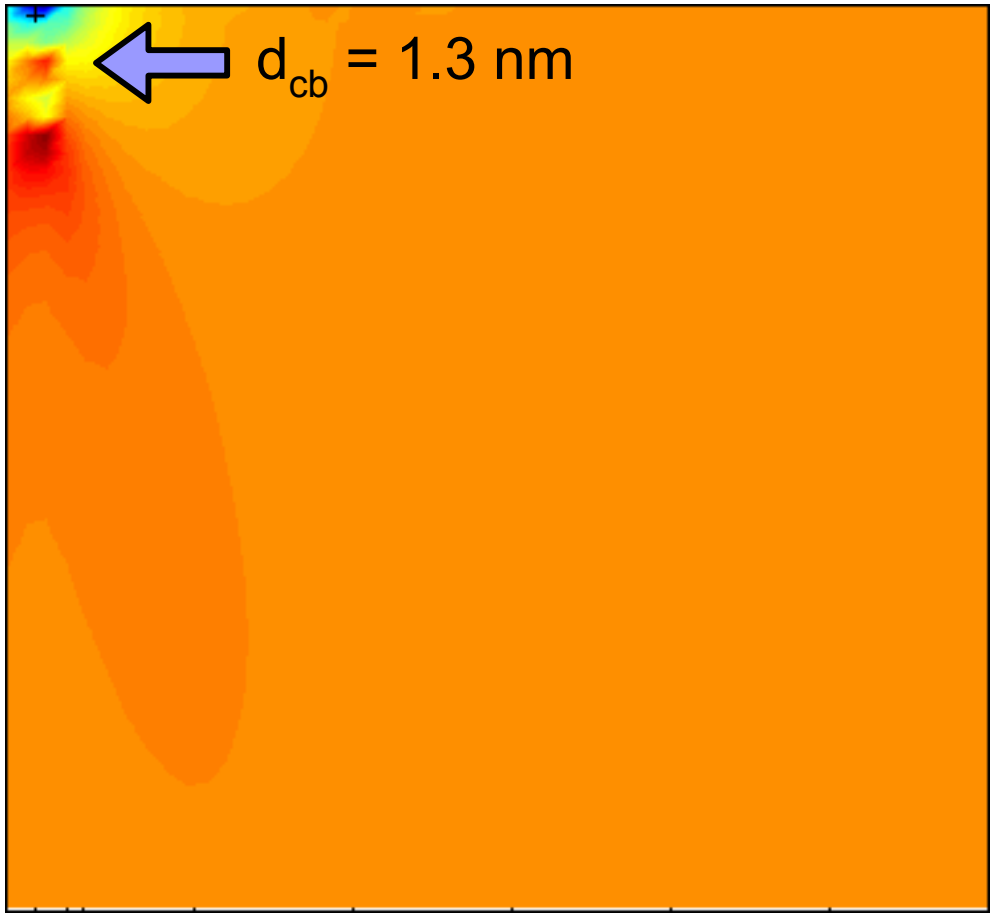


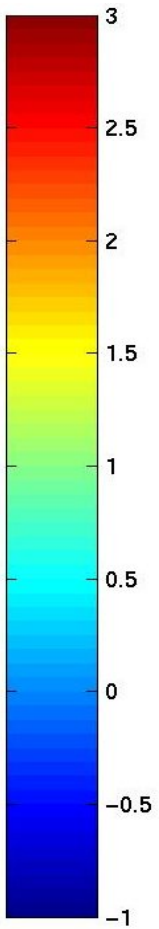
Critical condition for nucleation of PG dislocation from MD simulation:
Critical SIF

- 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**

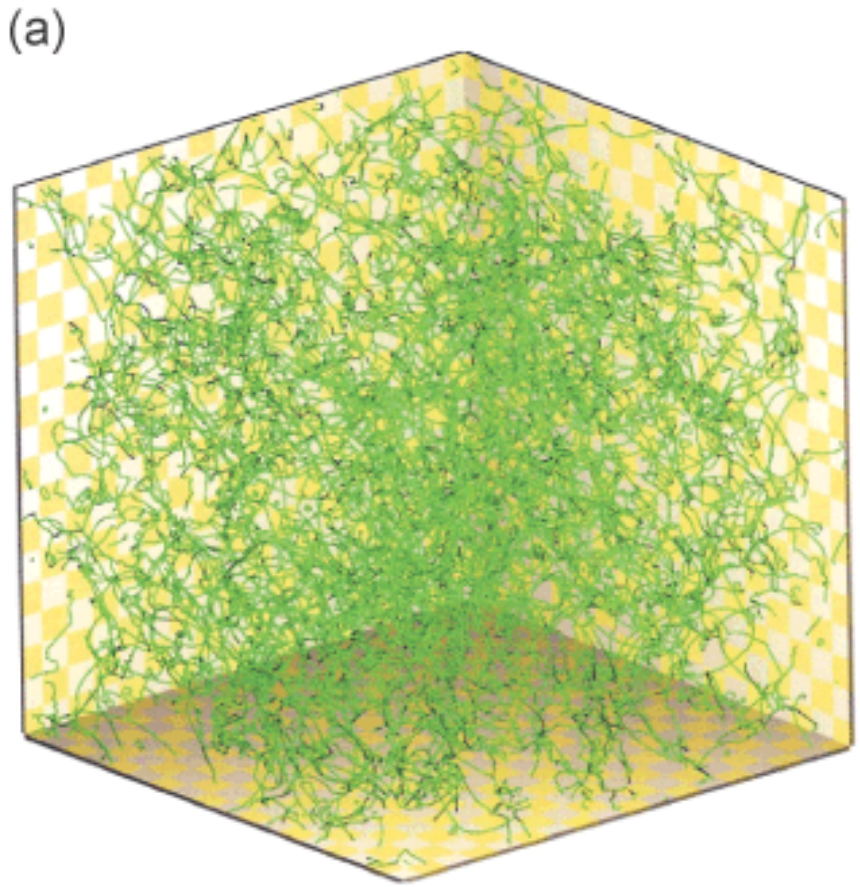
plastic relaxation under constant lateral displacement

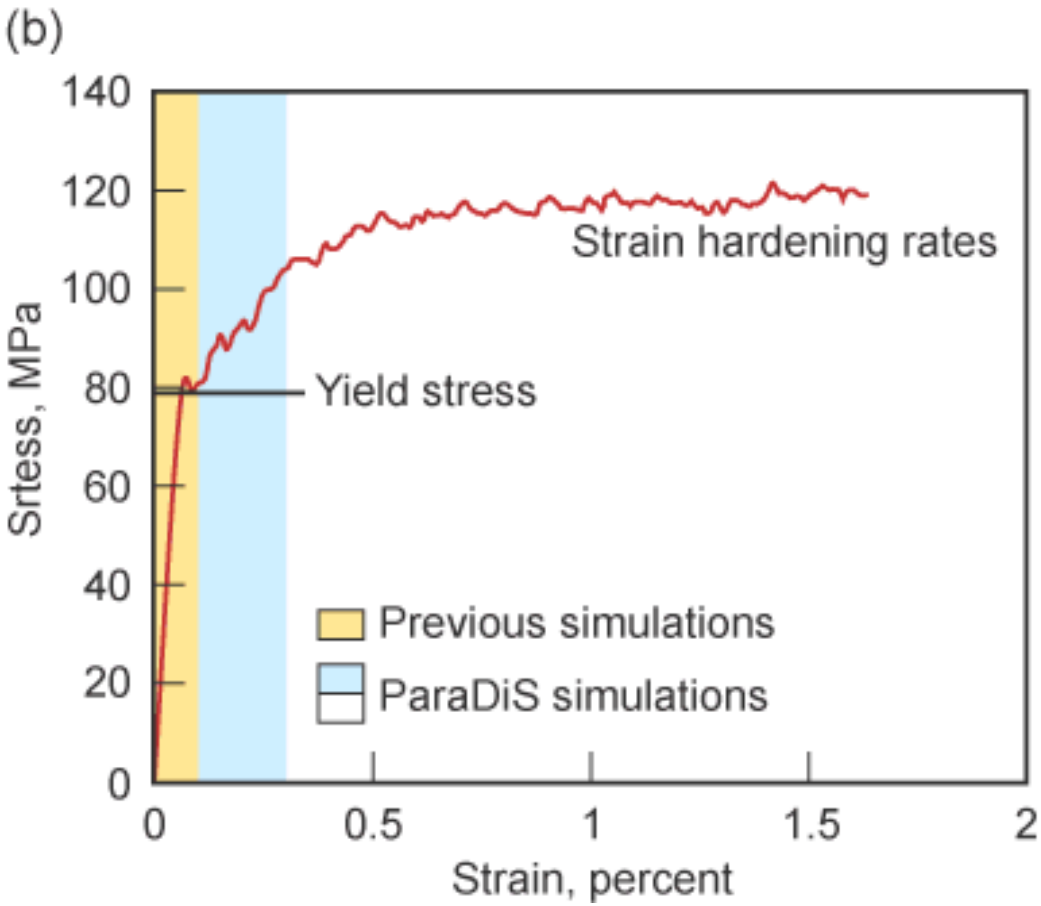
Glide source position adapted to MD results

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)

Mesoscale modeling





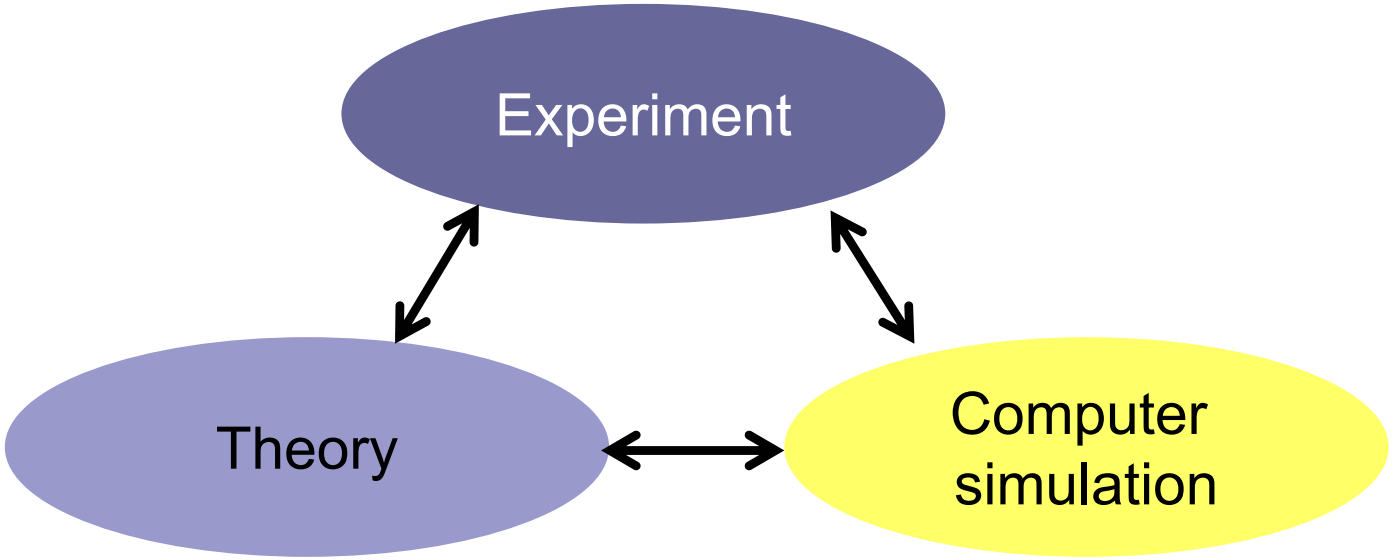
http://www-cms.llnl.gov/s-t/dislocation_dynamics.html

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 copper
- By direct numerical simulation, we have modeled the complex interaction of thousands of dislocations, and shown that there are three important mechanisms of work-hardening, which were – prior to our modeling – only known from indirect experiment or theory