Multiscale Materials Modeling

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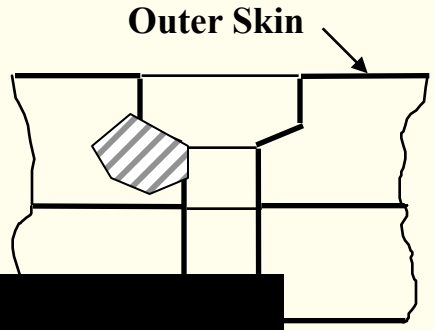
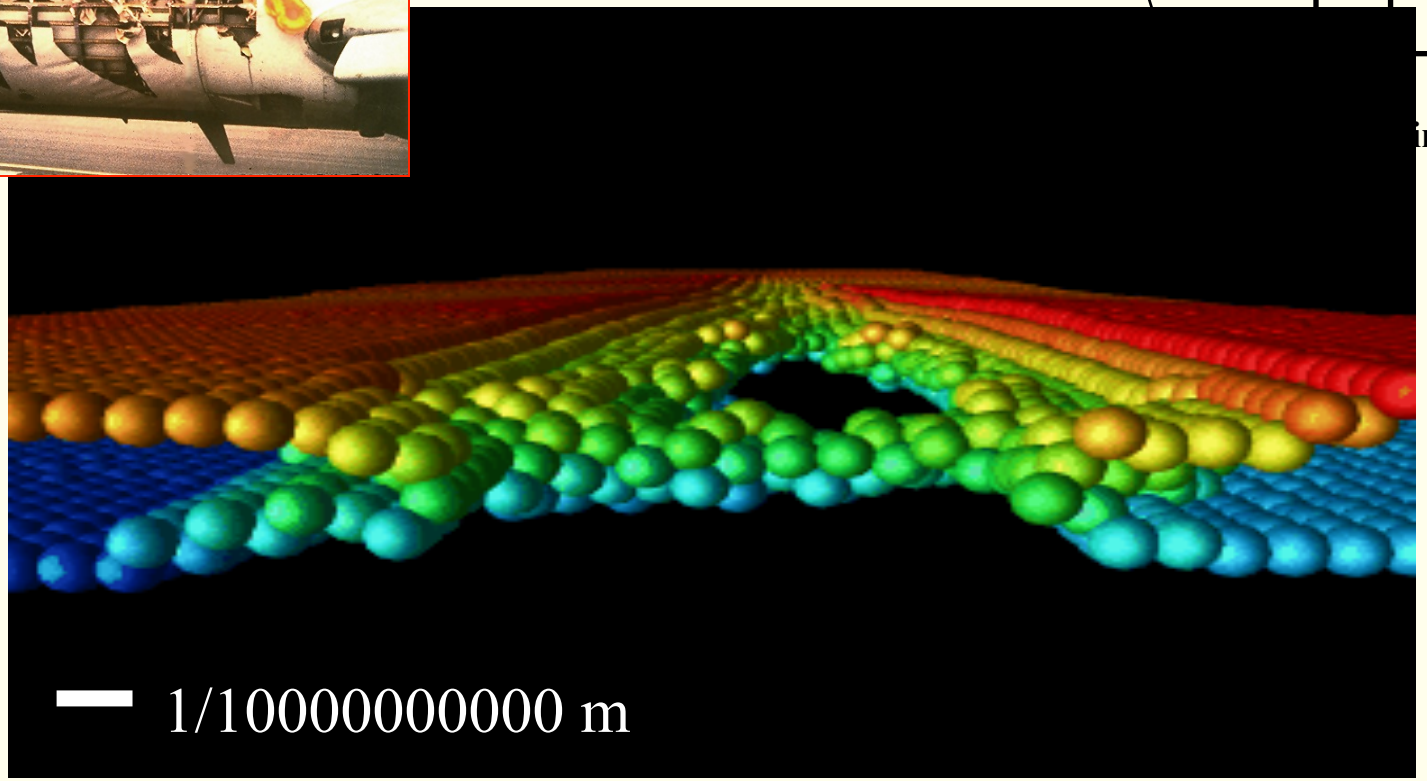
Computer Simulation and Physical Testing of Complex Fracturing Processes
Symposium in honor of Prof. Anthony R. Ingraffea on his retirement
September 27, 2014

Fatigue and fracture in metal: from cracks in the rivet holes to voids in grains to dislocation and atomistic fracture

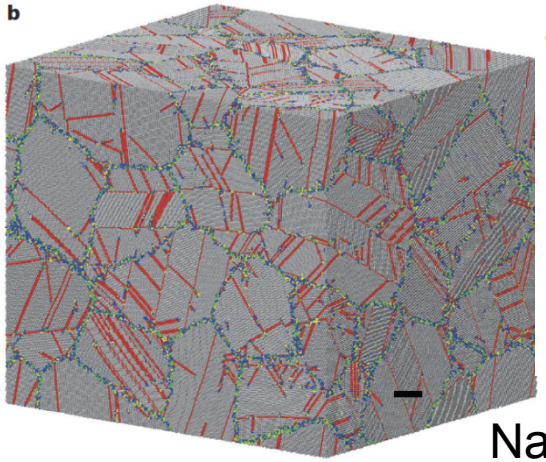
Cracking beneath a rivet

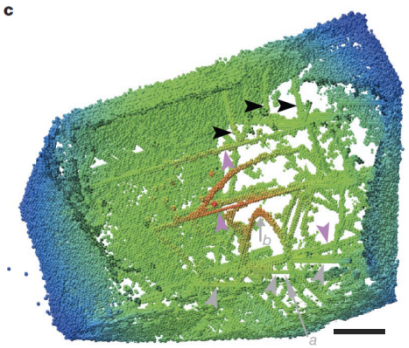




DISLOCATIONS AND MECHANICAL PROPERTY

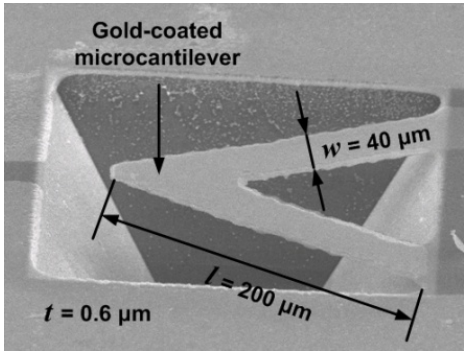
- Large-scale atomistic simulation opens a new way to study **mechanics of materials**.

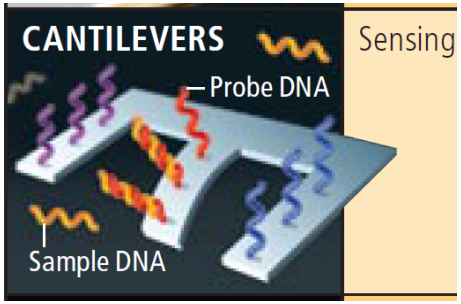




Nano-twinned Metal
Nature (2010)

~ 10^9 atoms





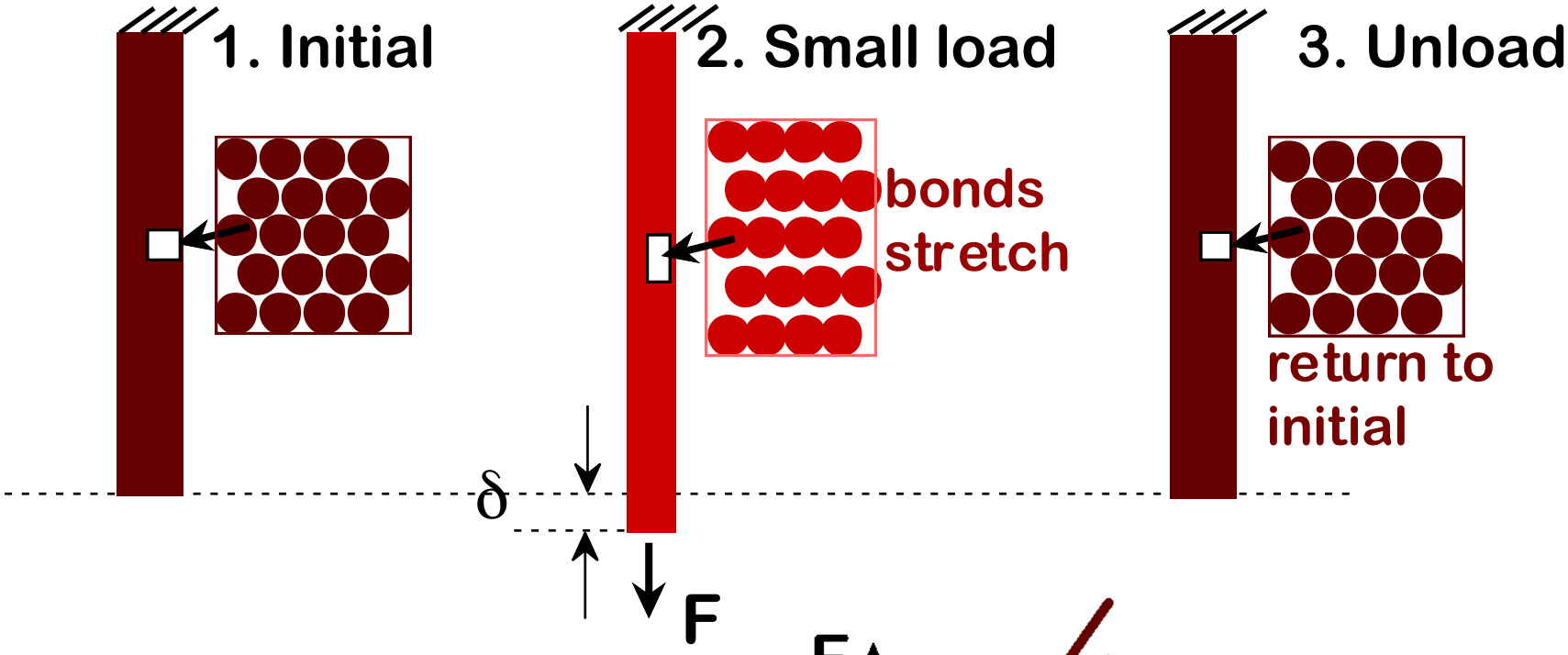
Nanomedicine targets cancer,
Scientific American, Feb 2009

200,000 x 40,000 x 600nm

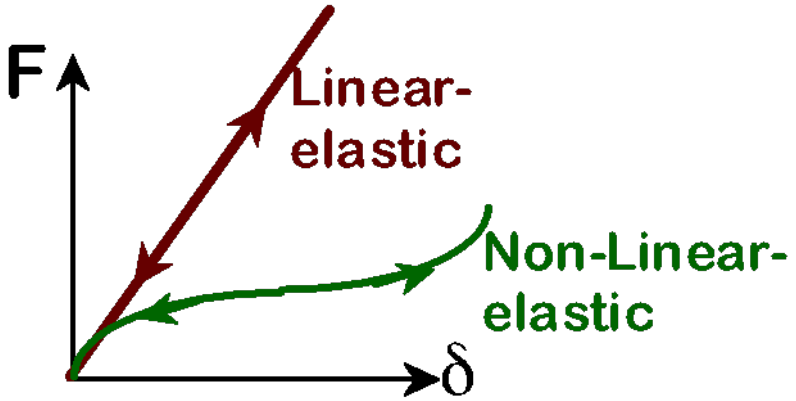
~ 10^{14} atoms

- (Key features) mechanisms and properties are emerged directly from fundamental evolution of atoms.

ELASTIC DEFORMATION

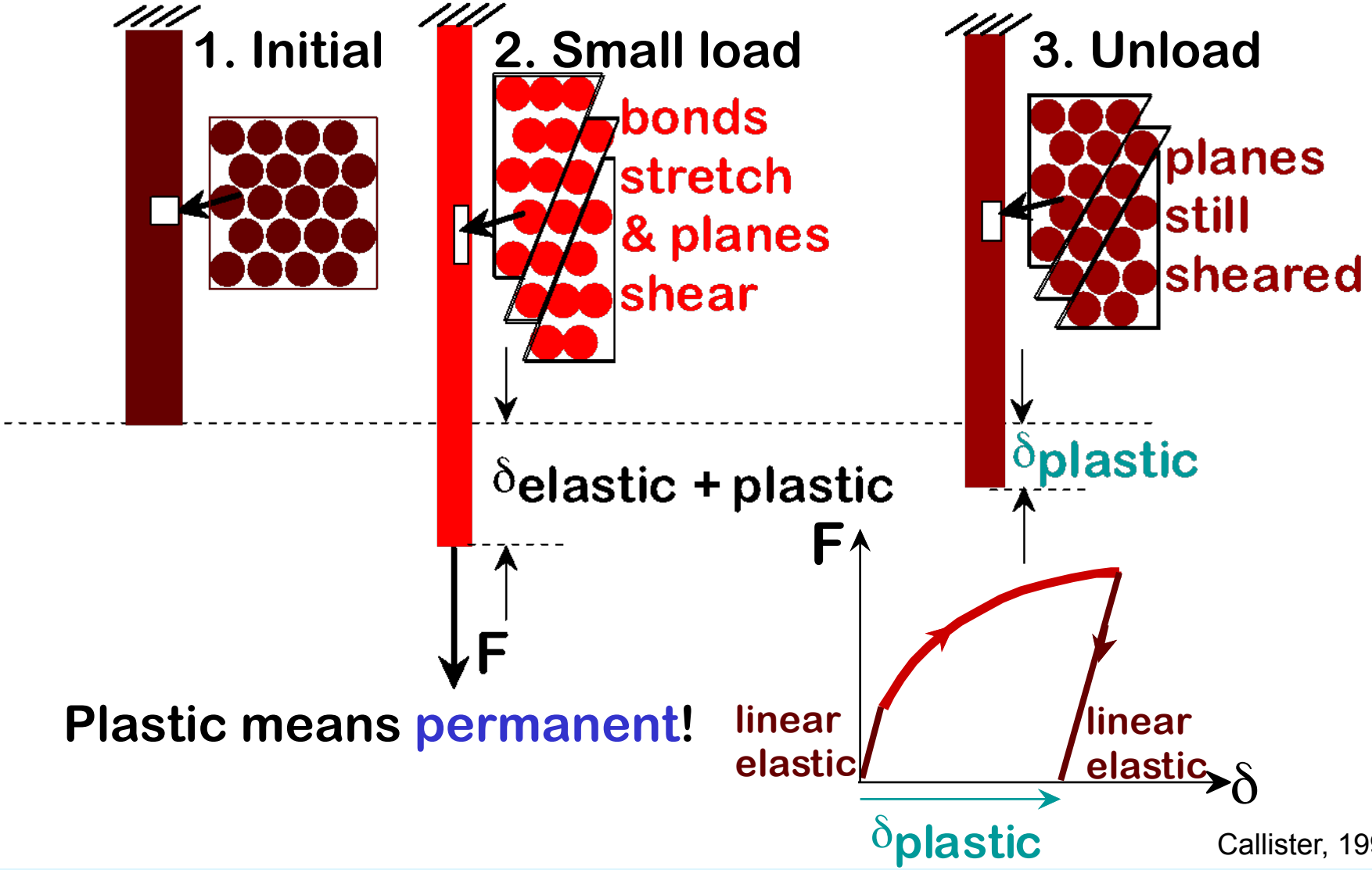


Elastic means reversible!



Callister, 1997

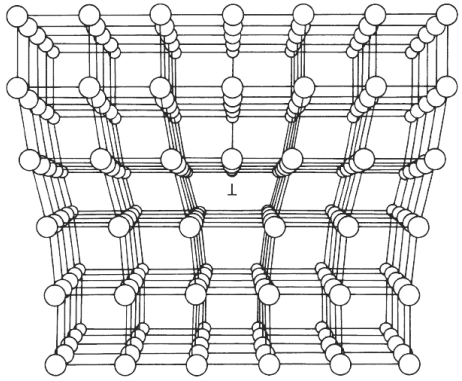
PLASTIC DEFORMATION (SHEAR and SLIP)



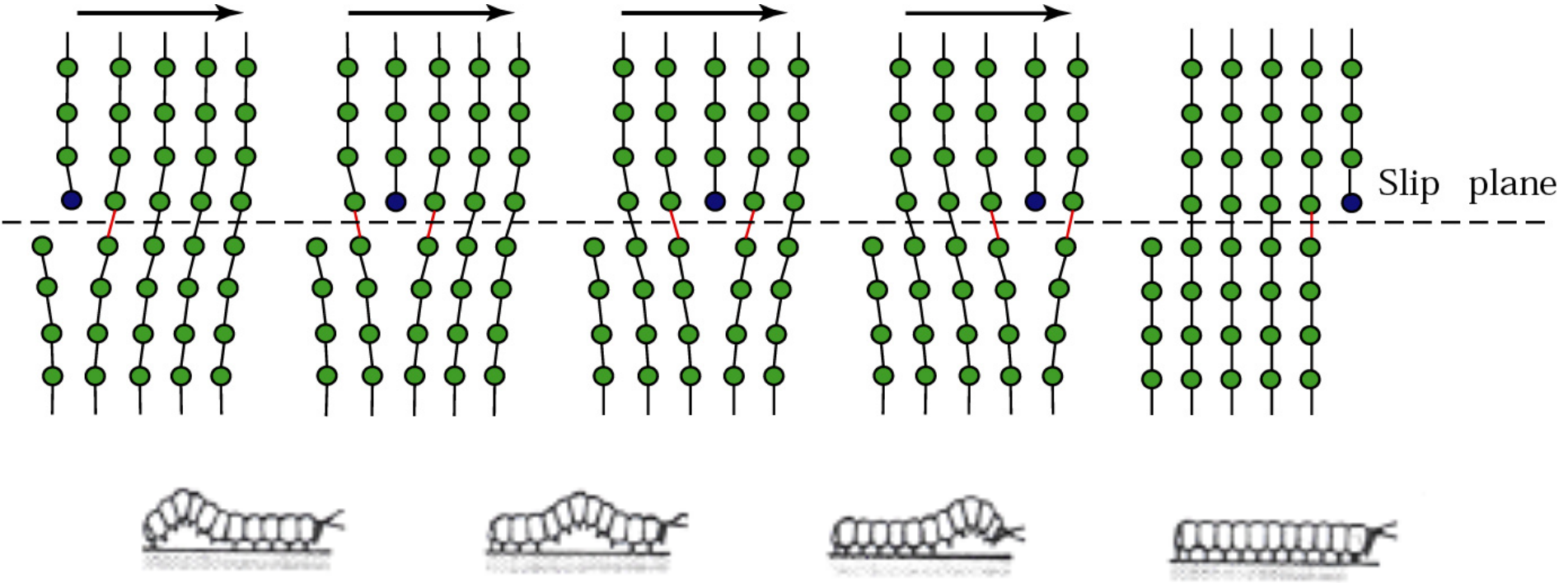
Plastic means permanent!

Callister, 1997

Dislocation and Plasticity

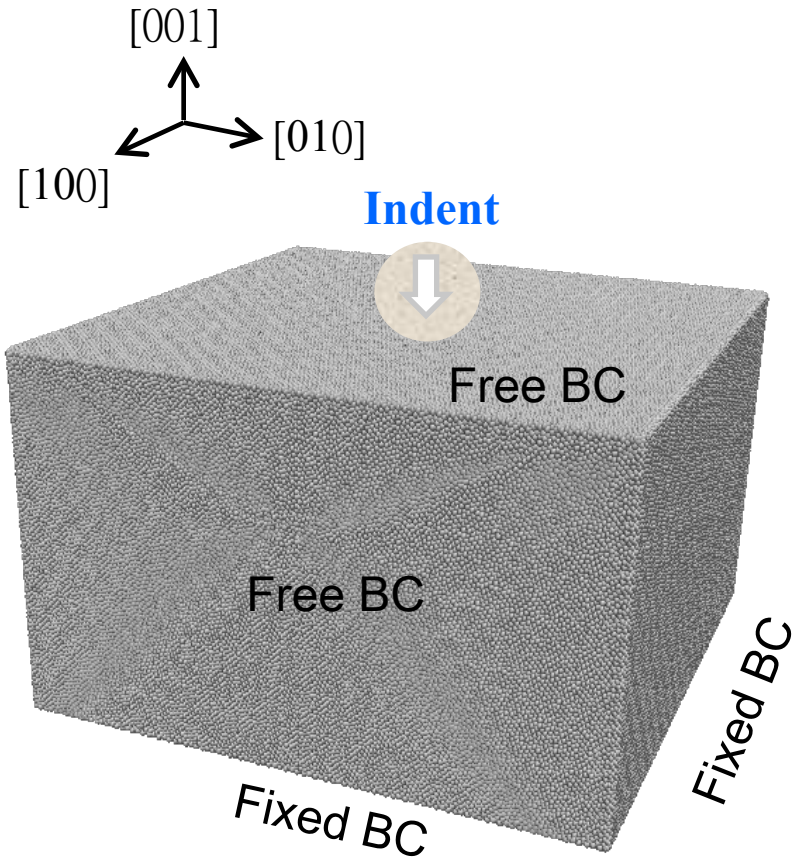


- Glide of dislocations results in slip, the most common manifestation of plastic deformation in **crystalline solids**.

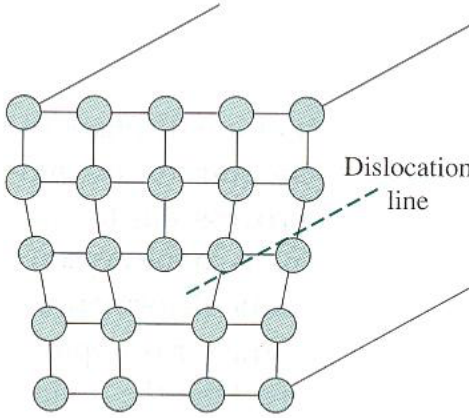


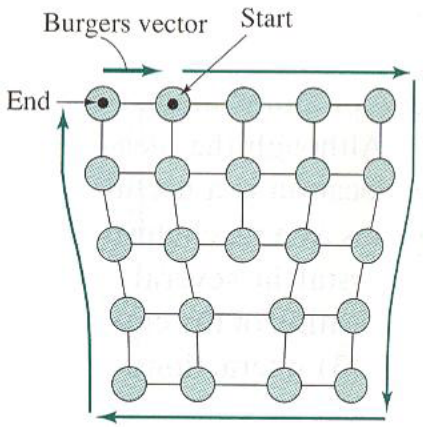
Atomistic Simulation Environment

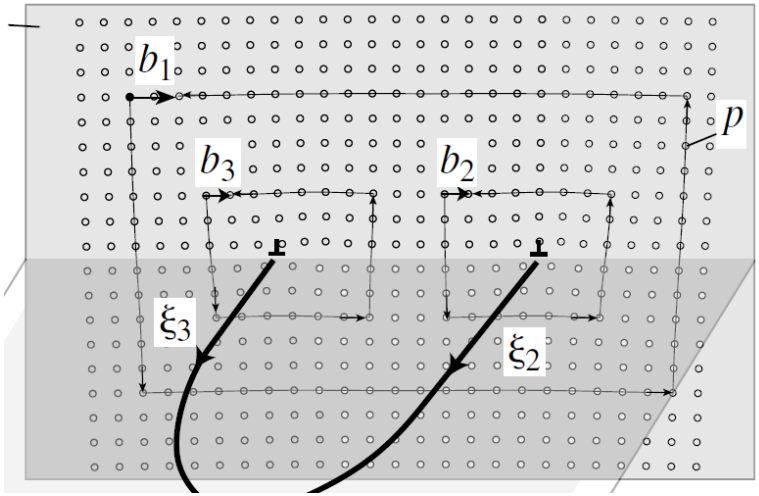
- Specimen samples
  - Contains ~10^8 atoms.
- Empirical interatomic potential: embedded atom method (EAM)
  - FCC metals (Baskes 1992).
- Quasi-static, conjugate gradient (CG) minimization.
- LAMMPS: an open source molecular dynamics program.

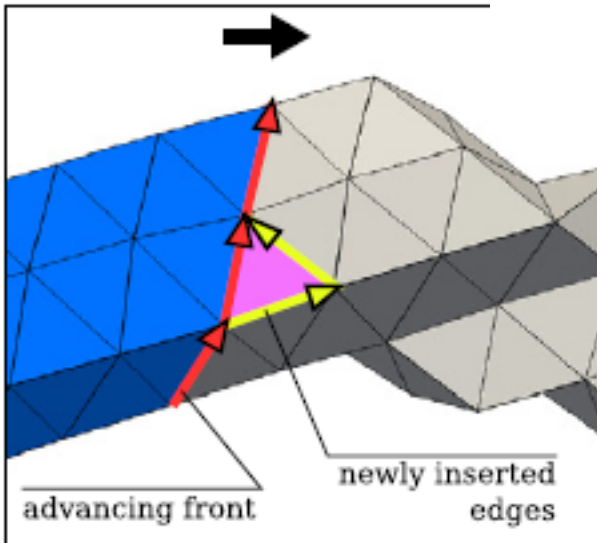


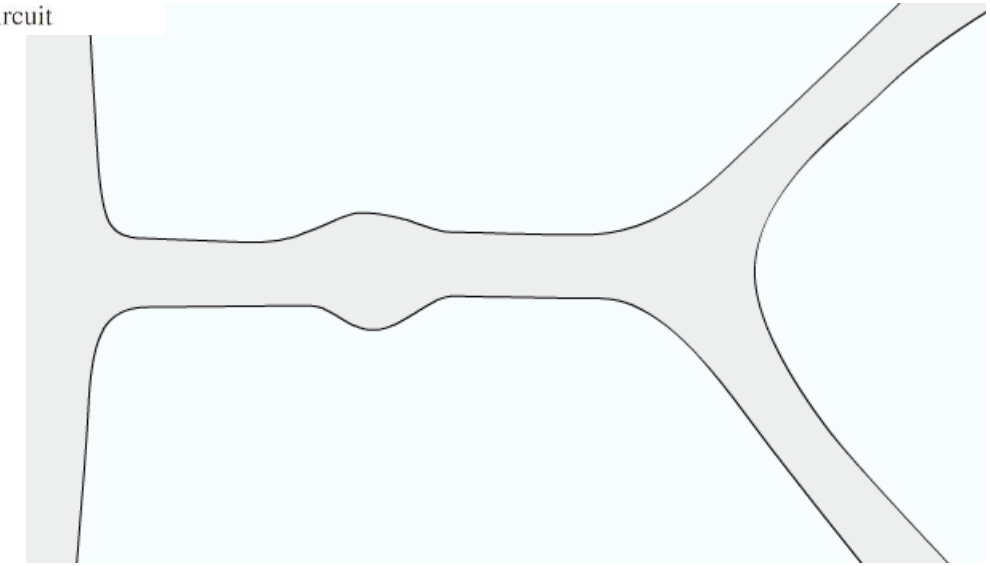
Dislocation Extraction From Burgers Circuit





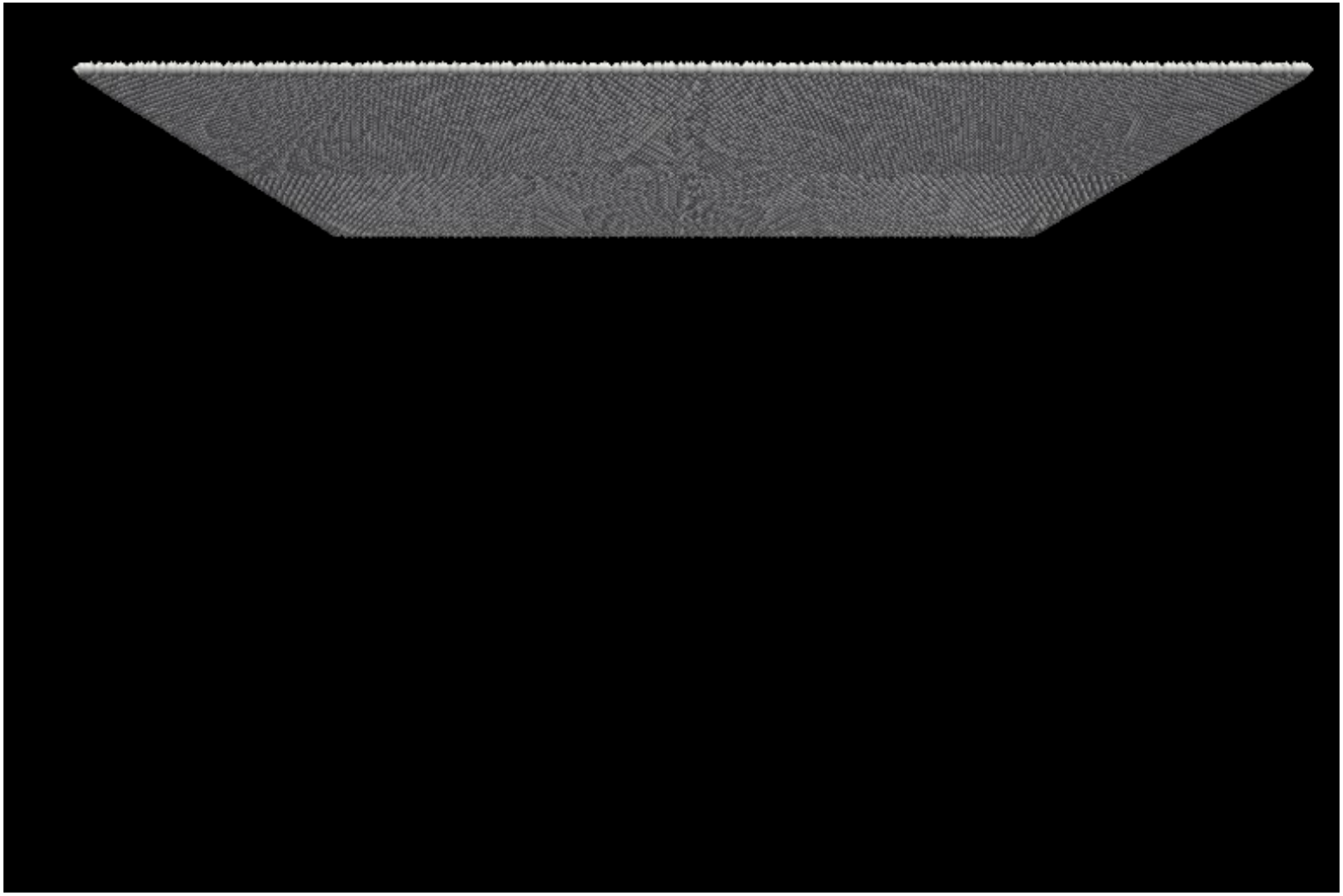






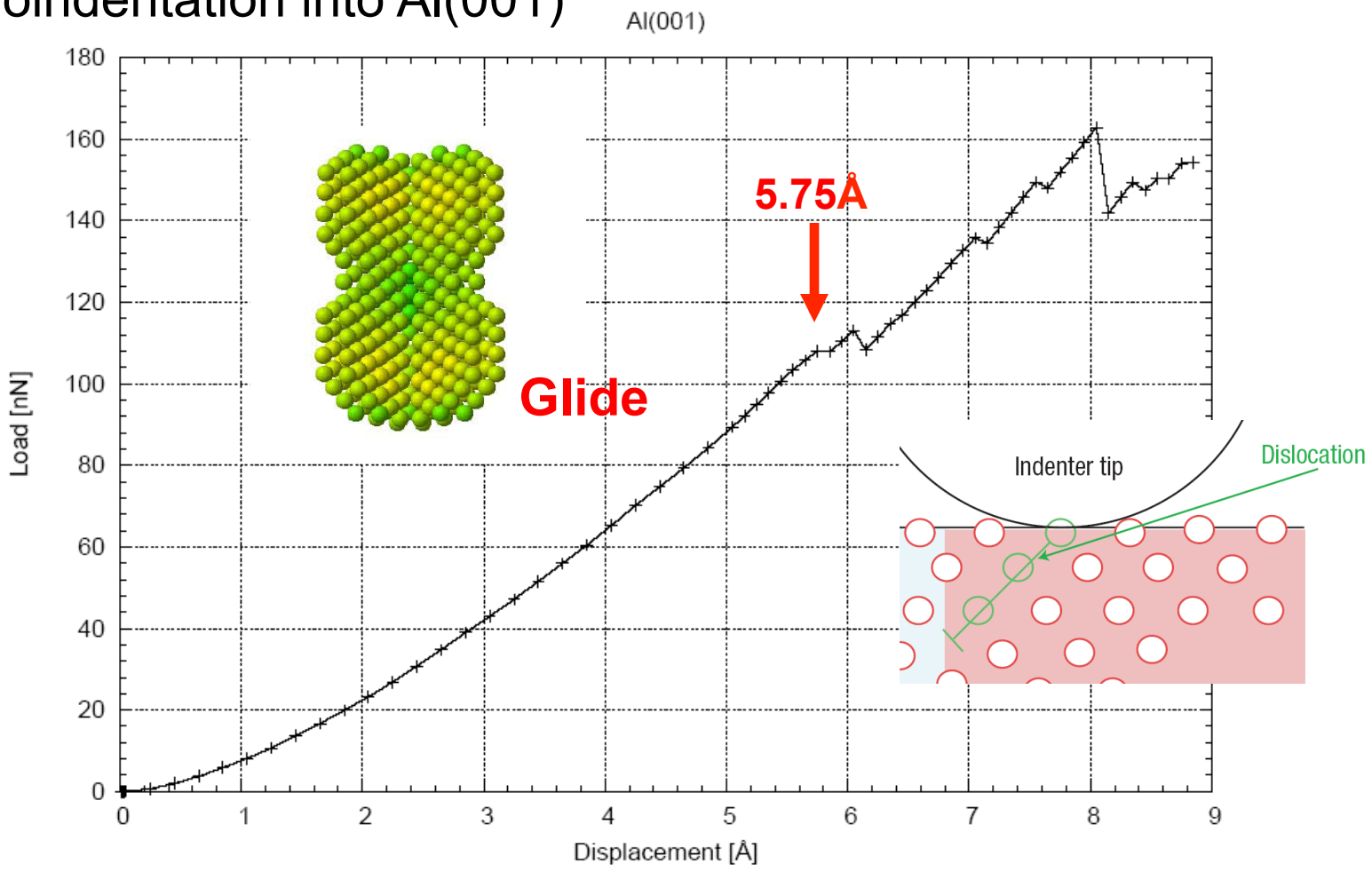
A. Stukowski and K. Albe, MSMSE, (2010) 085001.

Nanoindentation: Dislocation Evolution



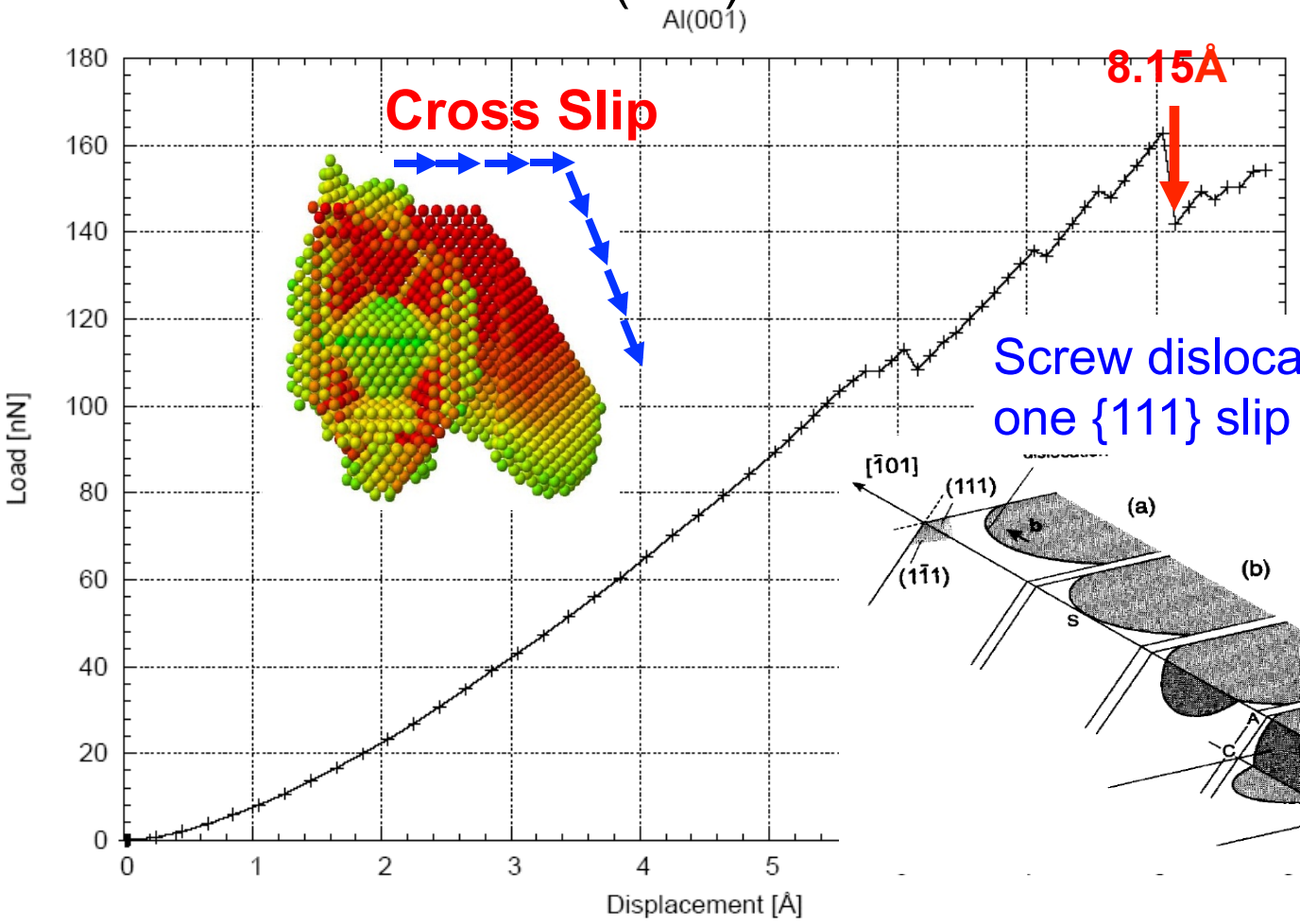
Dislocations Glide When $\tau > \tau_c$

Nanoindentation into Al(001)



Cross Slip of Screw Dislocations

Nanoindentation into Al(001)

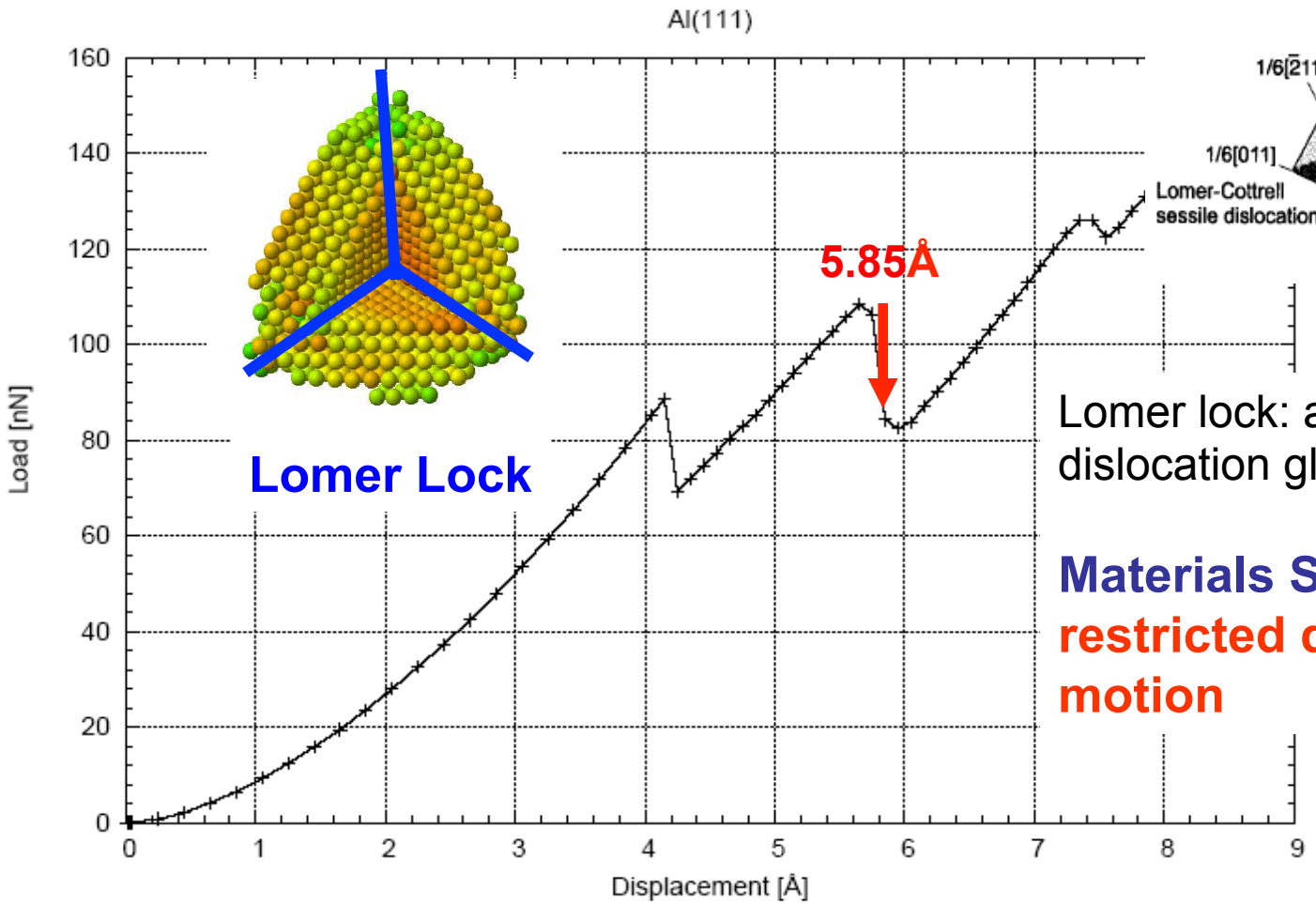


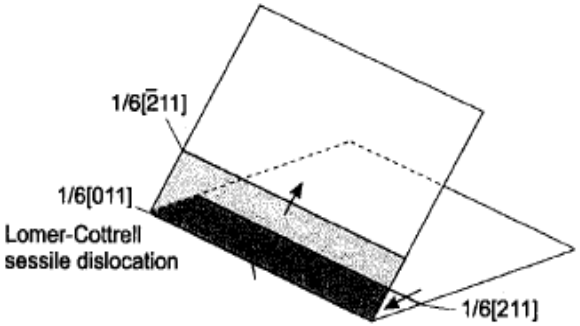
Multiple cross glide

Screw dislocation moves from one {111} slip plane to another.

Lomer Lock Blocks Dislocations

Nanoindentation into Al(111)



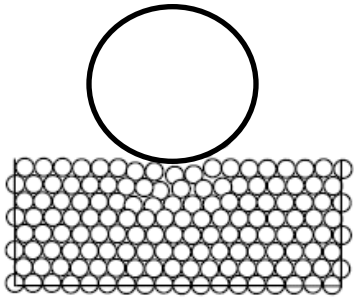


Lomer lock: a strong barrier to dislocation glides.

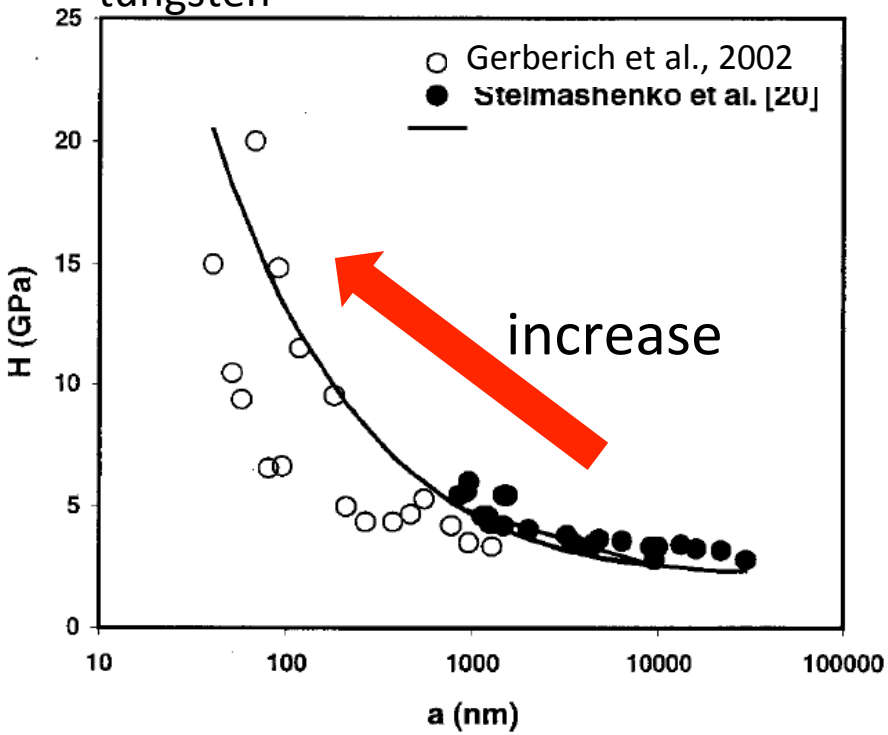
Materials Strength ≡ restricted dislocation motion

Indentation Size Effect (Smaller is Stronger)

Spherical indenter



tungsten

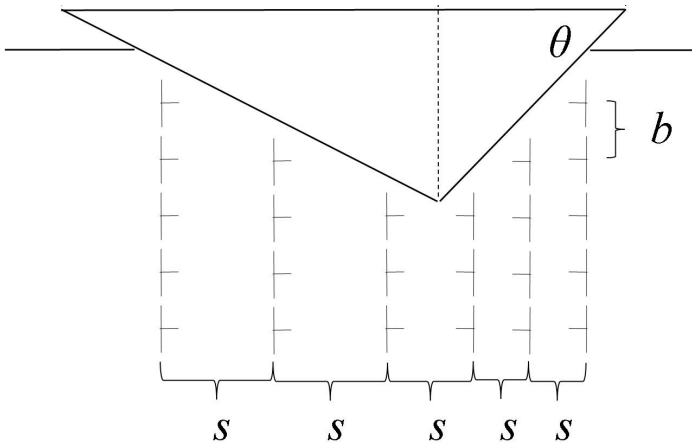


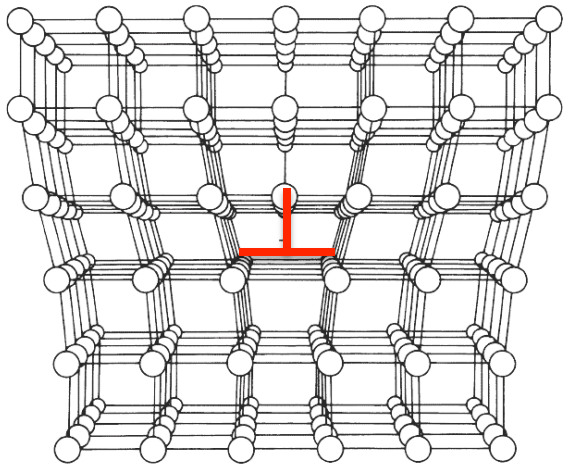
Gerberich et al. (2002), J of Applied Mechanics

Hardness increases when indenter radius decreases.

Indentation Size Effect: The Quest

- (Imagine) We push atoms into the underneath material.
- Atoms become extra planes of atoms (dislocations) in the original lattice.
- These dislocations are called geometrically necessary dislocations (GNDs).
- GNDs are believed to block other mobile dislocations thus contribute to hardening.
- The smaller indents, the higher **density** of GNDs, and thus stronger.

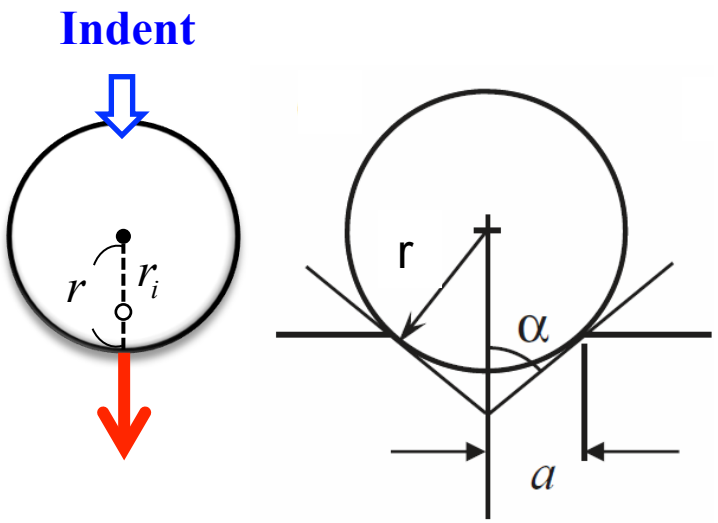


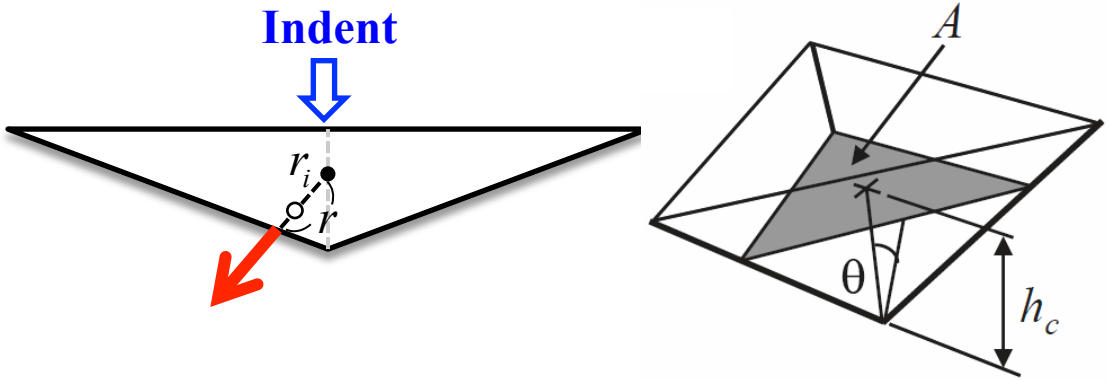


Repulsive Force Field for Indenters

$$F_i = \varepsilon (r - r_i)^2$$ (Plimpton 1995).

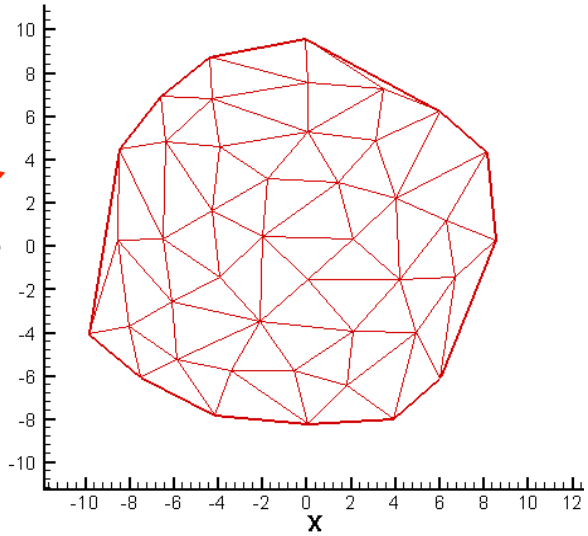
- Spherical Indenter
  - Smooth transition from elastic to elastic-plastic contact
- Berkovich Indenter
  - Routinely used in nanoindentation tests

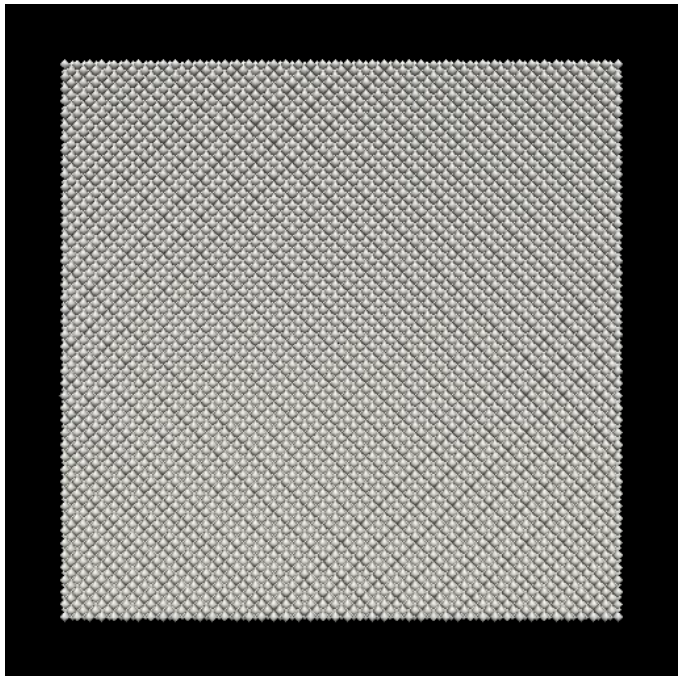


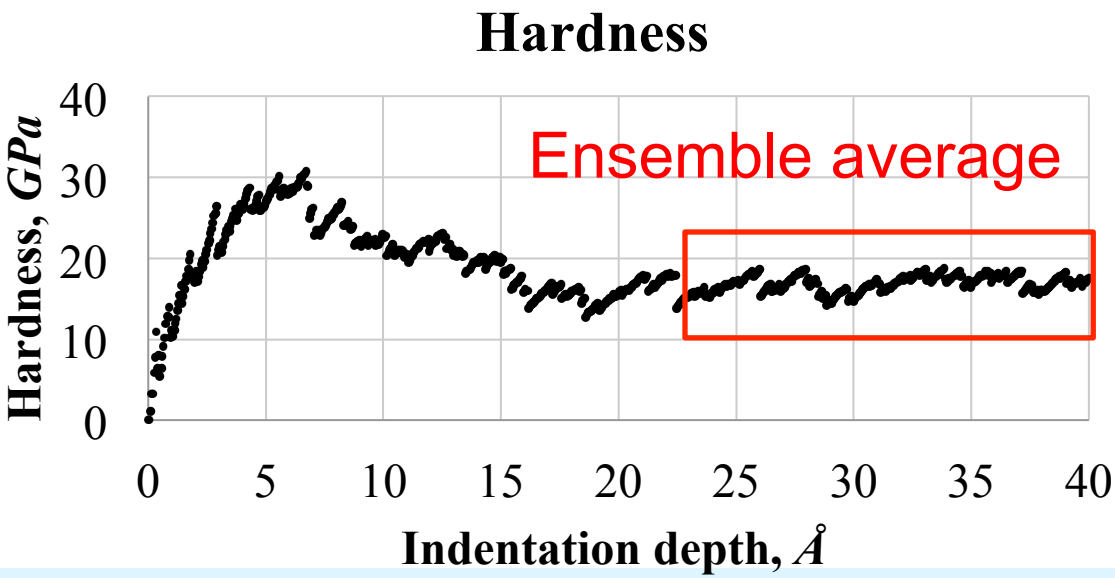


Hardness Calculation

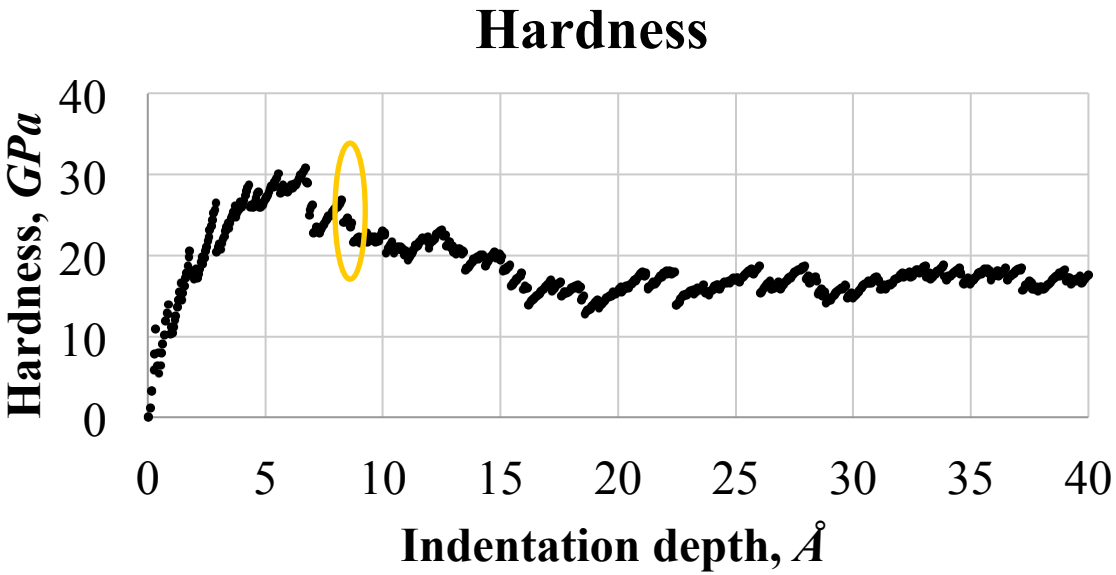
$$Hardness = \frac{P_{Load}}{A_{contact}}$$

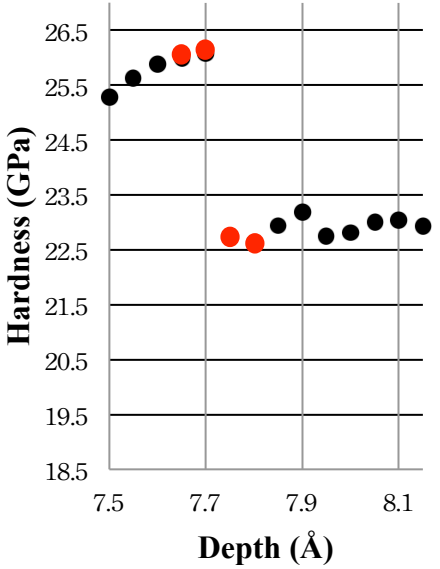


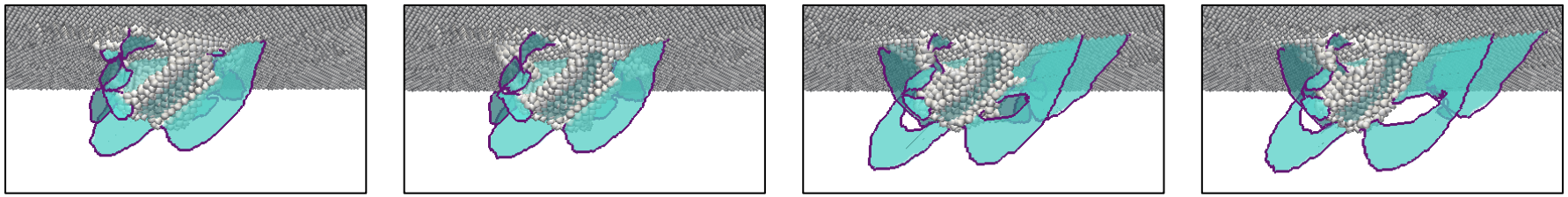




Hardness vs. Dislocation Evolution

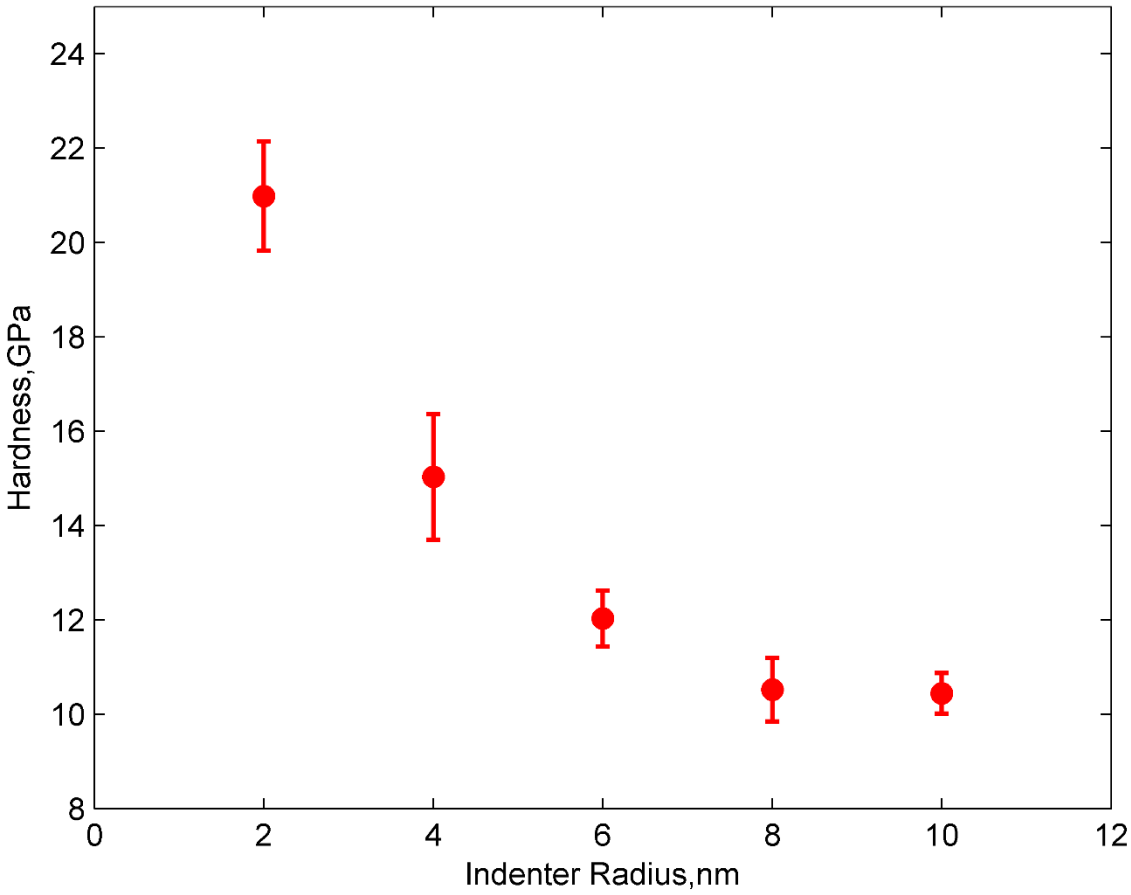






Materials Strength ≡ restricted dislocation motion.

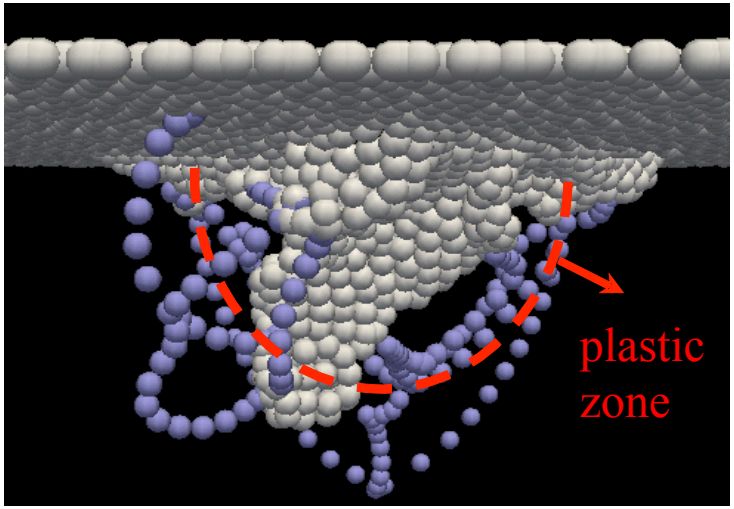
Hardness - Spherical

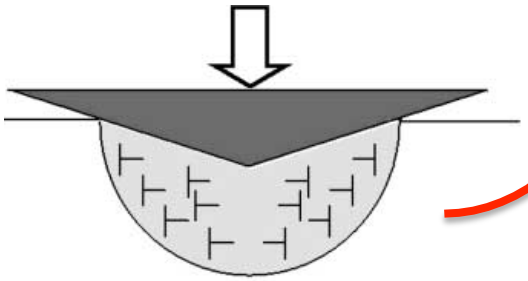


Quantify Density of Geometrically Necessary Dislocations (ρ_g)

Total length of dislocation lines

$$\rho_g = \frac{l}{V}$$





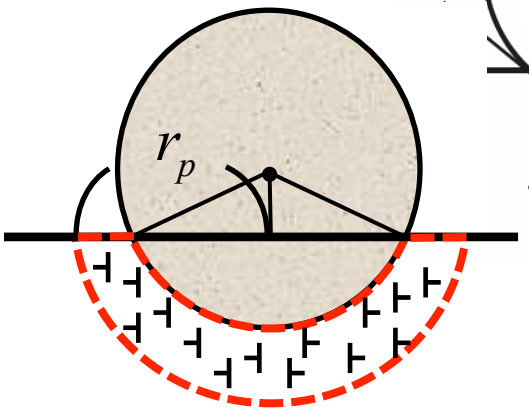
plastic zone

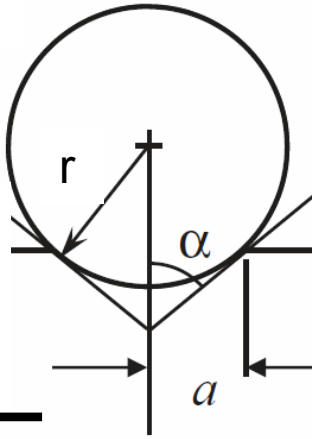
Plastic Zone Calculations

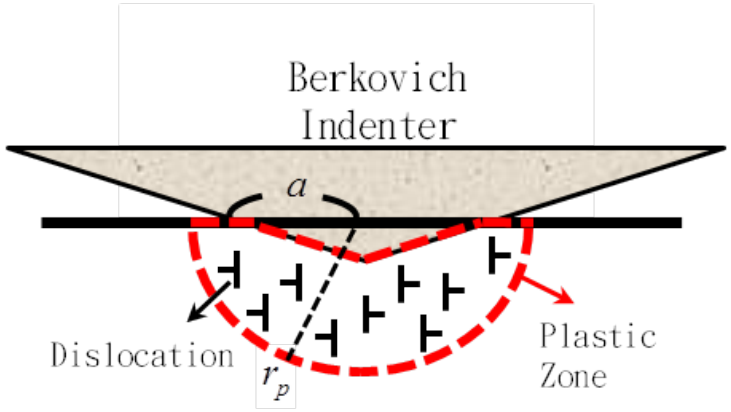
$$a = \sqrt{A_{contact} / \pi}$$

$$r_p = \sqrt[3]{(\frac{2}{3}\pi a^3 + V_{indenter,in}) * \frac{3}{2\pi}}$$

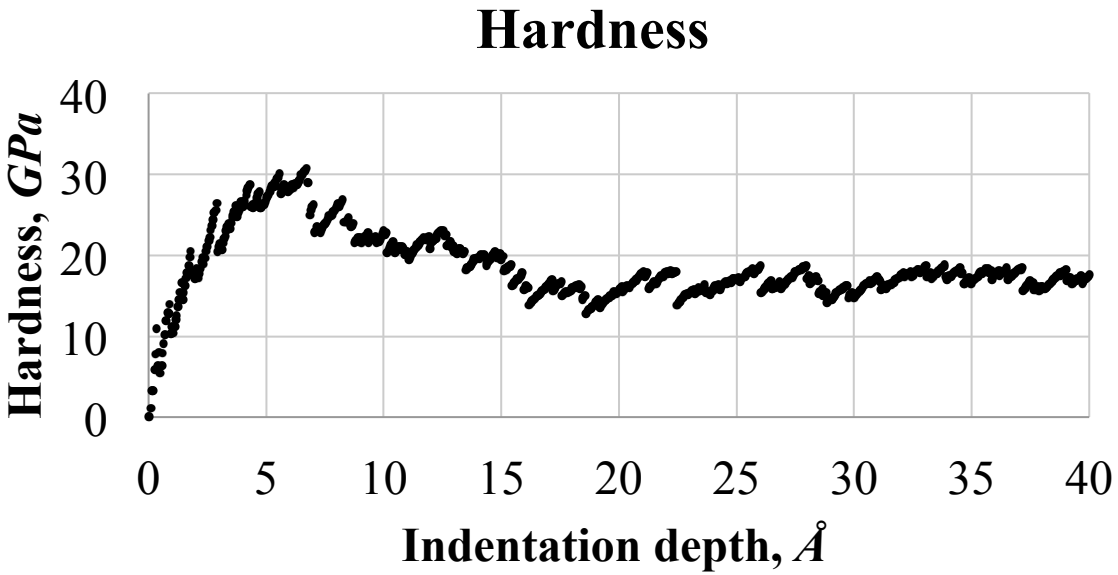
$$V_p = \frac{2}{3}\pi r_p^{\ 3} - V_{indenter,in}$$

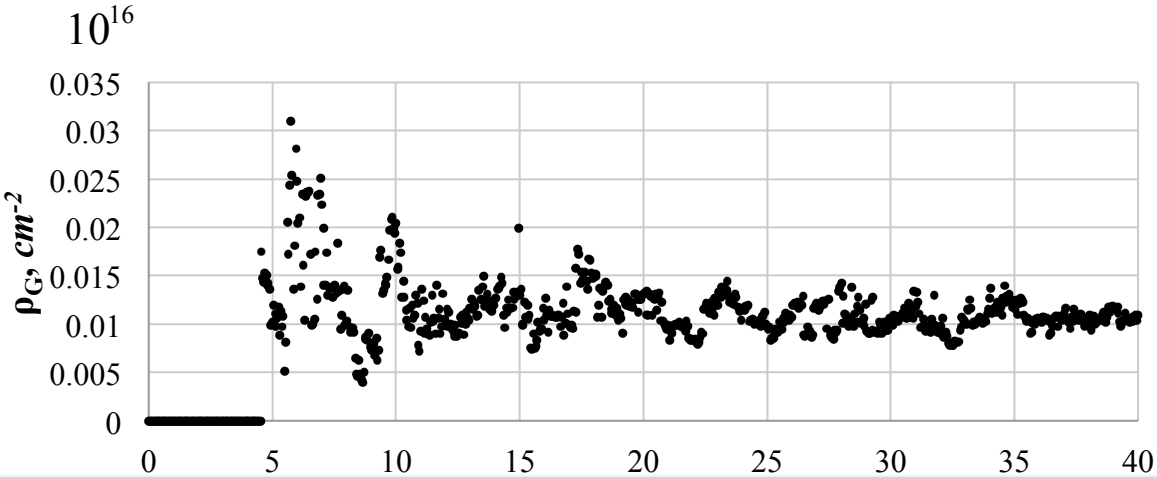






Hardness (Property) and GNDs (Mechanism)





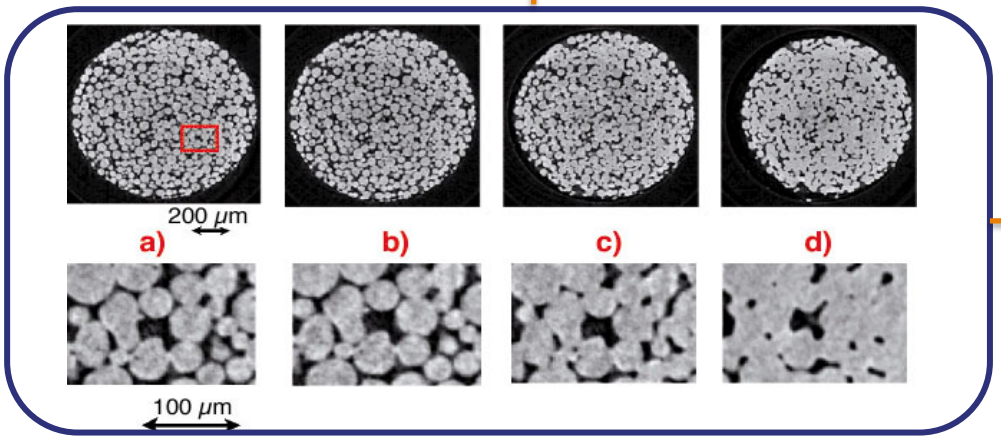
VOID NUCLEATION AND GROWTH

Ultra High Temperature Ceramics

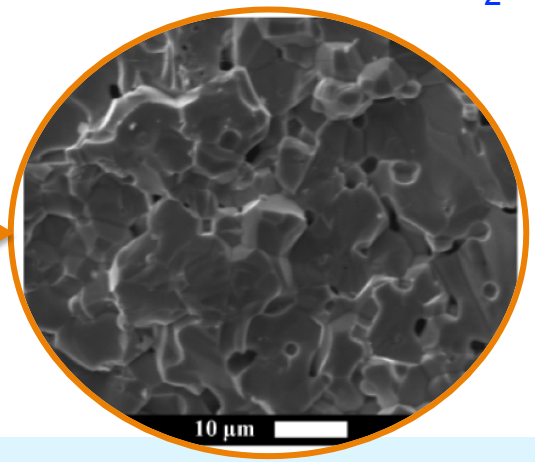
NASA http://apod.nasa.gov/apod/ap040329.html

DARPA Falcon Project http://www.space.com/12607-darpa-launches-hypersonic-glider-mach-20-test-flight.html

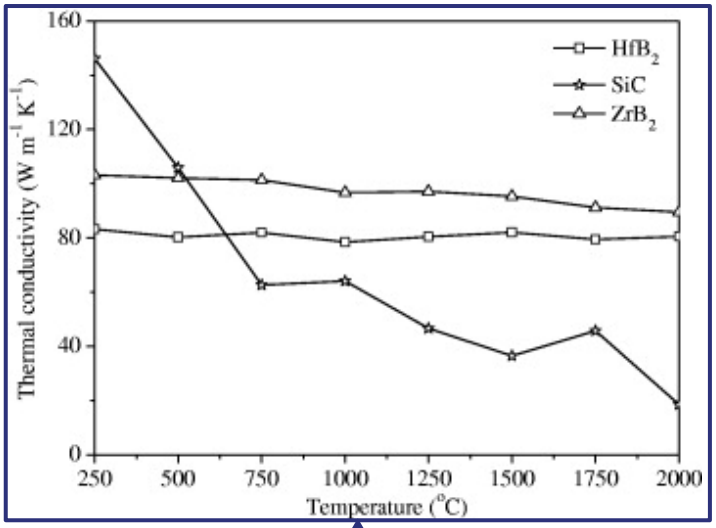
Sintering process of ZrB_2



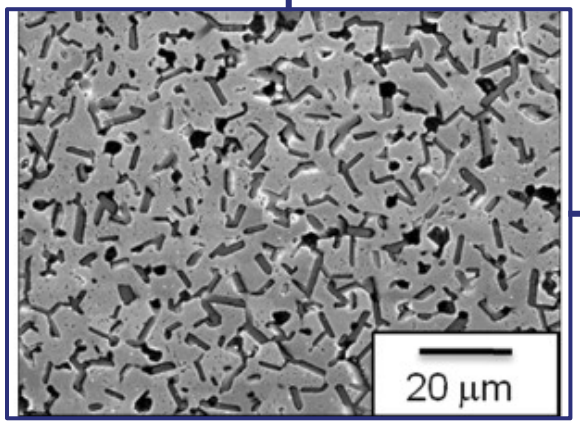
Microstructure of ZrB_2

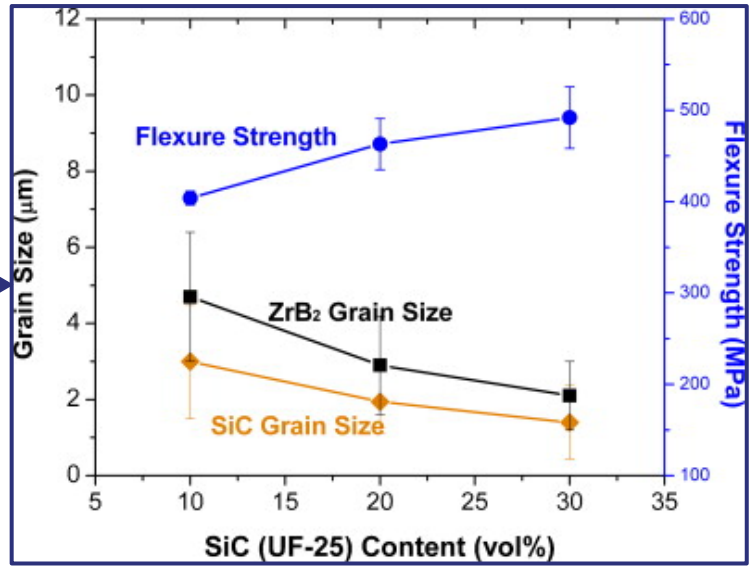


ZrB_2-SiC Ceramic Composites



ZrB_2 is one of the material candidates for UHTC: high strength, low density and excellent thermal properties

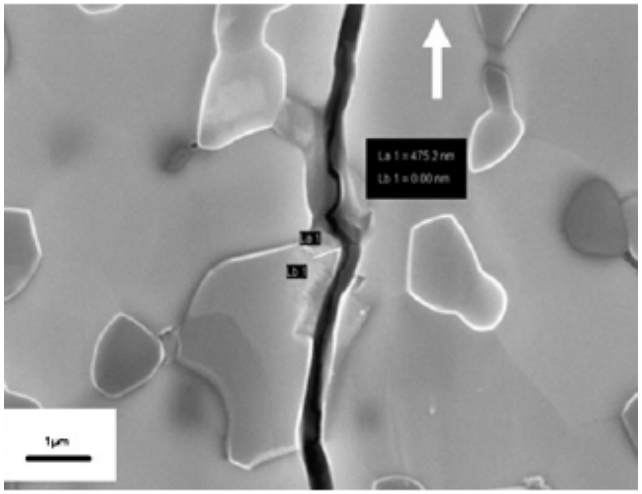


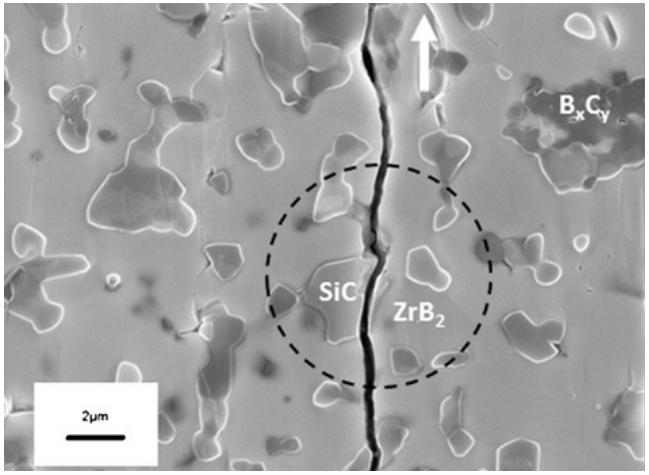


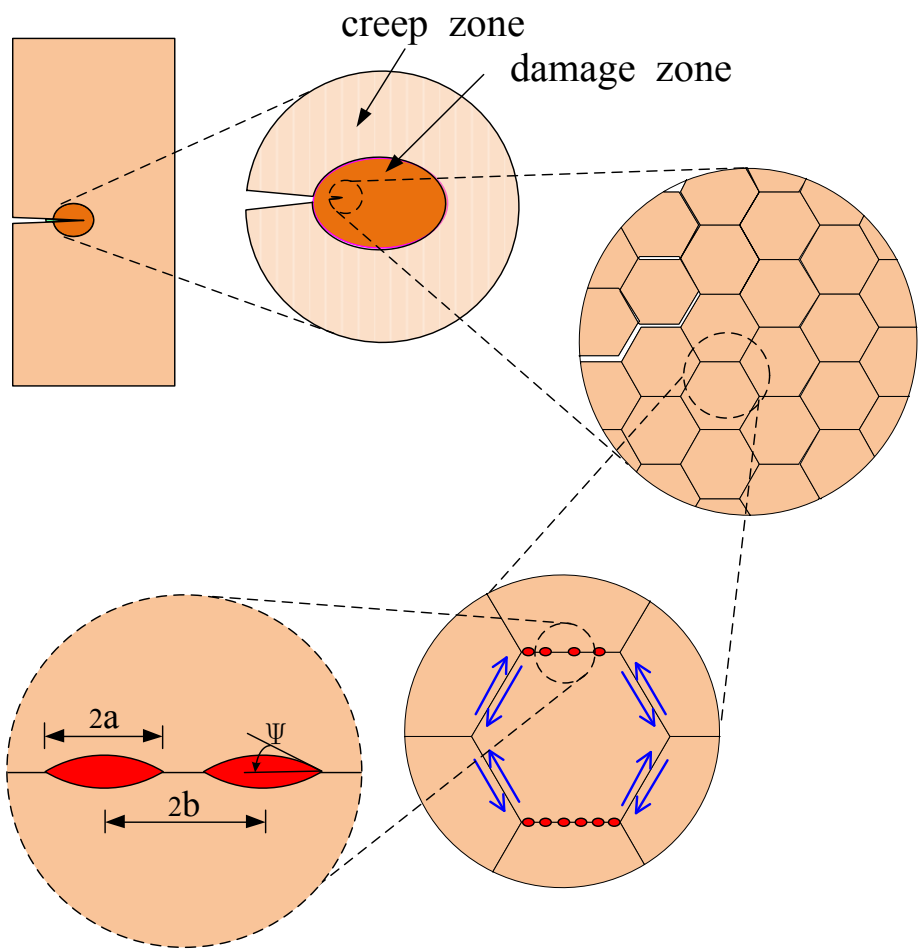
SiC content improves the flexure strength and toughness.

Modeling Intergranular Fracture

SEM image of ZrB_2-SiC composite at 1500°C CT test







Micromechanics Model: Simple Grain

- Constitutive model of ceramic grain
  - Superposition of strain rate

$$\dot{\varepsilon}_{ij} = \dot{\varepsilon}^{e}_{ij} + \dot{\varepsilon}^{cr}_{ij}$$

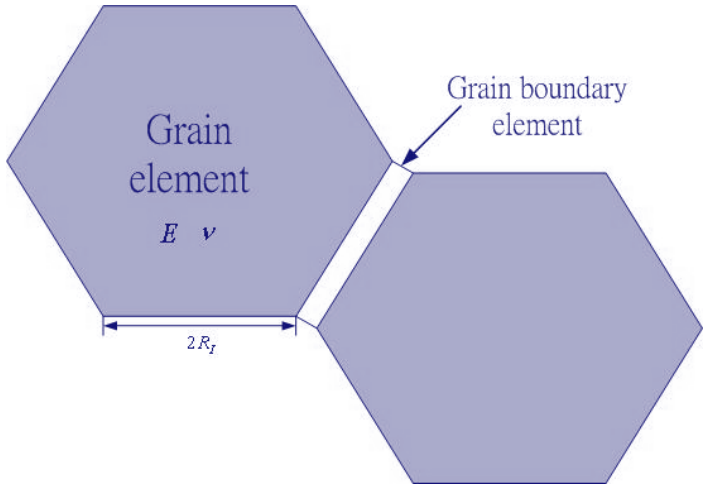
  - Stress

$$\sigma^{(m+1)}_{ij} = \mathbf{D}(\varepsilon^{(m+1)}_{ij} - \varepsilon^{cr(m+1)}_{ij})$$

$$\mathbf{D} = \frac{E}{(1+\nu)(1-2\nu)}\begin{bmatrix} 1-\nu & \nu & 0 \\ \nu & 1-\nu & 0 \\ 0 & 0 & 1-2\nu \end{bmatrix}$$

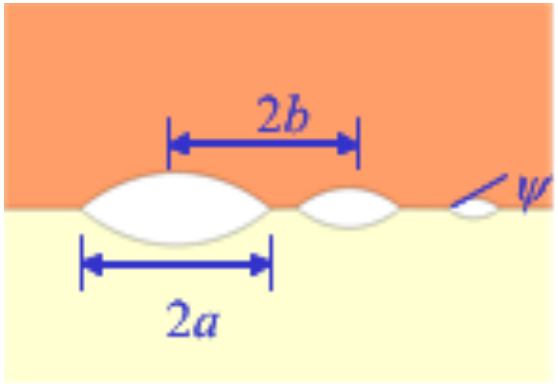
- Power law creep rate for a ceramic grain

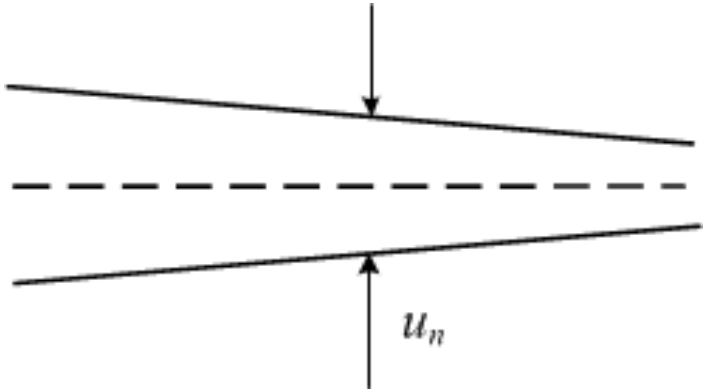
$$\dot{\varepsilon}^{cr}_{ij} = \frac{3}{2}\frac{S_{ij}}{\sigma_e}\dot{\varepsilon}_0 \exp\left(\frac{-Q}{RT}\right)\left(\frac{\sigma_e}{\sigma_0}\right)^n$$



Micromechanics Model: Grain Boundary

- Smeared out cohesive model for grain boundary





a: cavity radius
b: half cavity spacing
V: cavity volume

$$V = \frac{4}{3}\pi a^3 h(\psi)$$

and

$$h(\psi) = \frac{[(1+\cos\psi)^{-1} - \frac{1}{2}\cos\psi]}{\sin\psi}$$

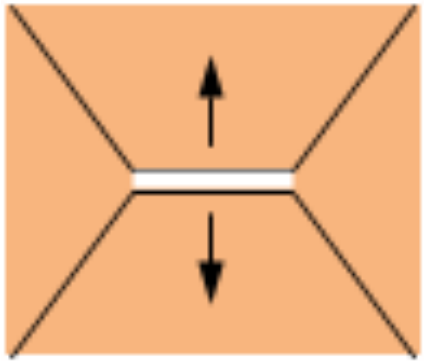
Grain separation in normal direction can be expressed by

$$u_n = \frac{V}{\pi b^2}$$

Micromechanics Model: Grain Boundary

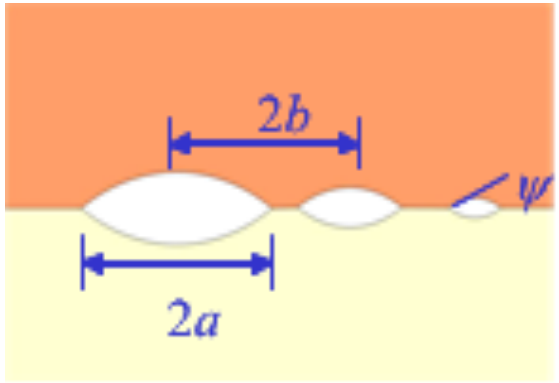
- Normal separation rate

$$\dot{u}_n = \frac{\dot{V}}{\pi b^2} - \frac{2V\dot{b}}{\pi b^3}$$



- **Three ingredients** in normal separation rate at grain boundary
  - Cavity nucleation
  - Cavity growth enabled by atom diffusion
  - Cavity growth enabled by creep

Cavity Nucleation



- Cavity density of undefomed grain boundary

$$N = \frac{1}{\pi b^2}$$

- The change rate of void spacing

$$\frac{\dot{b}}{b} = \frac{1}{2}(\dot{\varepsilon}_I + \dot{\varepsilon}_{II}) - \frac{1}{2}\frac{\dot{N}}{N}$$

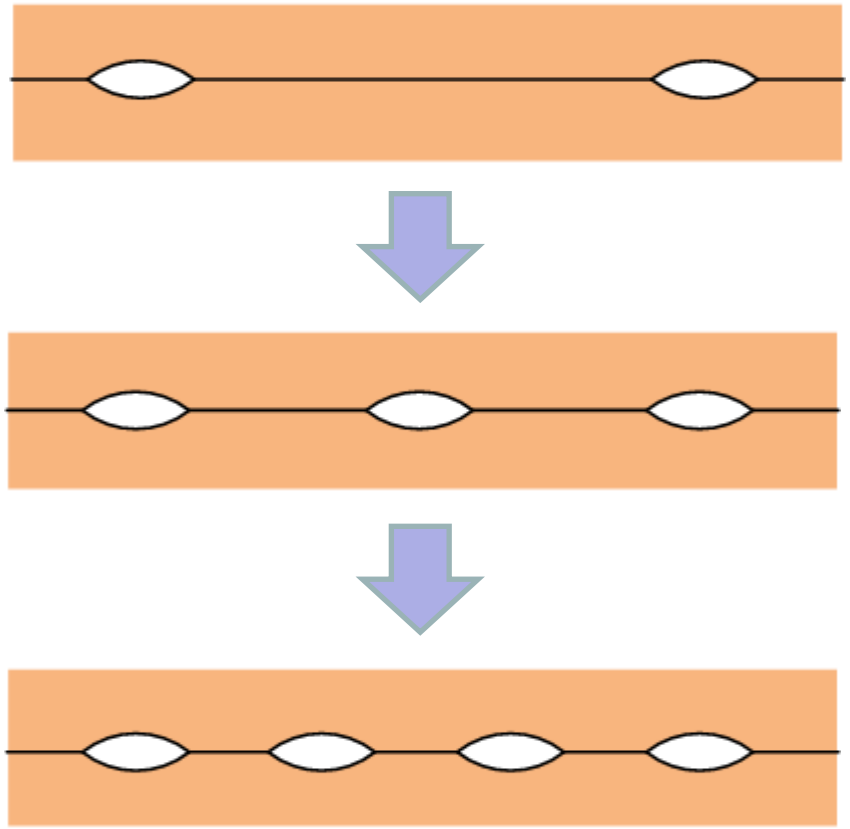
where $\dot{\varepsilon}_I$ and $\dot{\varepsilon}_{II}$ are the principal logarithmic strain rates at grain boundary

Cavity Nucleation Rule

- Cavity density rate

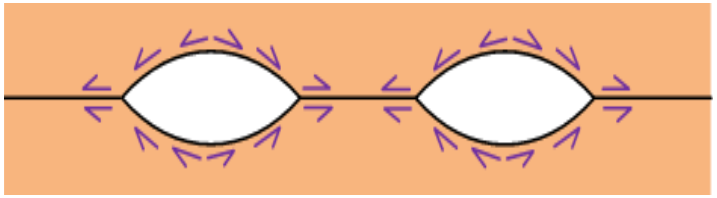
$$\dot{N} = F_n \left(\frac{\sigma_n}{\Sigma_0}\right)^2 \dot{\varepsilon}_e^C$$

F_n is material parameter, σ_n is normal traction, Σ_0 is a normalized factor, and $\dot{\varepsilon}_e^C$ is the effective strain which is the average value of adjacent grains.



Cavity Growth

- Cavity growth from diffusion



$$\dot{V}_1 = 4\pi D \frac{\sigma_n}{\ln(\frac{1}{f}) - \frac{1}{2}(3-f)(1-f)}$$

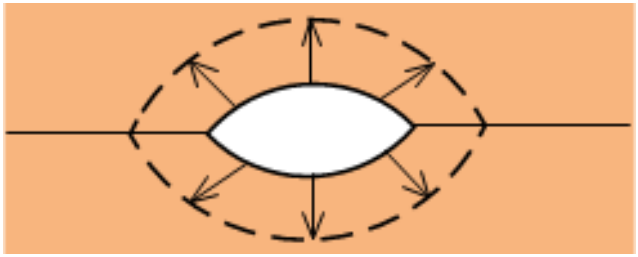
where

$$f = \max\left\{\left(\frac{a}{b}\right)^2, \left(\frac{a}{a+1.5L}\right)^2\right\}$$

and

$$L = \left[D\frac{\sigma_e}{\dot{\varepsilon}_e^c}\right]^{\frac{1}{3}}$$

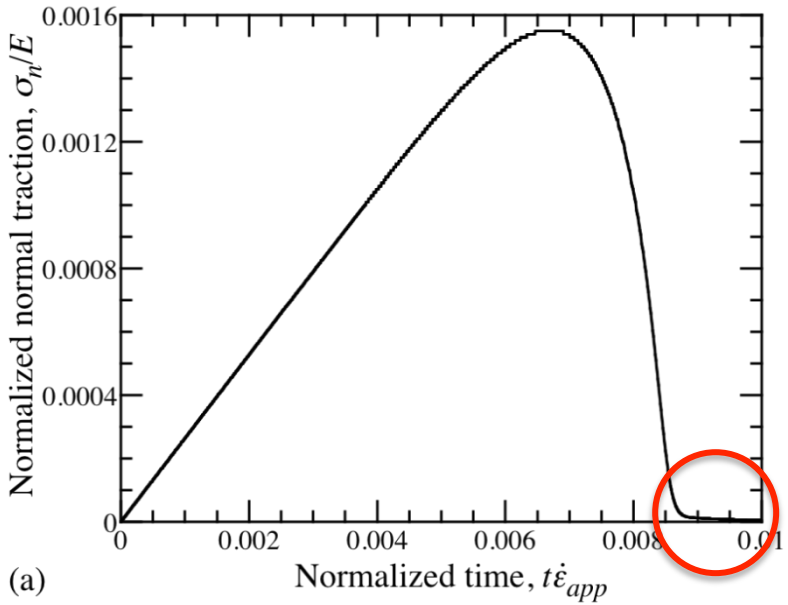
- Cavity growth from creep



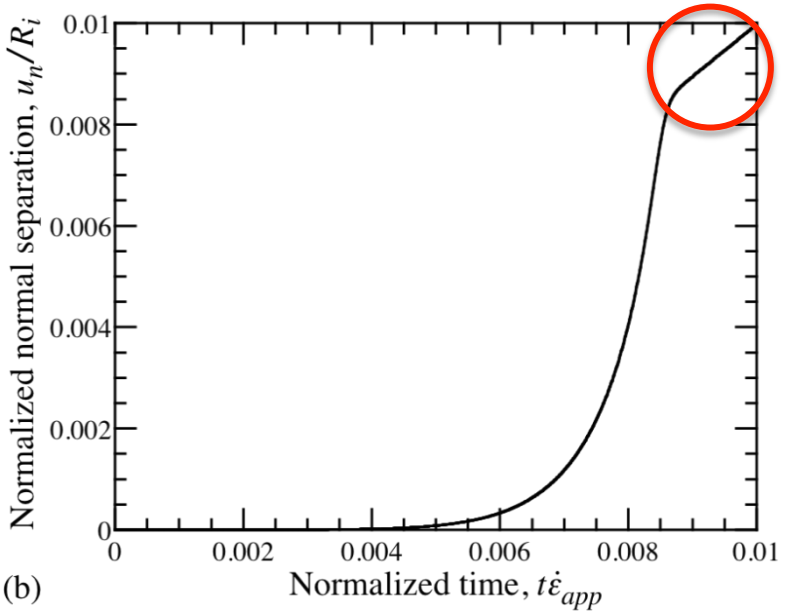
$$\dot{V}_2 = \begin{cases} \pm 2\pi\dot{\varepsilon}_e^c a^3 h(\psi)[\alpha_n \left|\frac{\sigma_m}{\sigma_e}\right| + \beta_n]^n, & \text{for} \pm \frac{\sigma_m}{\sigma_e} > 1 \\ 2\pi\dot{\varepsilon}_e^c a^3 h(\psi)[\alpha_n + \beta_n]^n \frac{\sigma_m}{\sigma_e}, & \text{for} \left|\frac{\sigma_m}{\sigma_e}\right| < 1 \end{cases}$$

where σ_e and σ_m are the average effective stress and mean stress from adjacent grains; and

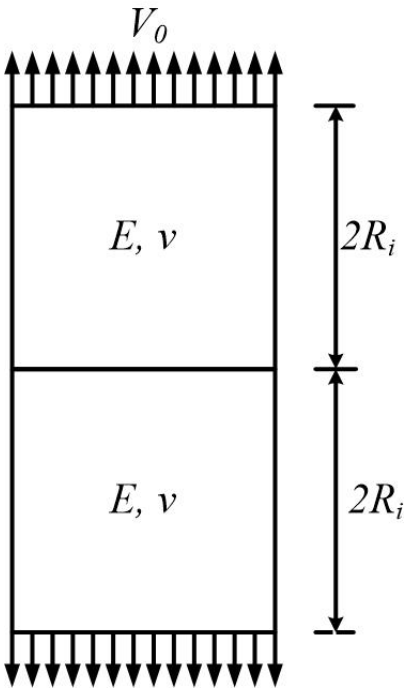
$$\alpha_n = \frac{3}{2n} \quad \beta_n = \frac{(n-1)(n+0.4319)}{n^2}$$

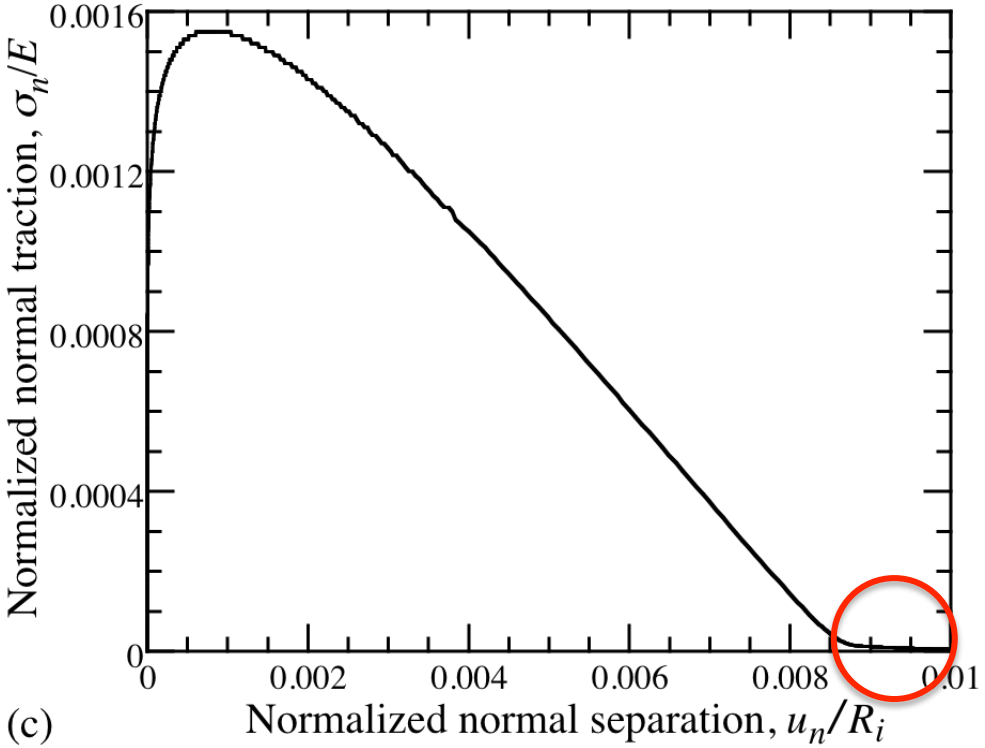

Normalized normal traction, σ_n/E
0.0016
0.0012
0.0008
0.0004
0
0
0.002
0.004
0.006
0.008
0.01
Normalized time, $t\dot{\varepsilon}_{app}$

(a)

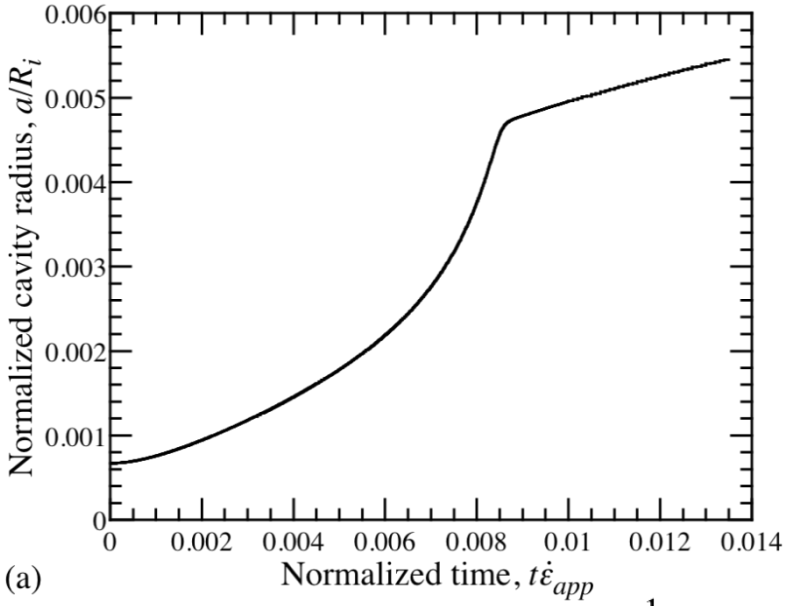

Normalized normal separation, u_n/R_i
0.01
0.008
0.006
0.004
0.002
0
0
0.002
0.004
0.006
0.008
0.01
Normalized time, $t\dot{\varepsilon}_{app}$

(b)

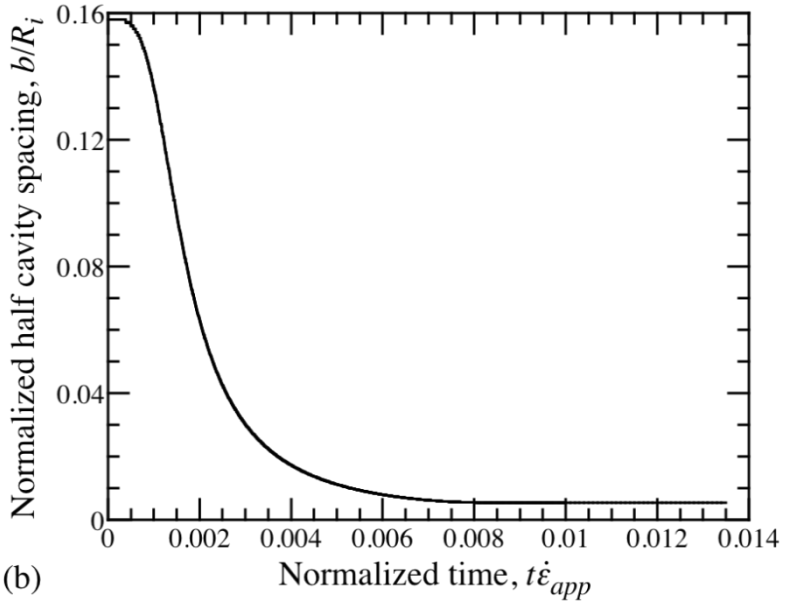

V_0
E, ν
$2R_i$
E, ν
$2R_i$


Normalized normal traction, σ_n/E
0.0016
0.0012
0.0008
0.0004
0
0
0.002
0.004
0.006
0.008
0.01
Normalized normal separation, u_n/R_i

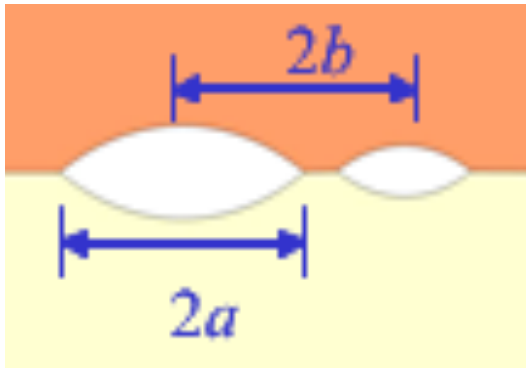
(c)

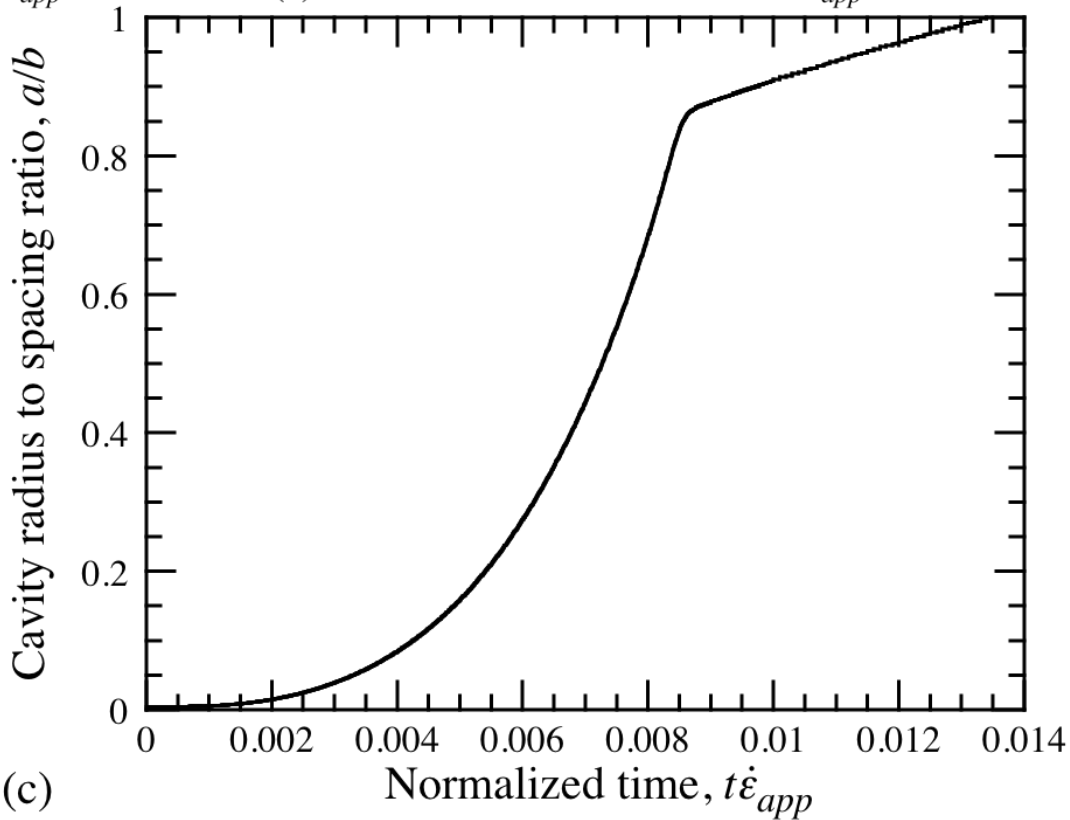

Normalized cavity radius, a/R_i
0.006
0.005
0.004
0.003
0.002
0.001
0
0 0.002 0.004 0.006 0.008 0.01 0.012 0.014
Normalized time, $t\dot{\varepsilon}_{app}$

(a)


Normalized half cavity spacing, b/R_i
0.16
0.12
0.08
0.04
0
0 0.002 0.004 0.006 0.008 0.01 0.012 0.014
Normalized time, $t\dot{\varepsilon}_{app}$

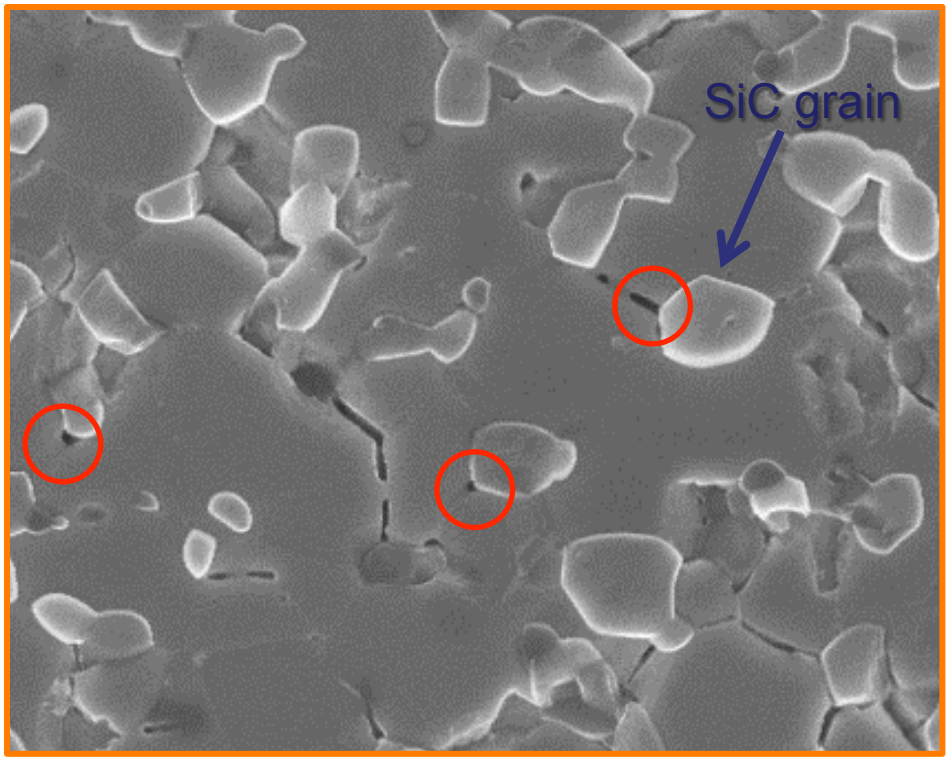
(b)


2b
2a


Cavity radius to spacing ratio, a/b
1
0.8
0.6
0.4
0.2
0
0 0.002 0.004 0.006 0.008 0.01 0.012 0.014
Normalized time, $t\dot{\varepsilon}_{app}$

(c)

Intergranular Fracture: Experimental Observation

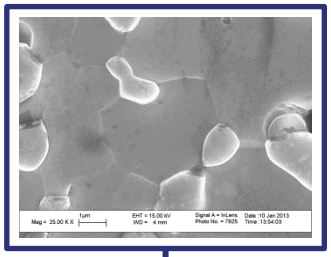


Micrograph at the tension side after creep test at 1700^{o}C

- SiC acts as microstructure anchors and some lead to cavitation but not all.
- SiC remains near constant shape (relatively high rigidity)
- Cavitation is only observed at high temperature region (above 1500^{o}C)
- About 5% cavitation is found at ZrB_2-SiC grain boundary and the rotation angle is less than 3^{o}

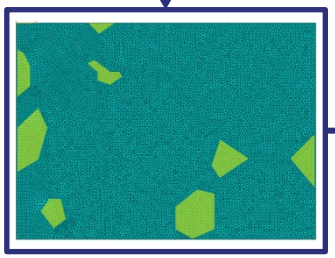
Polycrystalline Model

ZrB_2-SiC composite w/ Grain boundary elements



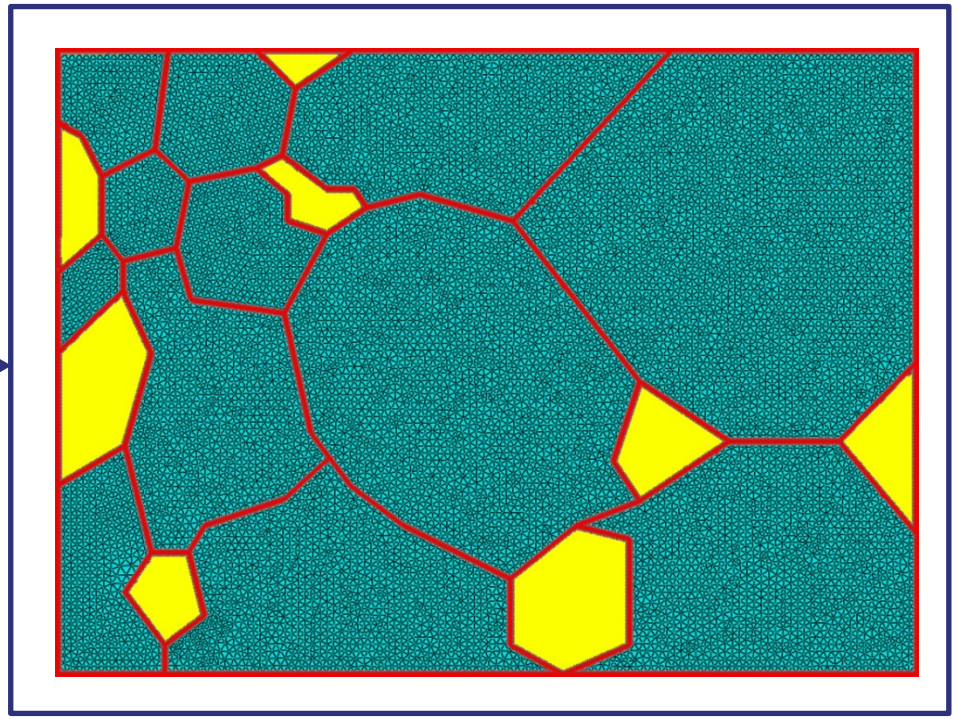
MATLAB image processing

*.py (Python script)

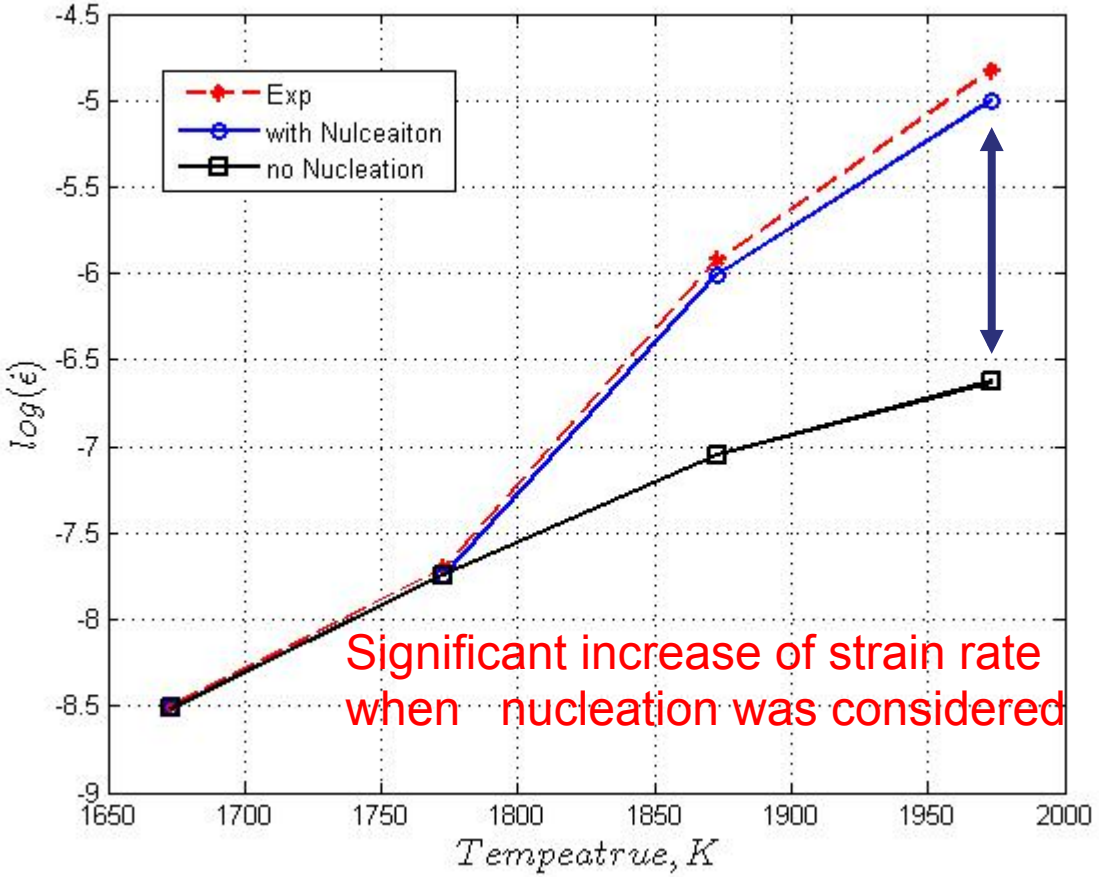


ABAQUS

MATLAB parser

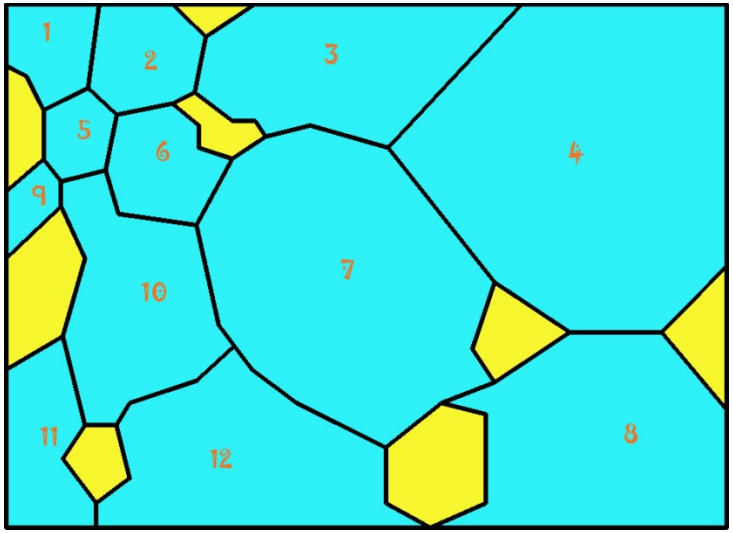


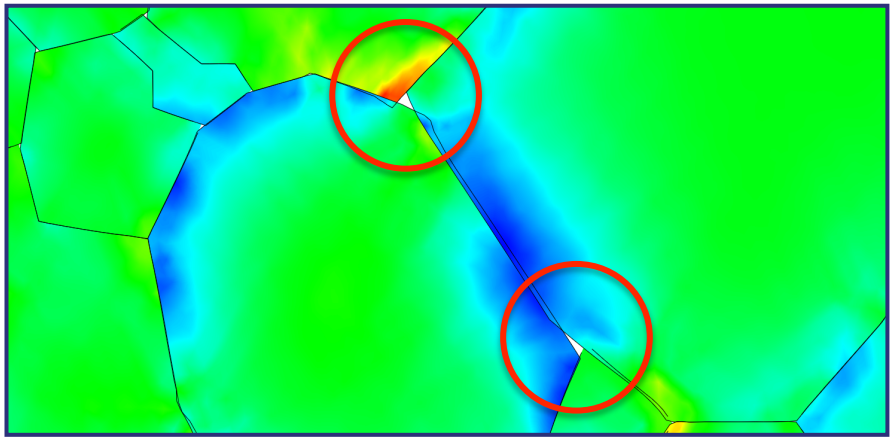
Comparison of Strain Rate



- Simulation results show a significant variation when cavitation nucleation was assigned.
- Simulation with nucleation allowed at ZrB_2-SiC interface show a great agreement with experiment data

Grain Rotation





scale 100 times. Nucleation occurs at ZS grain boundary as softening

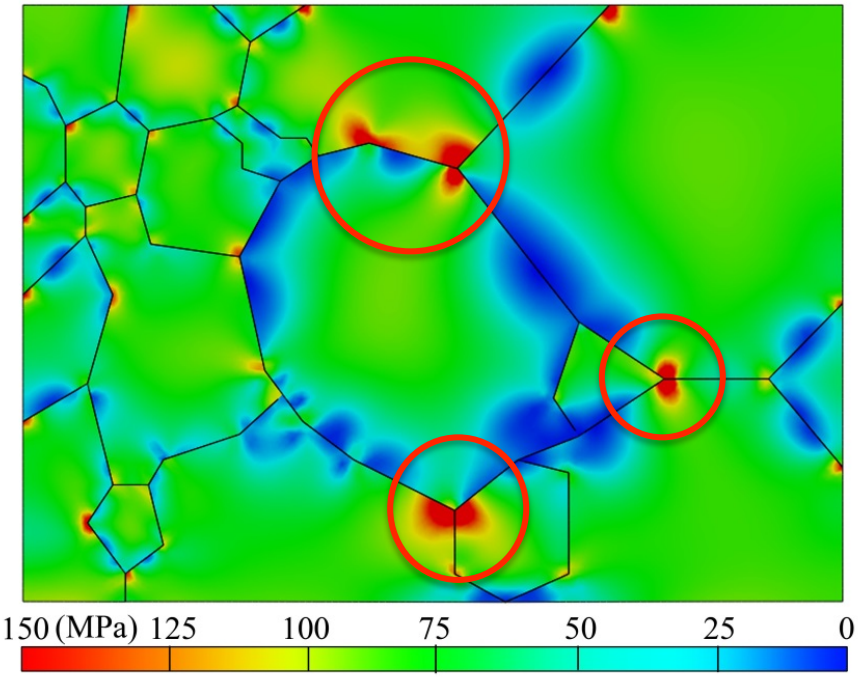
(a) Without nucleation

ID	1	2	3	4	5	6	7	8	9	10	11	12
Angle	0.004	0.008	0.011	0.004	0.015	0.007	0.035	0.008	0.030	0.004	0.003	0.014

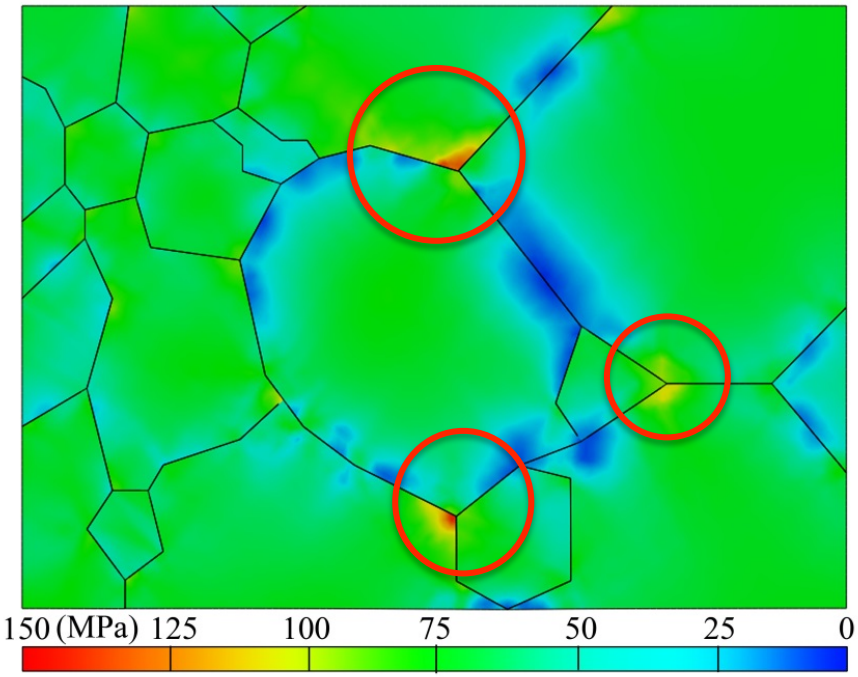
(b) With nucleation @ ZS grain boundary

ID	1	2	3	4	5	6	7	8	9	10	11	12
Angle	0.02	0.17	0.37	0.09	2.14	1.37	2.67	0.13	0.22	0.01	0.04	0.12

Tensile Stress Contour



without nucleation

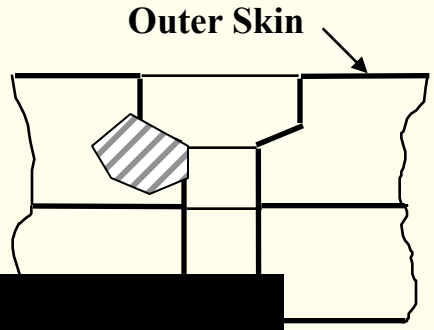


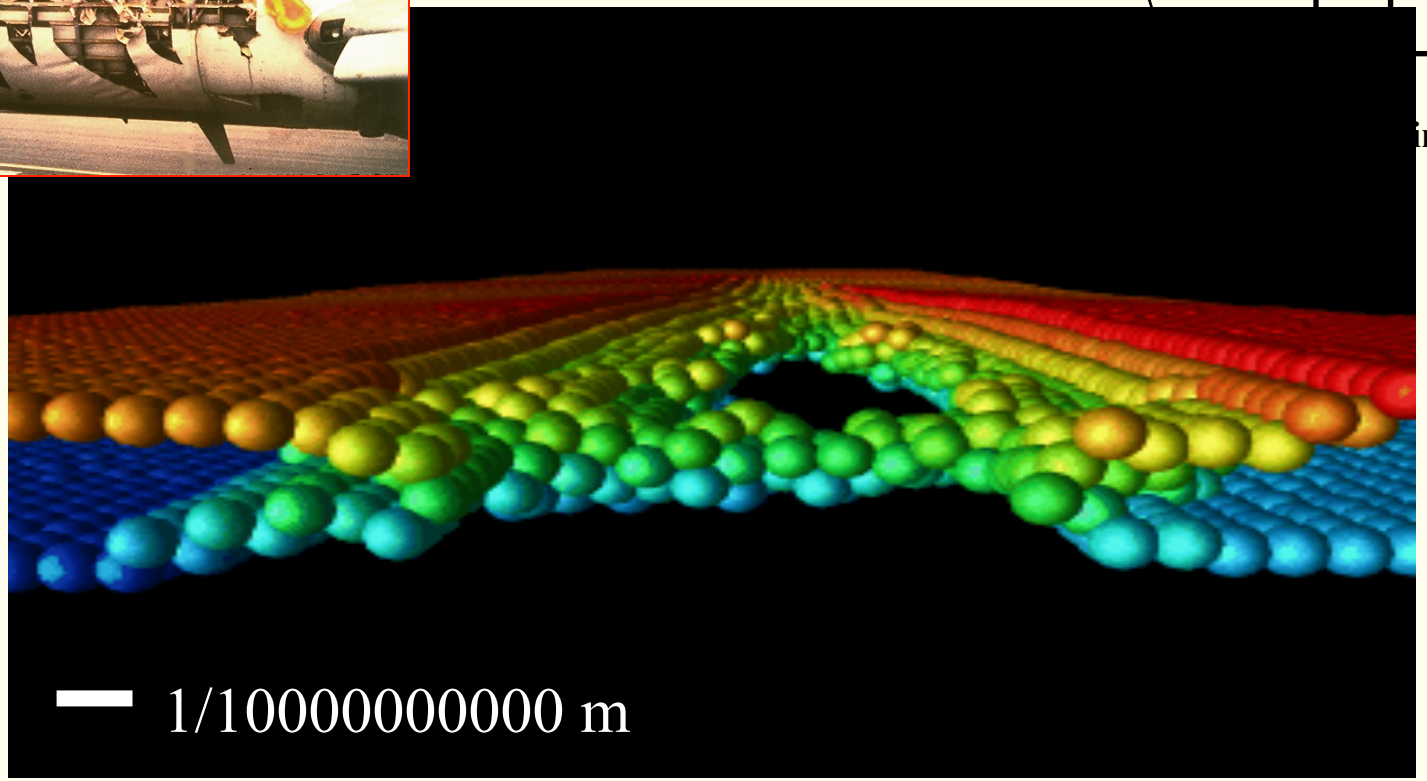
nucleation at ZrB_2-SiC

Severe stress concentration at ZrB_2-SiC grain boundary when nucleation is not allowed.

Fatigue and fracture in metal: from cracks in the rivet holes to voids in grains to dislocation and atomistic fracture

Cracking beneath a rivet





"Crystals are like people, it is the defects in them which tend to make them interesting!"

- Colin Humphreys

From Tony, 1991.12

DAVID (Chuin-Shan) CHEN !!!

THIS IS A PUBLIC THANK YOU
FOR BEING AN **OUTSTANDING**
TA
IN CE 673

STUDENTS AND PROFESSOR
ALIKE APPLAUD YOU
FOR YOUR KNOWLEDGE, CARING,
AND ACCESSIBILITY.

Glorious Ascend (精彩綻放)

Driven and Determine

Achieving one's dream in the most Gracious Manner

Braving all Obstacles with Confidence and

Emerged as a Glorious Winner