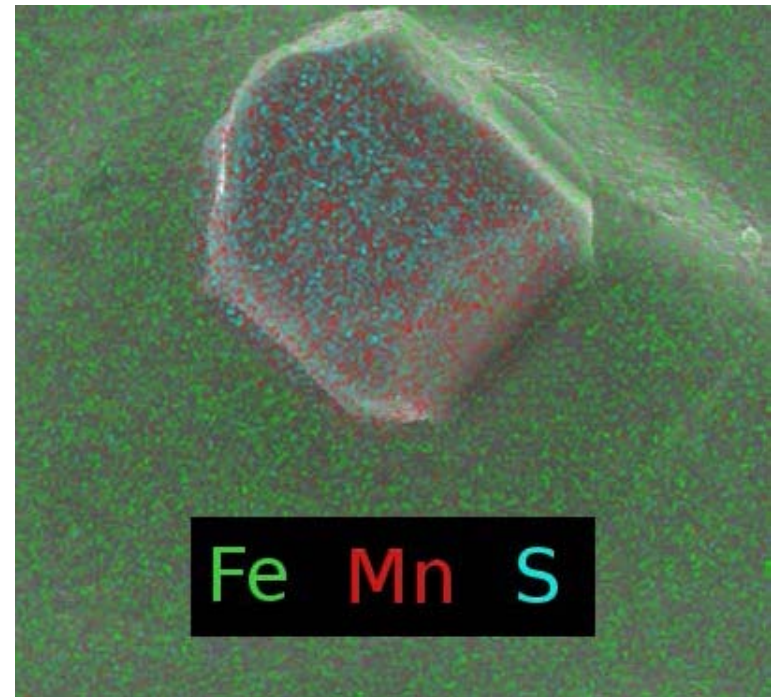


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# A Survey of Crystalline Defects

# Outline – Defects

- 0D Defects
  - Vacancies & Interstitials
- 1D Defects (Dislocations)
- 2D Defects
  - Grain & twin boundaries
- 3D Defects
  - Coherent vs. incoherent inclusions, precipitates



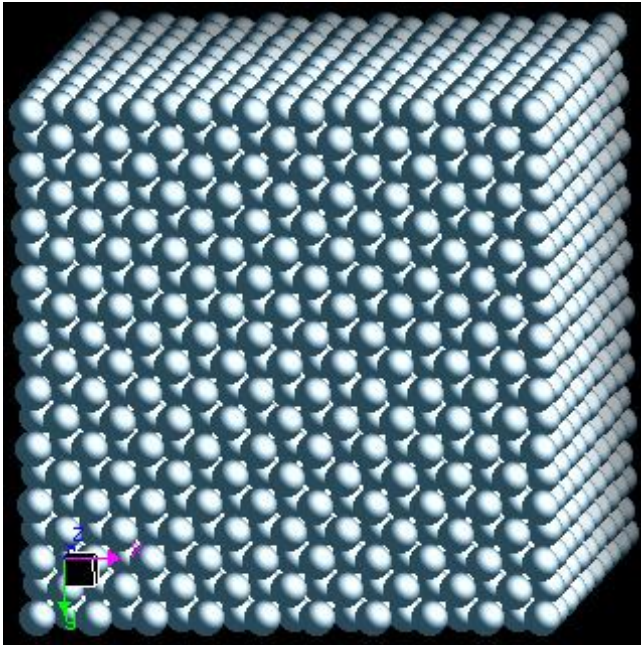
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Single crystal of MnS, space group  $Fm\bar{3}m$ , FCC crystal structure

# Crystalline Solids

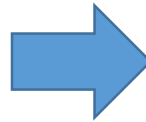
[http://www.webelements.com/calcium/crystal\\_structure.html](http://www.webelements.com/calcium/crystal_structure.html)

- Periodic, long-range ordered structures



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Face centered cubic calcium  
crystal structure



Single crystals of calcium metal  
under kerosene

# Form Follows Structure

[http://www.zkg.de/en/artikel/bildpopup\\_en\\_1698578.html?image=5](http://www.zkg.de/en/artikel/bildpopup_en_1698578.html?image=5)

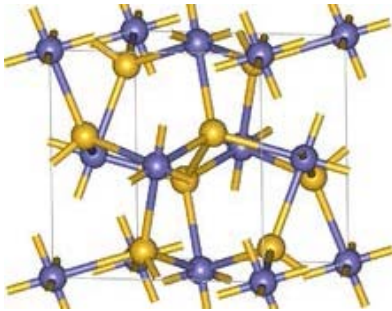
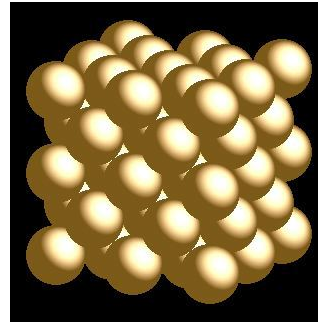
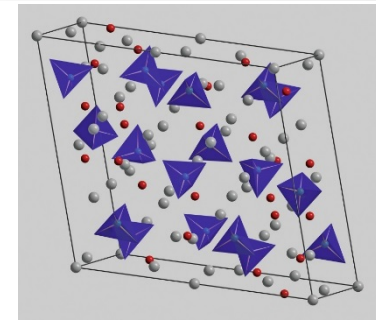


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Courtesy of Mark Winter.  
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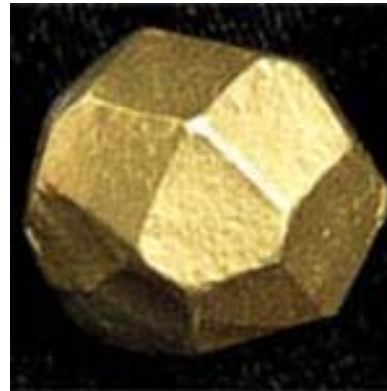
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**Pyrite ( $\text{FeS}_2$ ), simple cubic (SC)**

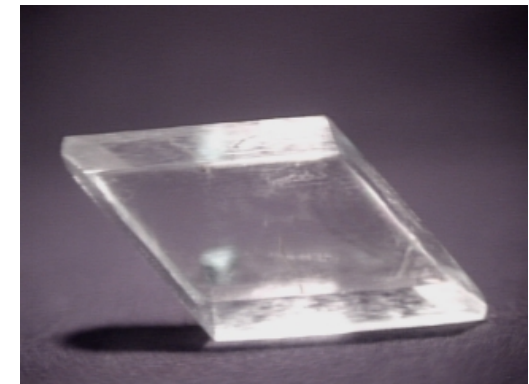
[Wikimedia Commons](#)



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**Gold (Au), face centered cubic (FCC)**

[http://www.palaminerals.com/news\\_2007\\_v2.php](http://www.palaminerals.com/news_2007_v2.php)



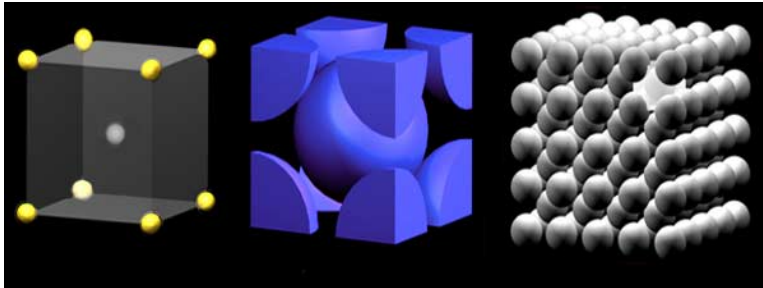
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**Gypsum, monoclinic**

<http://www.galleries.com/minerals/symmetry/monoclin.htm>

# Grain vs. Crystal Structure

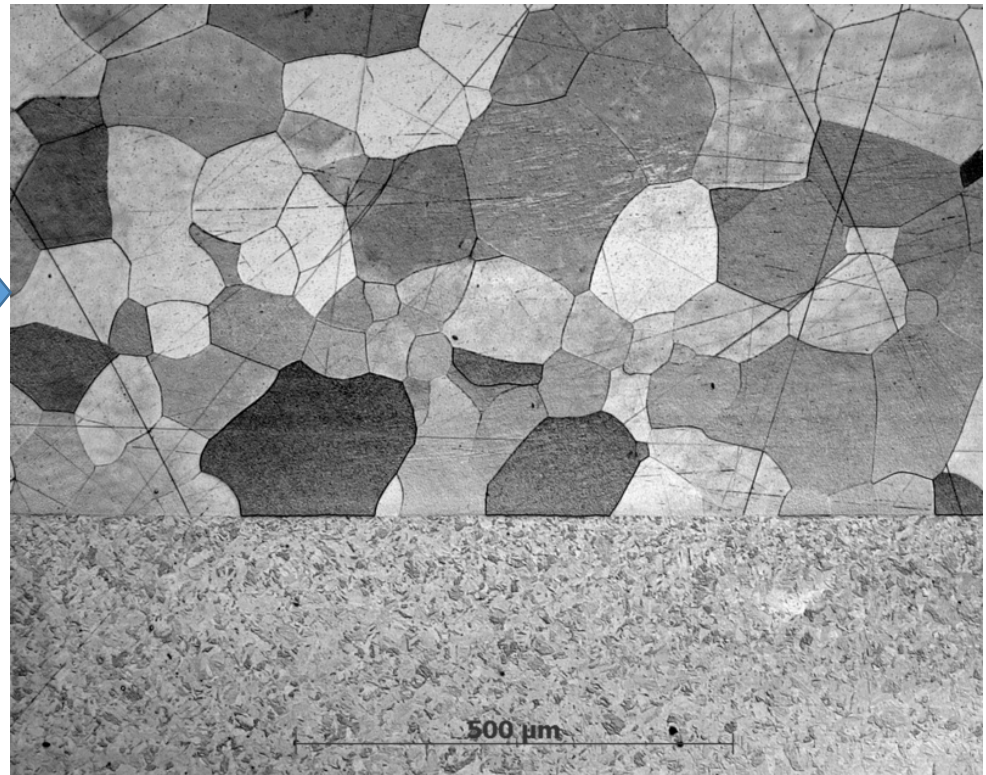
- Why do grains look more spherical, when crystal structures are cubic?



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<https://www.nde-ed.org/EducationResources/CommunityCollege/Materials/Graphics/CrystalStructure/BCC.jpg>

Body centered cubic (BCC) iron crystal structure (left), micrograph of Fe-12Cr-2Si (right)

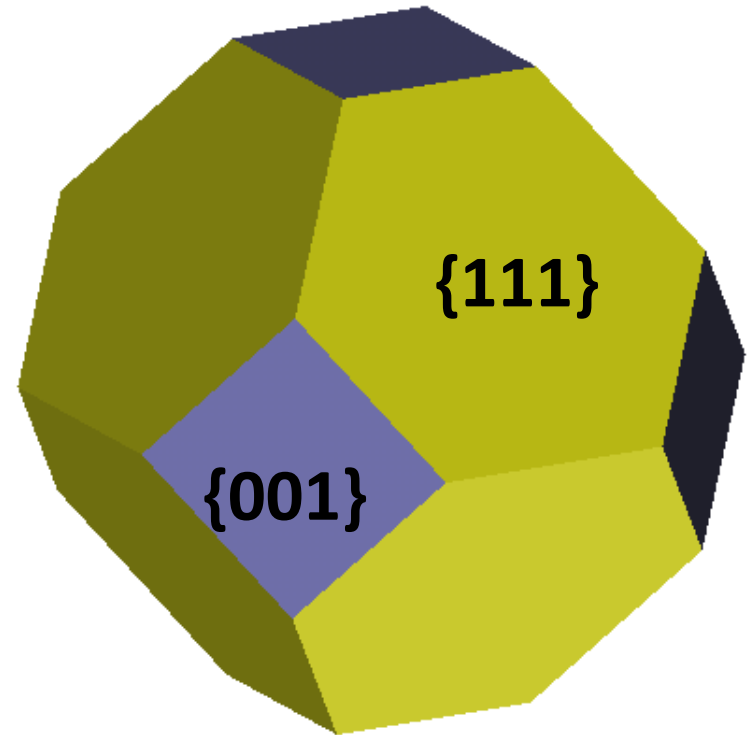


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# Grain vs. Crystal Structure

---

- Wulff crystals describe *lowest energy* surfaces
- Exposing *close packed planes* lowers surface energy

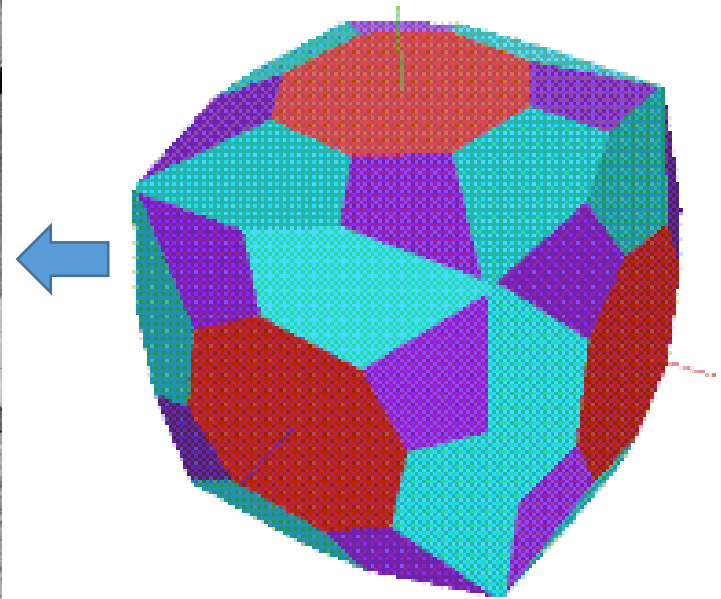
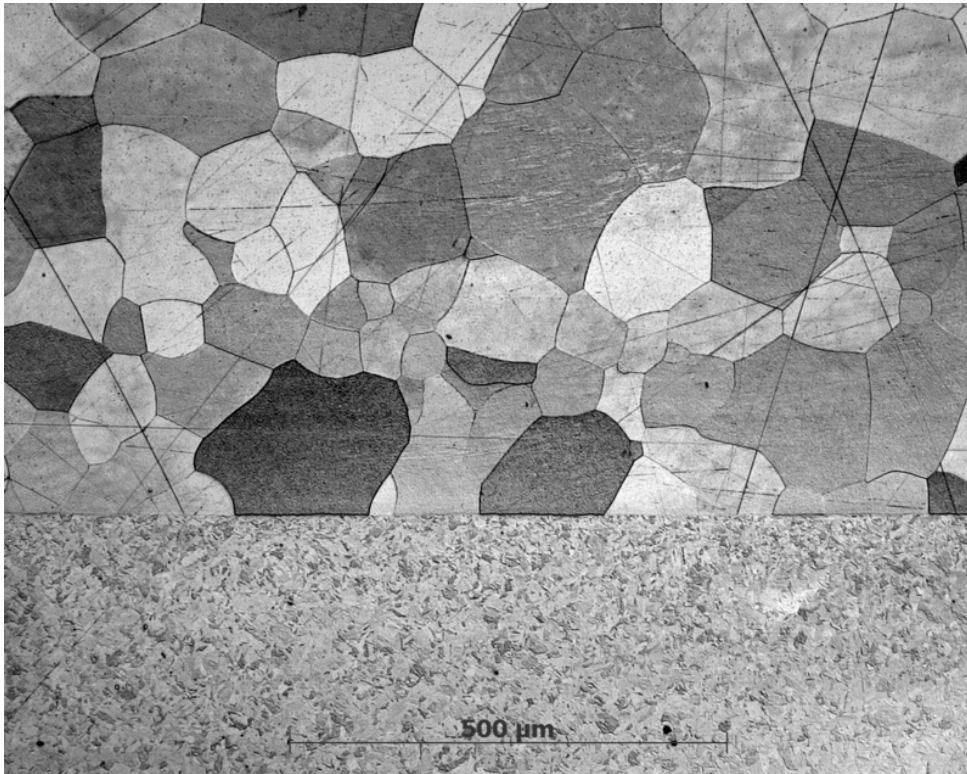


This image is in the public domain.

<http://www.ctcms.nist.gov/wulffman/examples.html>

# Grain vs. Crystal Structure

- We see 2D slices of Wulff crystals as grains!



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<http://www.ctcms.nist.gov/wulffman/examples.html>

# Point Defects (0D) – Vacancies

---

Was, p. 163

[Was, Gary S. *Fundamentals of Radiation Materials Science*, p. 163.  
ISBN: 9783540494713.] removed due to copyright restrictions.



# Point Defects (0D) – Multiple Vacancies

Was, p. 163

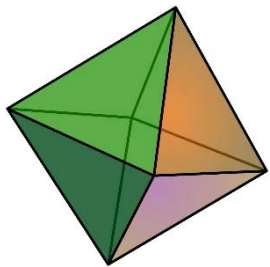
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[Was, Gary S. *Fundamentals of Radiation Materials Science*, p. 163.  
ISBN: 9783540494713.] removed due to copyright restrictions.

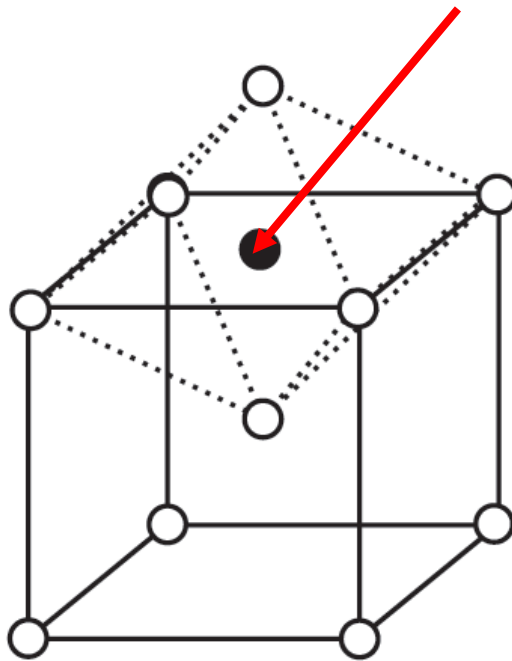
# Point Defects (0D) – Interstitials

Was, p. 157

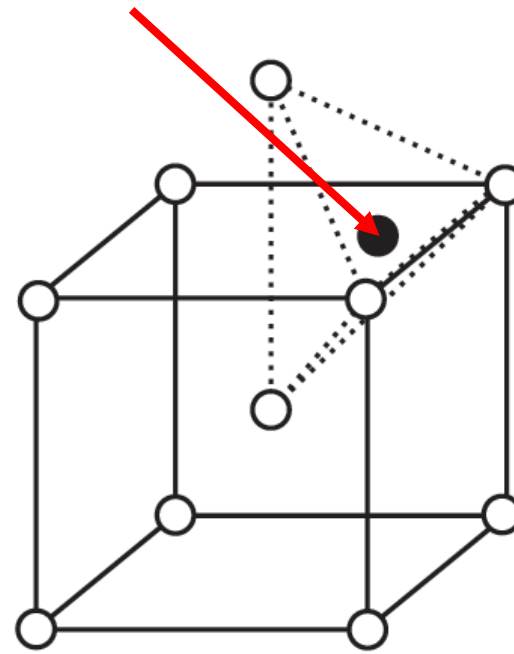
- Extra atoms shoved into the crystal lattice



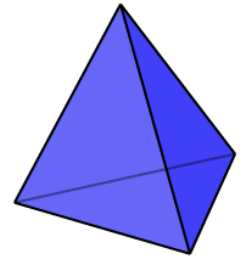
Octahedron



Octahedral interstitial in BCC lattice



Tetrahedral interstitial in BCC lattice



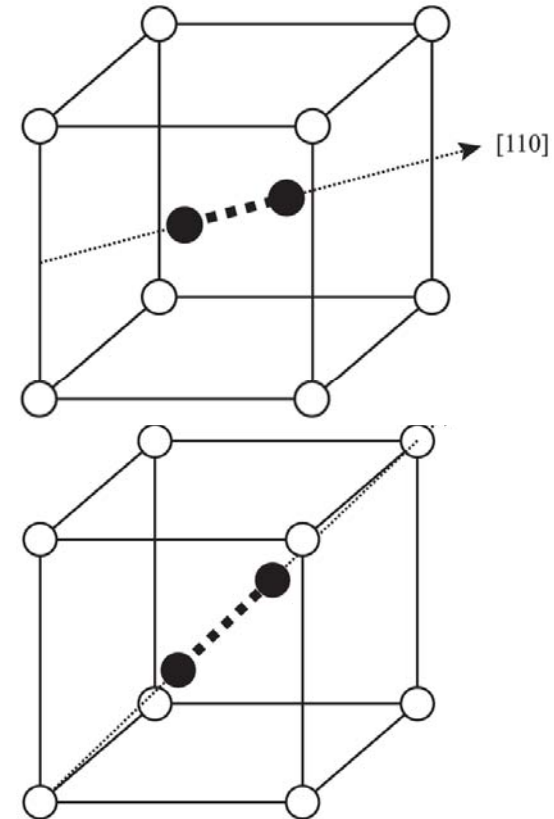
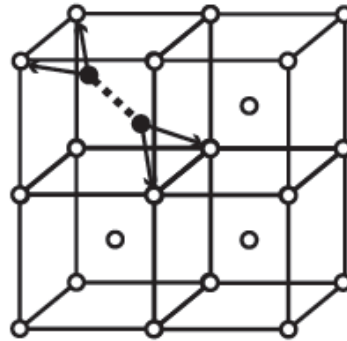
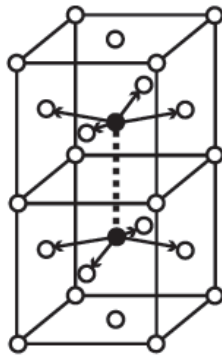
Tetrahedron

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# Point Defects (0D) – Split Interstitials

Was, p. 159

- Dumbbells are often lower energy configurations
- Also much easier to diffuse
  - One interstitial can “knock” the other in their common direction
  - Lower distance to movement



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# Point Defect Energies

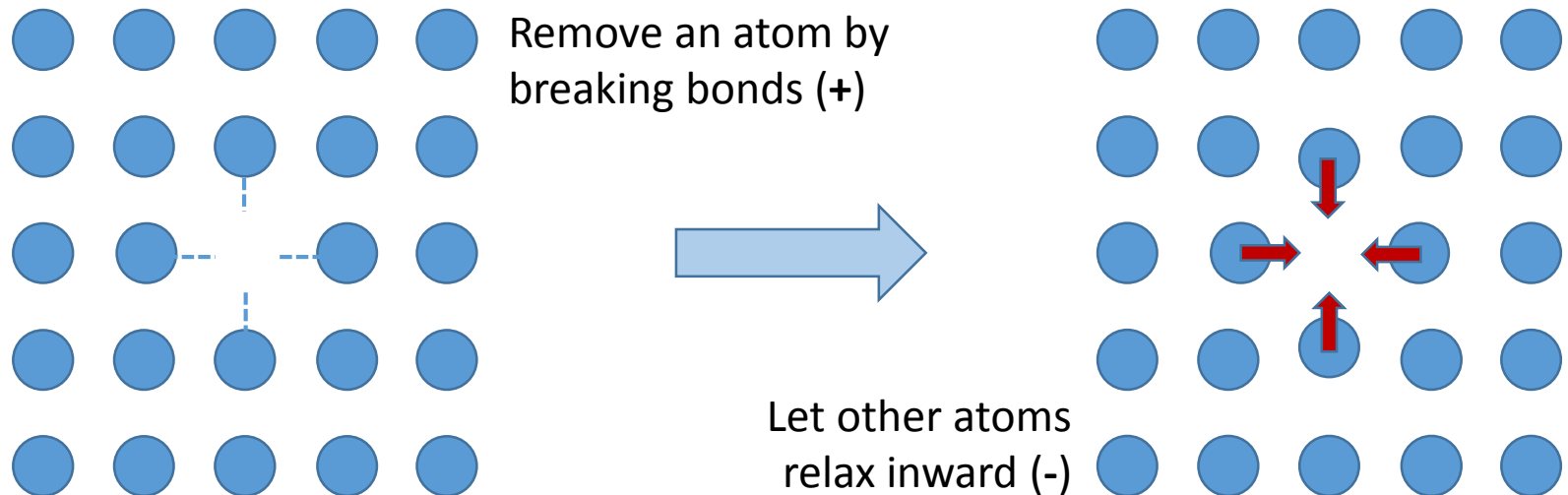
Was, p. 160

	Symbol	Unit	Al	Cu	Pt	Mo	W
<b>Interstitials</b> <b>Harder to make, easier to move</b>							
Relaxation volume	$V_{relax}^i$	Atomic vol.	1.9	1.4	2.0	1.1	
Formation energy	$E_f^i$	eV	3.2	2.2	3.5		
Equilibrium concentration at $T_m^*$	$C_i(T_m)$	–	$10^{-18}$	$10^{-7}$	$10^{-6}$		
Migration energy	$E_m^i$	eV	0.12	0.12	0.06		0.054
<b>Vacancies</b> <b>Easier to make, harder to move</b>							
Relaxation volume	$V_{relax}^v$	Atomic vol.	0.05	–0.2	–0.4		
Formation energy	$E_f^v$	eV	0.66	1.27	1.51	3.2	3.8
Formation entropy	$S_f^v$	k	0.7	2.4			2
Equilibrium concentration at $T_m^*$	$C_v(T_m)$	–	$9 \times 10^{-6}$	$2 \times 10^{-6}$			$4 \times 10^{-5}$
Migration energy	$E_m^v$	eV	0.62	0.8	1.43	1.3	1.8
Activation energy for self-diffusion	$Q_{vSD}$	eV $Q_a$	1.28	2.07	2.9	4.5	5.7

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# Point Defect Energetics

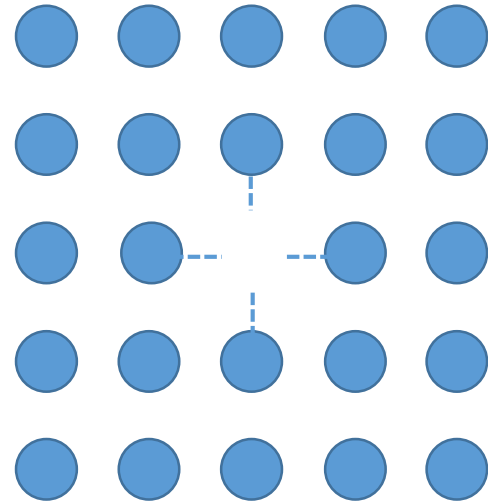
- How much energy to make a vacancy?



# Point Defect Energetics

- How much energy to make a vacancy?
- Fe-Fe bond dissociation energy:  
$$118 \frac{\text{kJ}}{\text{mol}} = 1.22\text{eV} [1]$$
  - Fe-Fe cluster calculations give  
0.64eV [2]
- Z=8 in BCC Fe: 5.12 – 9.76eV

Remove an atom by  
breaking bonds (+)

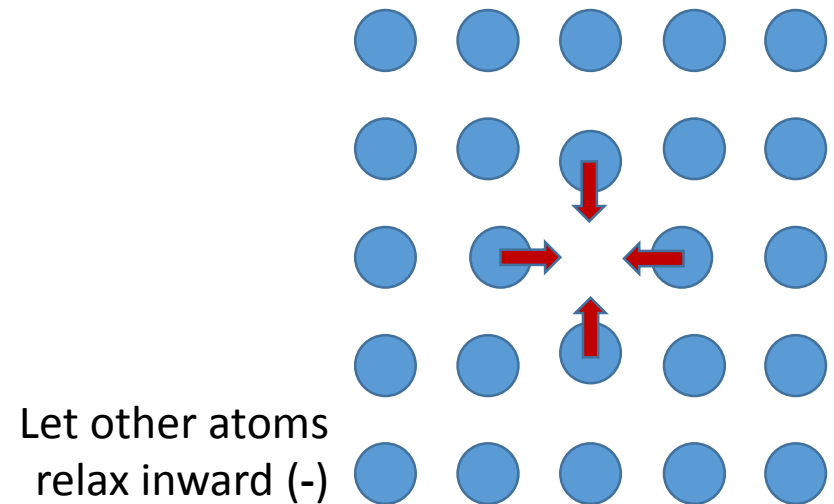


[1] Y-R Luo. "Bond Dissociation Energies." CRC Handbook (2009)

[2] T. Nakazawa, T. Igarashi, T. Tsuru, Y. Kaji, *Comp. Mater. Sci.*, 46(2):367-375 (2009)

# Point Defect Energetics

- $Z=8$  in BCC Fe:  
 $5.12 [2] - 9.76 [1] eV$
- Molecular dynamics (MD) calculations [3] show:  
 $E_{Vacancy} = 1.83 eV$
- Difference due to crystal relaxation



[1] Y-R Luo. "Bond Dissociation Energies." CRC Handbook (2009)

[2] T. Nakazawa, T. Igarashi, T. Tsuru, Y. Kaji, *Comp. Mater. Sci.*, 46(2):367-375 (2009)

[3] B. D. Wirth et al. *J. Nucl. Mater.*, 244:185:194 (1997)

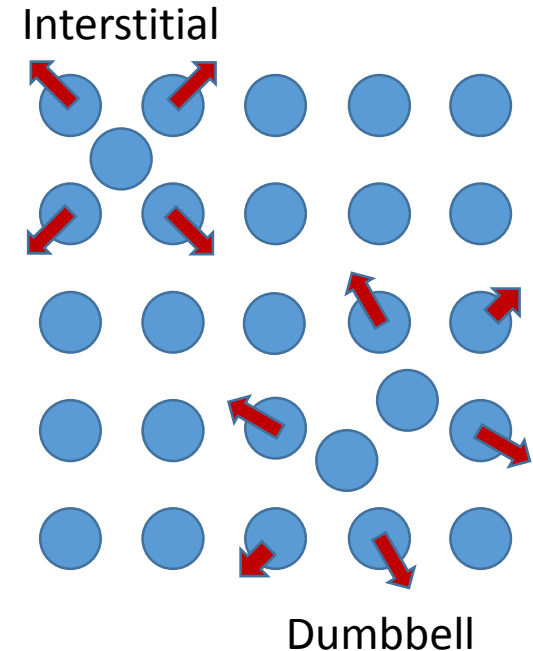
# Point Defect Energetics

- Which interstitial is most stable?

Relaxed structure and formation properties of point-defects in  $\alpha$ -iron <sup>21</sup>

Defect	Atomic positions (a)	Formation energy (eV)	Formation volume ( $\Omega$ )
< 110 > dumbbell	(0.245, 0.245, 0.5) (0.755, 0.755, 0.5)	4.76	1.43
< 111 > dumbbell	(0.291, 0.291, 0.291) (0.709, 0.709, 0.709)	4.87	1.74
< 111 > crowdion	(0.331, 0.331, 0.331) (0.749, 0.749, 0.749) (1.167, 1.167, 1.167)	4.91	1.77
vacancy		1.83	0.93

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 Source: Wirth, B. D., et al. "Energetics of Formation and Migration of Self-interstitials and Self-interstitial Clusters in  $\alpha$ -iron." *Journal of Nuclear Materials* 244, no. 3 (1997): 185-94.



B. D. Wirth et al. *J. Nucl. Mater.*, 244:185:194 (1997)

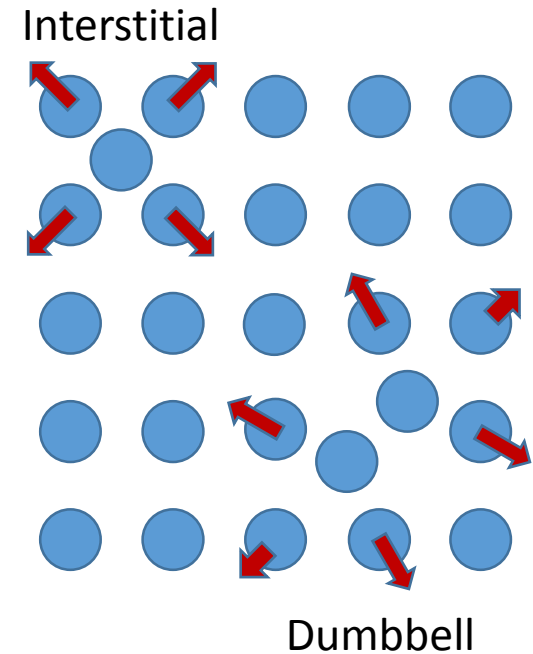


# Point Defect Energetics

- Which interstitial is most stable?

Relaxed structure and formation properties of point-defects in  $\alpha$ -iron <sup>31</sup>

Defect	Atomic positions (a)	Formation energy (eV)	Formation volume ( $\Omega$ )
< 110 > dumbbell	(0.245, 0.245, 0.5) (0.755, 0.755, 0.5)	4.76	1.43
< 111 > dumbbell	(0.291, 0.291, 0.291) (0.709, 0.709, 0.709)	4.87	1.74
< 111 > crowdion	(0.331, 0.331, 0.331) (0.749, 0.749, 0.749) (1.167, 1.167, 1.167)	4.91	1.77



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 Source: Wirth, B. D., et al. "Energetics of Formation and Migration of Self-interstitials and Self-interstitial Clusters in  $\alpha$ -iron." *Journal of Nuclear Materials* 244, no. 3 (1997): 185-94.

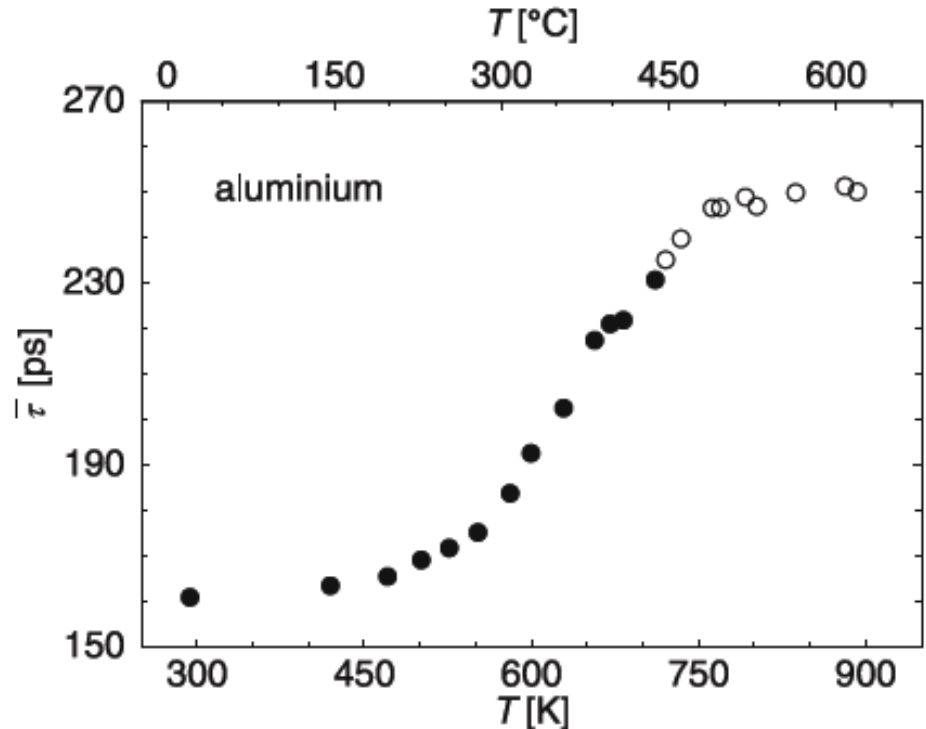
B. D. Wirth et al. *J. Nucl. Mater.*, 244:185:194 (1997)

- Does it matter?

# Direct Measurement of $C_{1V}^{eq}$

Mehrer, p. 78

- Positron annihilation spectroscopy (PAS)
  - Shoot positrons into material, they annihilate very quickly with local electrons
  - Positrons can bind to vacancy, which has a reduced electron cloud
  - Lasts longer!



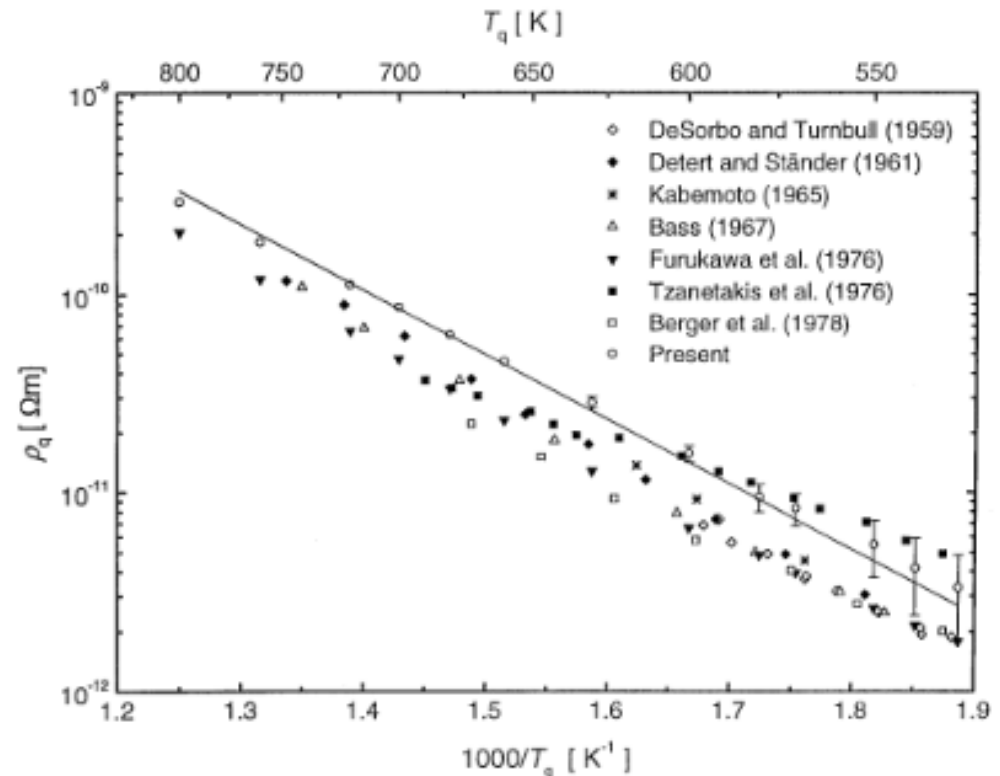
Mean positron lifetime in aluminum

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# Direct Measurement of $C_{1V}^{eq}$

A. Khellaf et al., Mater. Trans. 43(2):186 (2002)

- Quenching resistance measurements
  - Heat material to high temperature, quench, measure resistivity
  - Resistivity directly proportional to vacancy concentration
  - Measured at liquid-He temperature



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# Dislocations (1D)

Was, p. 268

---

- Extra half-plane of atoms shoved into the lattice
- Two types: **Edge & Screw**

[Fig. 7.2 in p. 268 from Was, Gary S. *Fundamentals of Radiation Materials Science*, ISBN: 9783540494713] removed due to copyright restrictions.

# Dislocations (1D)

Was, p. 268

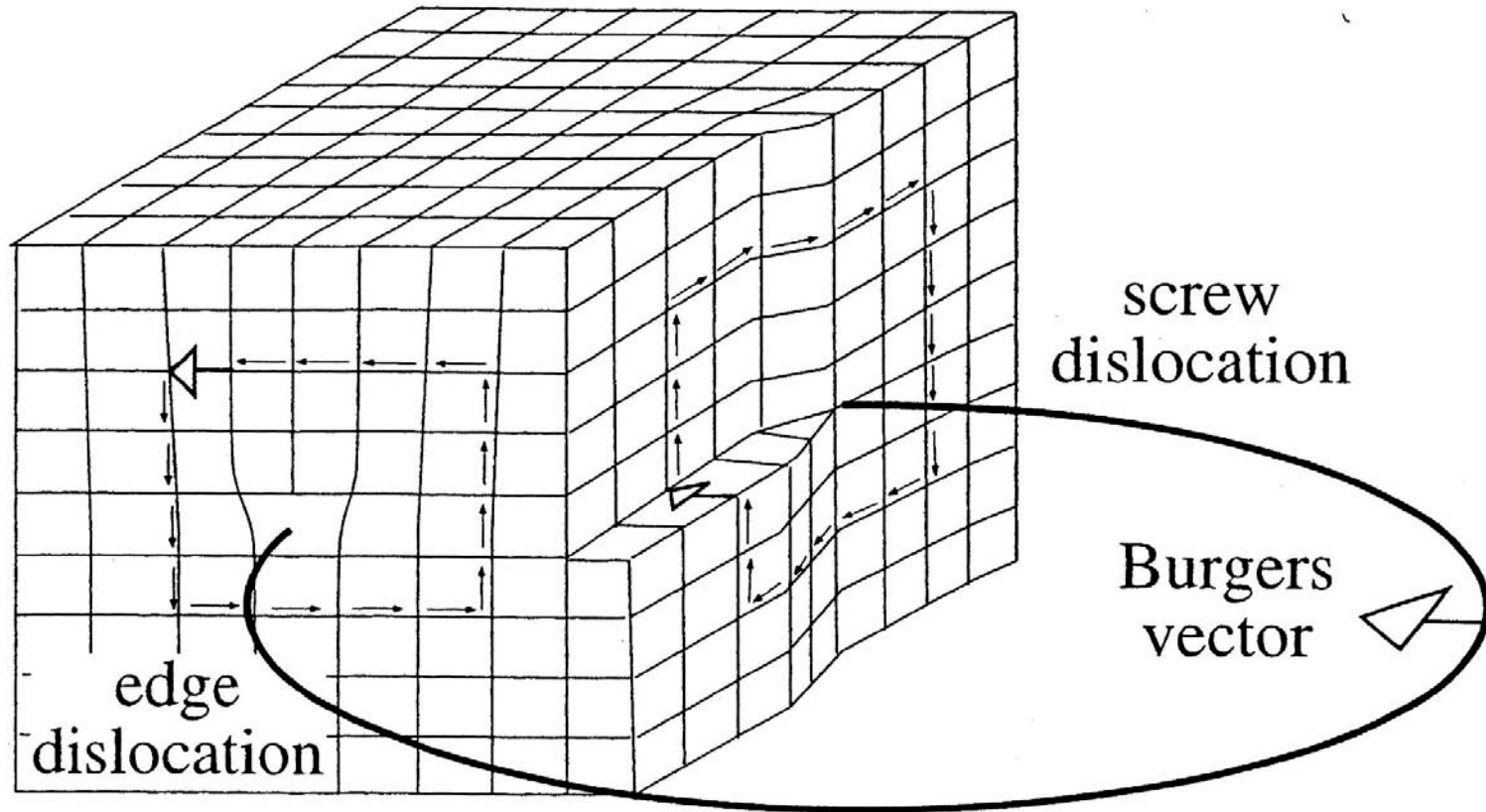
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- Extra half-plane of atoms shoved into the lattice
- Two types: Edge & Screw

[Fig. 7.3 in p. 268 from Was, Gary S. *Fundamentals of Radiation Materials Science*, ISBN: 9783540494713] removed due to copyright restrictions.

# Edge vs. Screw Dislocations

Passchier and Trouw, "Microtectonics," p. 33 (2005)

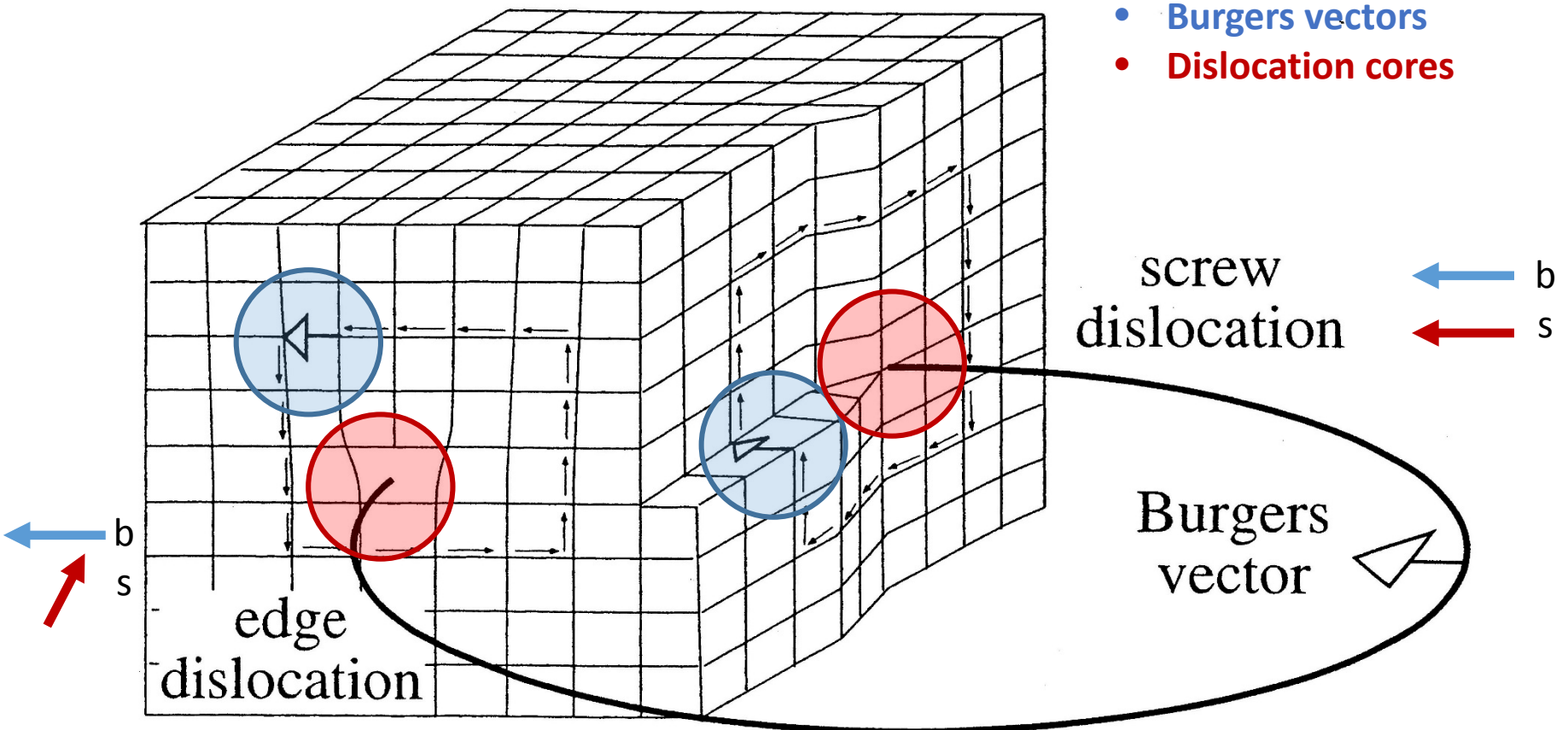


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# Edge vs. Screw Dislocations

Passchier and Trouw, "Microtectonics," p. 33 (2005)

- Burgers vectors
- Dislocation cores

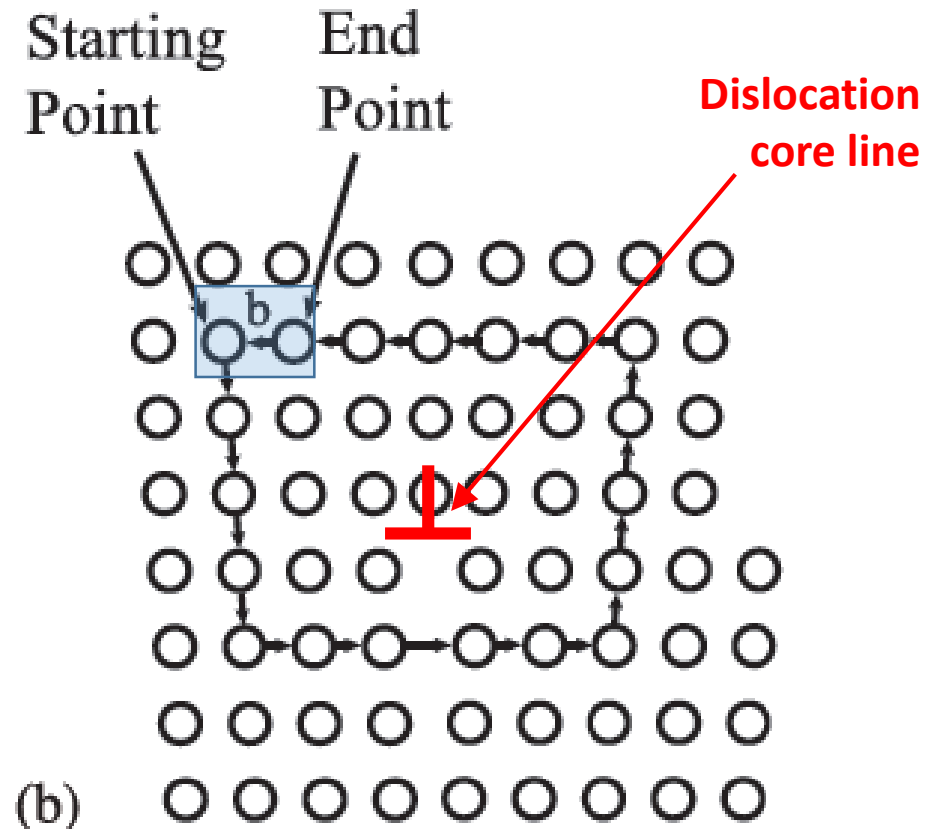


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# The Burgers Vector

Was, p. 275

- Start at one atom, make a circle around the dislocation core
- The *Burgers Vector* is the direction you move to reach your starting point
- Example: Edge disloc.



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# Dislocation Glide

Was, p. 272

---

- Movement one plane at a time along the slip direction

[Fig. 7.8 in p. 272 from Was, Gary S. *Fundamentals of Radiation Materials Science*, ISBN: 9783540494713] removed due to copyright restrictions.

# Edge Dislocation Glide

---



A video is played in class to demonstrate the concept.

<http://youtu.be/kk2oOxSDQ7U>

# Dislocation Glide

---

- Movement one plane at a time along the slip direction

[Fig. 7.9 from Was, Gary S. *Fundamentals of Radiation Materials Science*. ISBN: 9783540494713] removed due to copyright restrictions.

# Dislocation Climb

Was, p. 273

---

- Vacancy diffusion to dislocation core
  - Vacancies are attracted to the compressive stress at core

[Fig. 7.12 in p. 273 from Was, Gary S. *Fundamentals of Radiation Materials Science*, ISBN: 9783540494713] removed due to copyright restrictions.

# Dislocation Kinks, Jogs

Allen, "Kinetics of Materials," p. 116

- Dislocations preferentially move on slip systems
  - Certain directions of easier movement
  - Close packed planes slip in close packed directions

Crystal structure	Slip plane	Slip direction	Number of nonparallel planes	Slip directions per plane	Number of slip systems
Face-centered cubic	{111}	$\langle 1\bar{1}0 \rangle$	4	3	12 = (4 × 3)
Body-centered cubic*	{110}	$\langle \bar{1}11 \rangle$	6	2	12 = (6 × 2)
	{112}	$\langle 11\bar{1} \rangle$	12	1	12 = (12 × 1)
	{123}	$\langle 11\bar{1} \rangle$	24	1	24 = (24 × 1)
Hexagonal close-packed†	{0001}	$\langle 11\bar{2}0 \rangle$	1	3	3 = (1 × 3)
	{10 $\bar{1}$ 0}	$\langle 11\bar{2}0 \rangle$	3	1	3 = (3 × 1)
	{10 $\bar{1}$ 1}	$\langle 11\bar{2}0 \rangle$	6	1	6 = (6 × 1)

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# Dislocation Motion

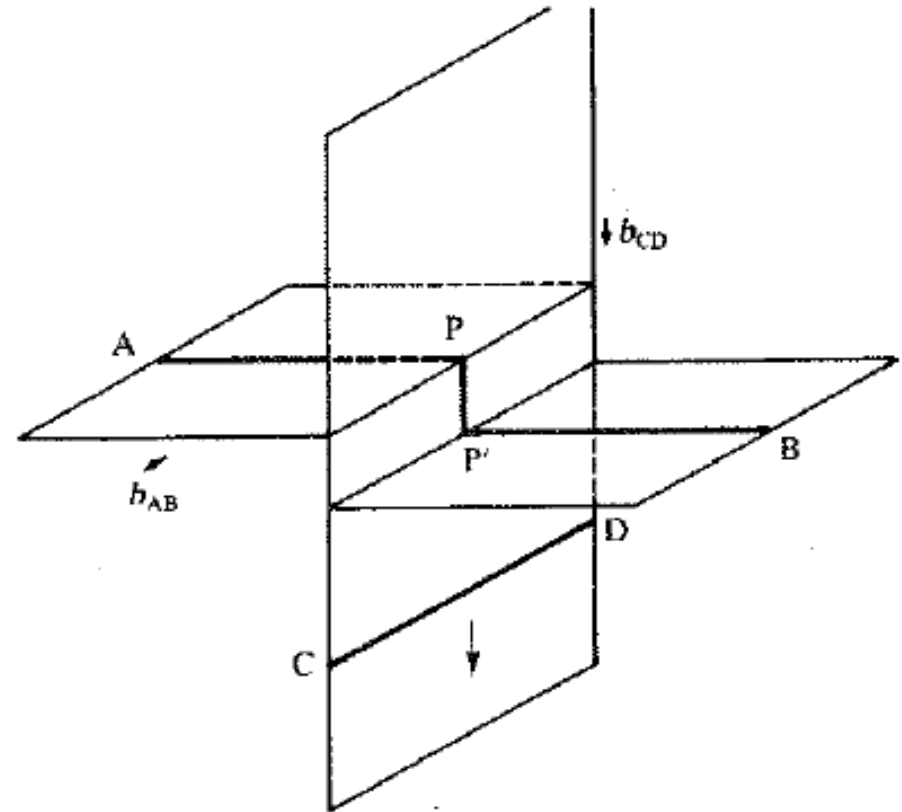
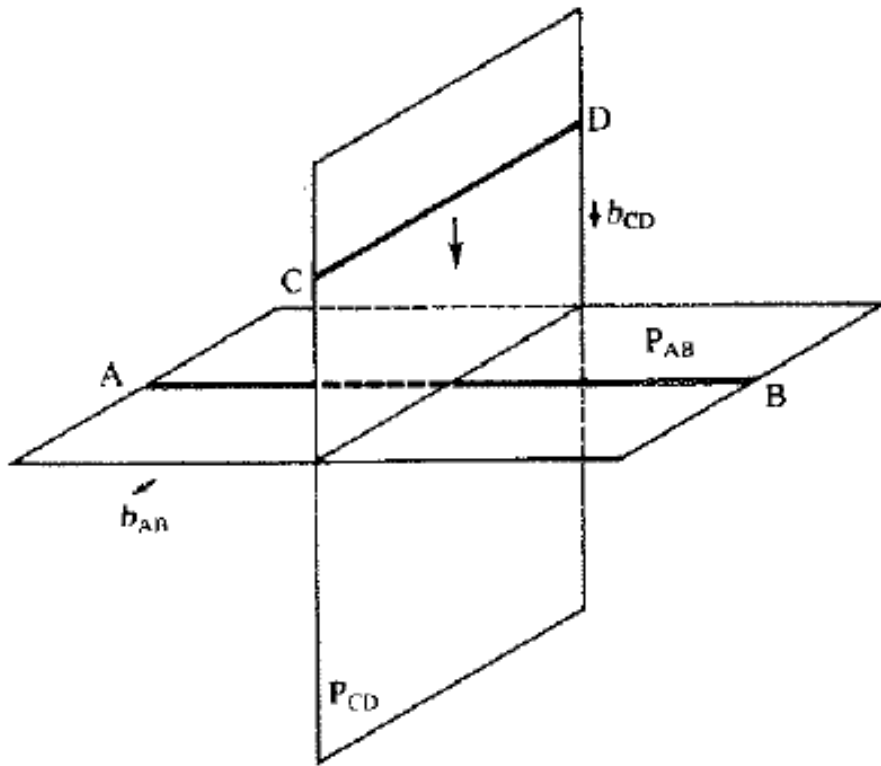
Was, p. 277

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[Fig. 7.18 in p. 277 from Was, Gary S. *Fundamentals of Radiation Materials Science*, ISBN: 9783540494713] removed due to copyright restrictions.

# Glissile vs. Sessile Sections

Allen, "Kinetics of Materials," p. 124

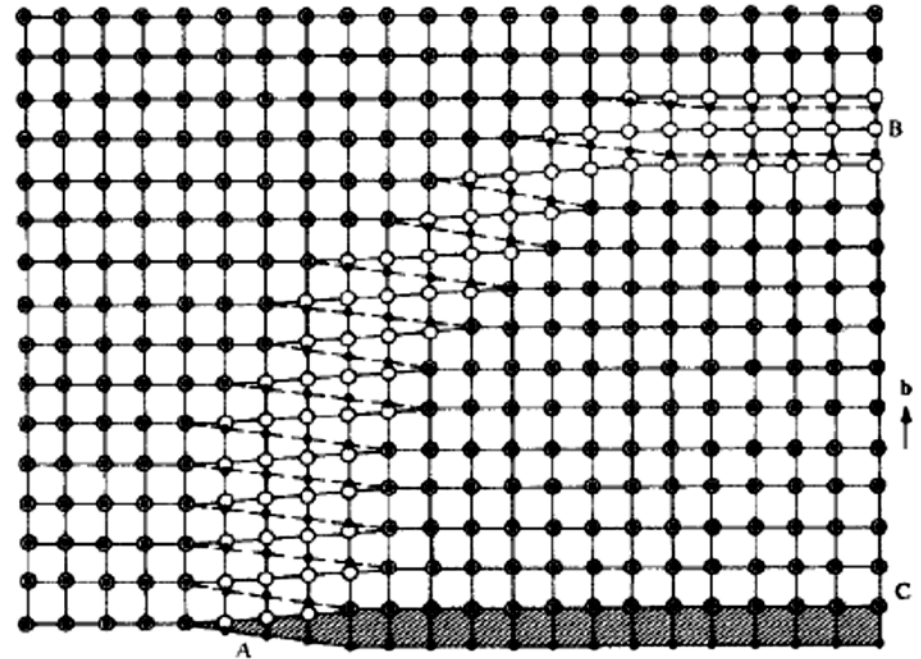
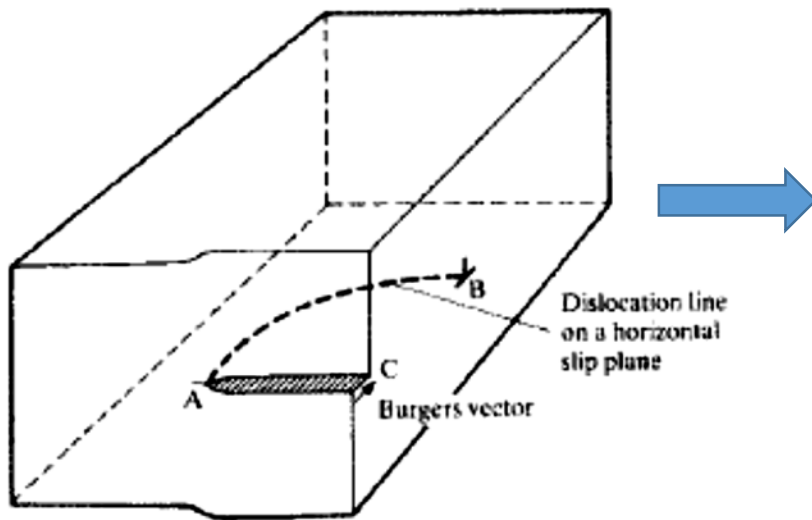


Two edge dislocations moving towards each other form a *sessile* jog

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# Dislocation Loops

- Loops have mixed edge/screw character
  - May be circular planes of atoms between two planes

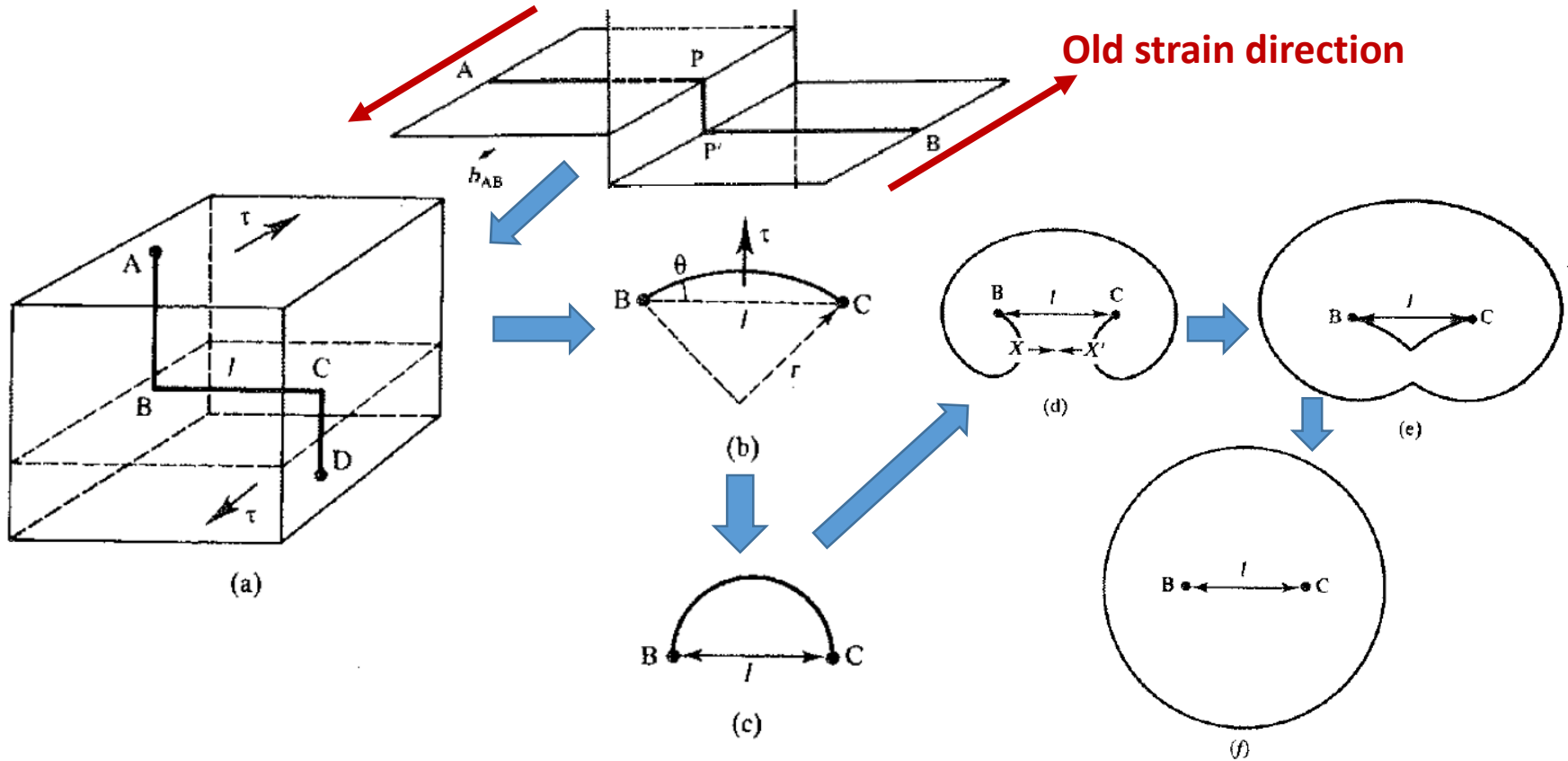


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# Dislocation Loop Sources

- Come from sessile sections of dislocations



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# Dislocation Videos!

<http://www.numodis.fr/tridis/TEM/mechanisms/multiplication.html>

---



**Dislocation sources in Mo-5Nb**

A video is played in class to demonstrate the concept.

# Dislocation Videos!

<http://www.numodis.fr/tridis/TEM/mechanisms/multiplication.html>

---



**A Frank-Read Source in Silicon** A video is played in class to demonstrate the concept.

# Dislocation Videos!

<http://www.numodis.fr/tridis/TEM/mechanisms/multiplication.html>

---



**Dislocation source in Ge at high temperature**

A video is played in class to demonstrate the concept.

# Dislocation Videos!

<http://www.numodis.fr/tridis/TEM/mechanisms/multiplication.html>

---



**Dislocation sources and pileup in Ge**

A video is played in class to demonstrate the concept.

# Dislocation Videos!

<http://www.numodis.fr/tridis/TEM/mechanisms/multiplication.html>

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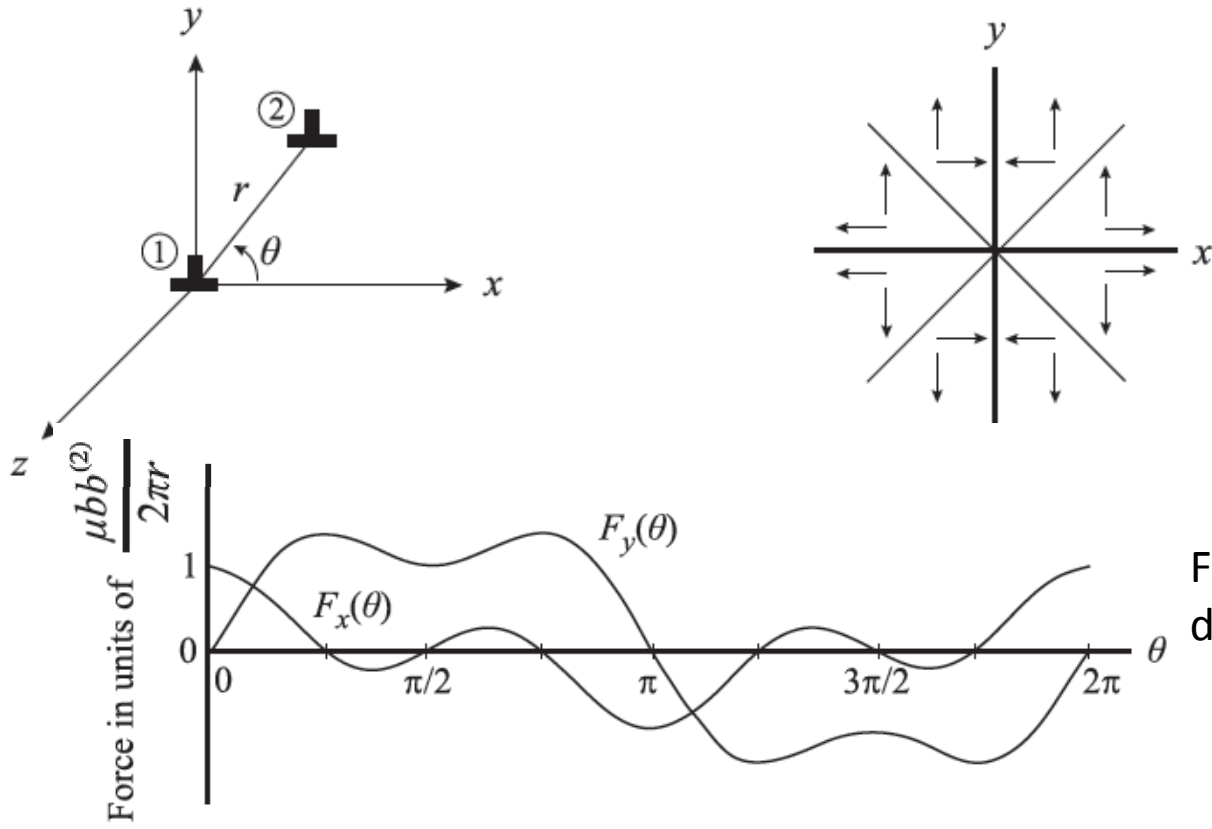
**Dislocation sources in Si**

A video is played in class to demonstrate the concept.

# Forces Between Edge Dislocations

Was, p. 289-290

- X & Y forces, no Z-force



## Peach-Kohler Equation

Burgers vector of dislocation (2) transposed

Line vector of dislocation (2) transposed

$$\mathbf{f} = \underline{\underline{b}}_{(2)}^T \underline{\underline{\sigma}}_{(1)} \times \underline{\underline{s}}_{(2)}$$

Force vector on dislocation (2)

Stress tensor induced by dislocation (1)

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# All Together: Loops, Movement, Pileup

Dislocations moving & piling up in Inconel 617 (Ni-based alloy) under *in-situ* straining in the TEM



<http://youtu.be/r-geDwE8Z5Y>

A video is played in class to demonstrate the concept.



# Grain Boundaries (2D)

<http://www-hrem.msm.cam.ac.uk/gallery/>

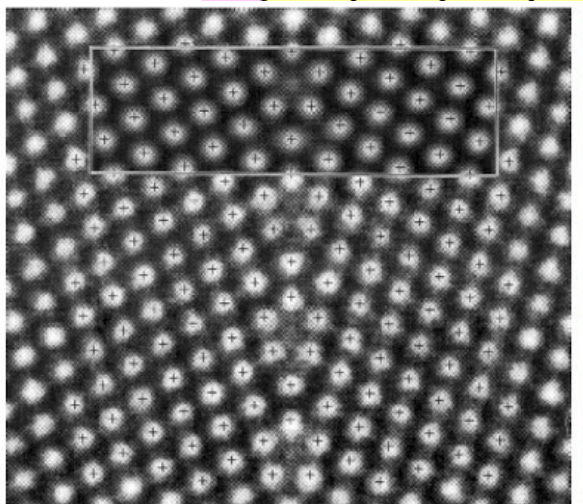
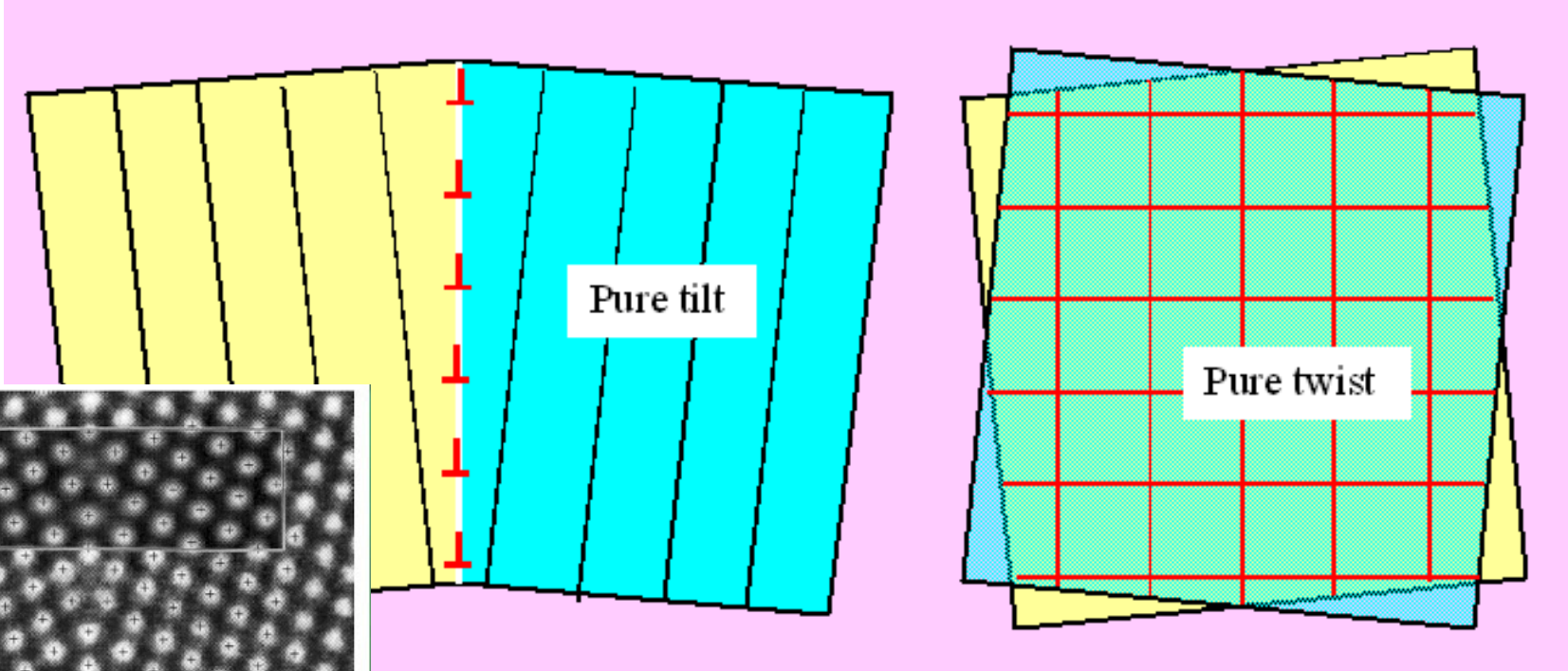
- Regions of different orientation
  - May also be different crystal structure



TEM image of a grain boundary in pure Al

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# GBs can be Lines of Dislocations



Tilt grain boundary in Al  
This image is in the public domain.

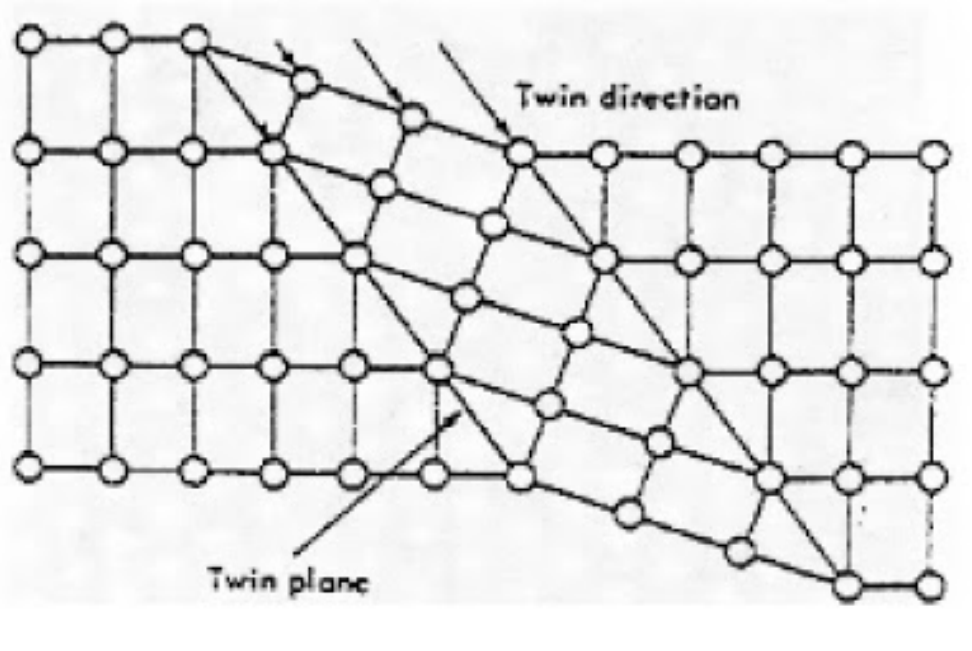
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[http://www.tf.uni-kiel.de/matwis/amat/def\\_en/kap\\_7/backbone/r7\\_2\\_1.html](http://www.tf.uni-kiel.de/matwis/amat/def_en/kap_7/backbone/r7_2_1.html)

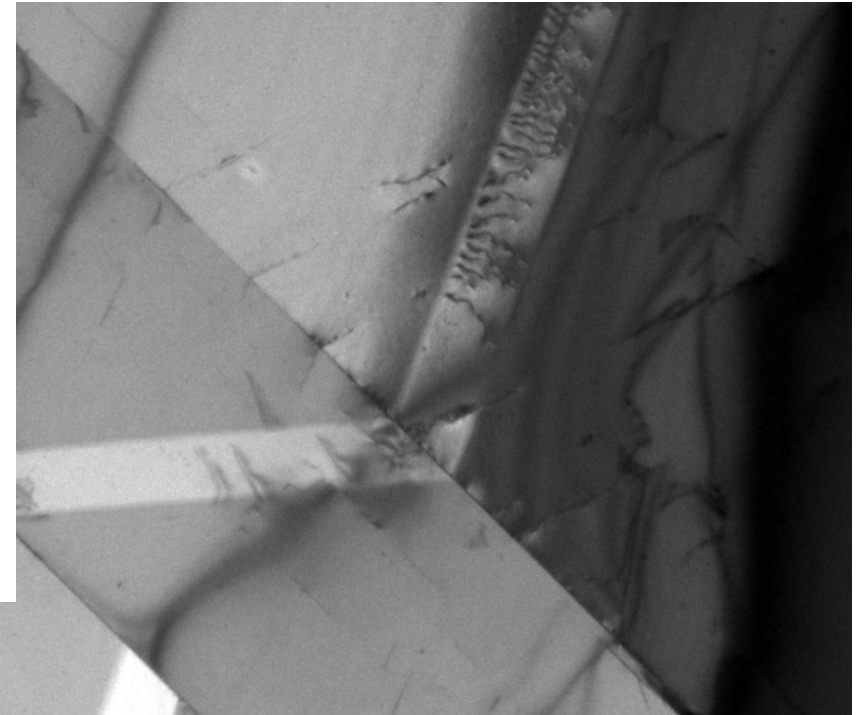
<http://moisespinedacaf.blogspot.com/>

# Twinning

- Alternate plastic deformation mechanism



[http://dcg.materials.drexel.edu/?page\\_id=14#nuclear](http://dcg.materials.drexel.edu/?page_id=14#nuclear)



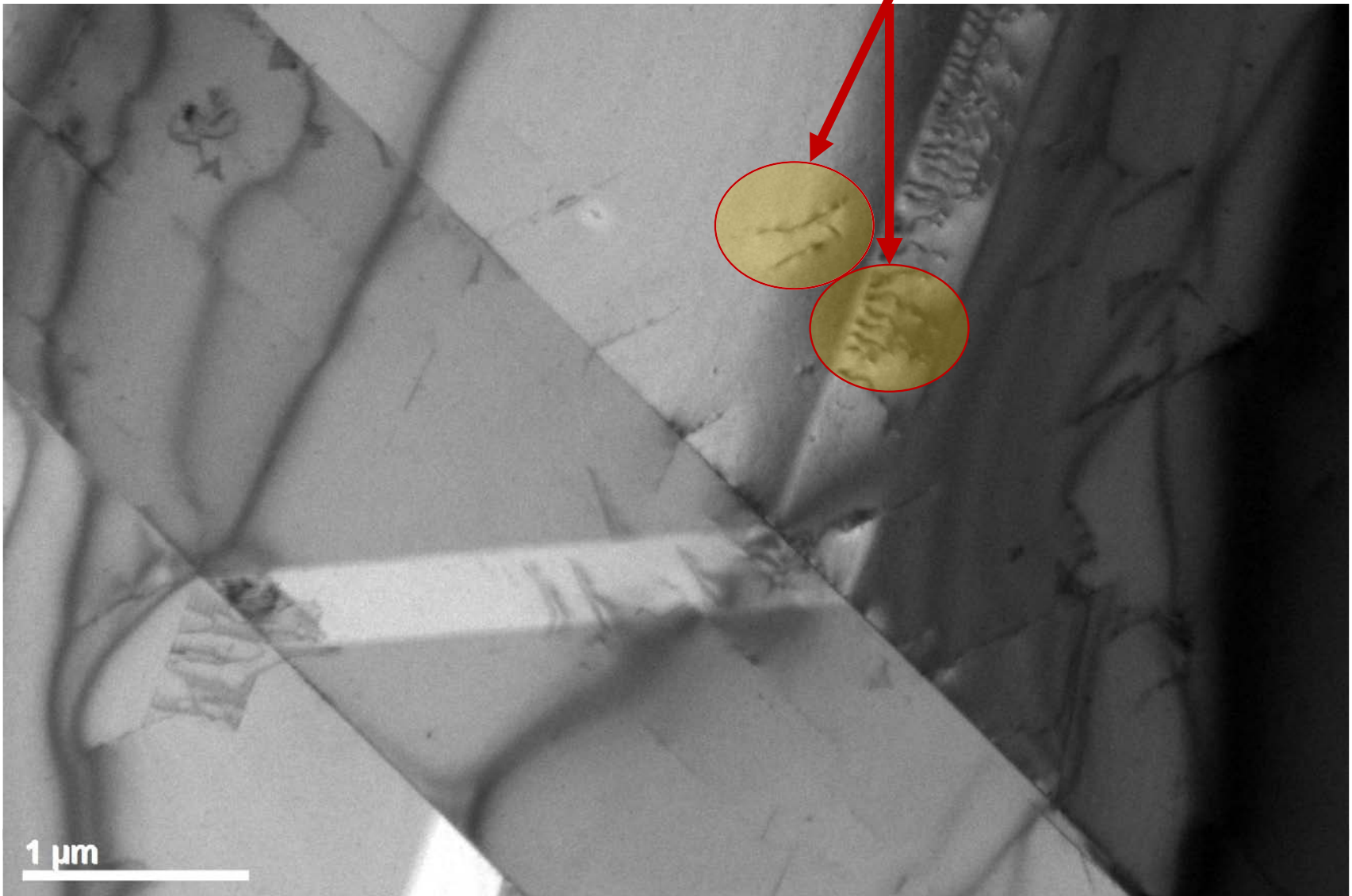
Twinning observed in irradiated  
reactor pressure vessel steel

1  $\mu\text{m}$

Courtesy of Dynamic Characterization Group, property of Drexel University. Used with permission.

# Twinning

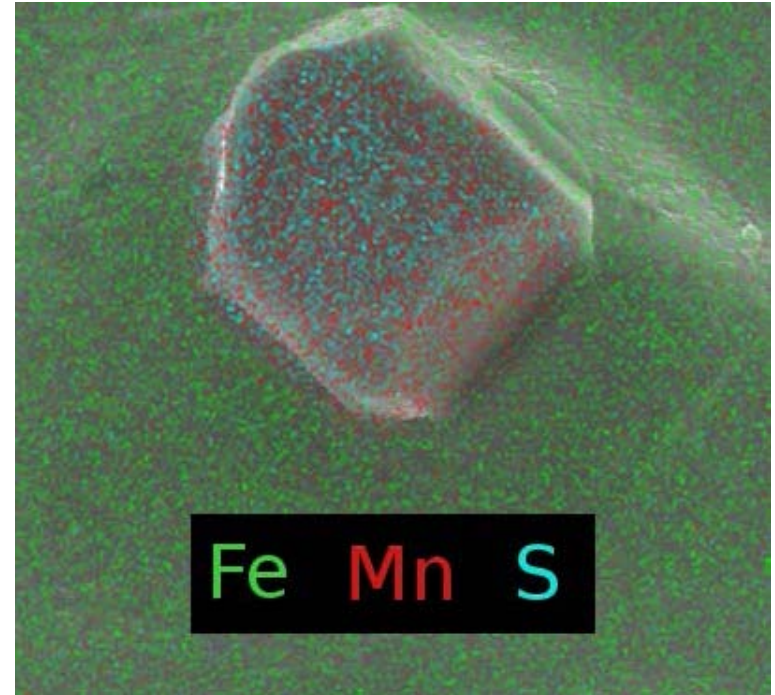
Differently oriented dislocations  
inside/outside twin boundary!



Courtesy of Dynamic Characterization Group, property of Drexel University. Used with permission.

# Inclusions (3D)

- Other phases trapped within base material
- Examples:
  - Secondary particle precipitates in Zircalloys
  - Carbides in steels
  - $Y_2O_3$  particles in Oxide Dispersion Strengthened (ODS) steels

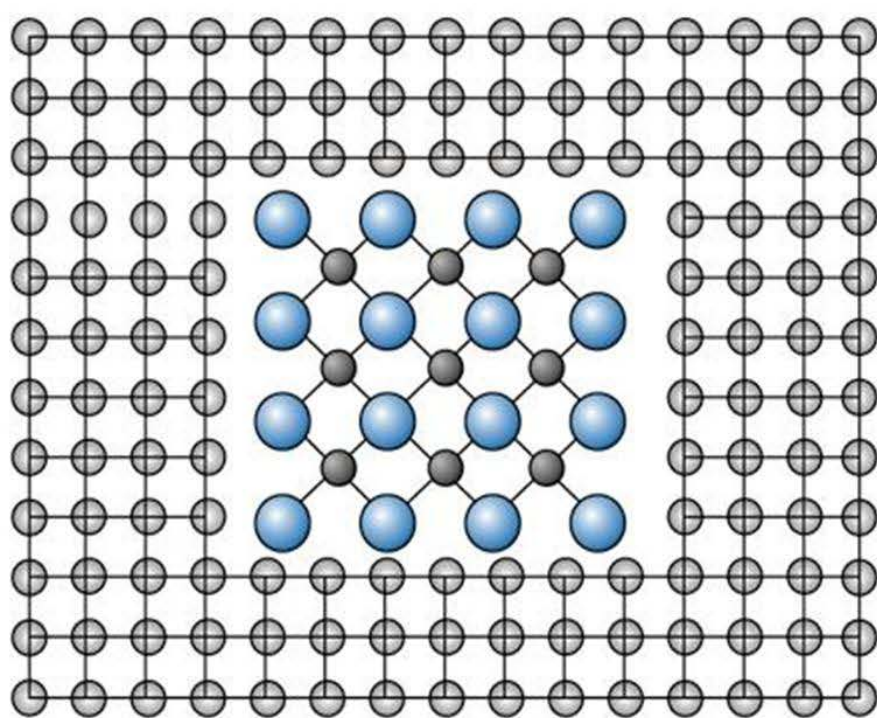


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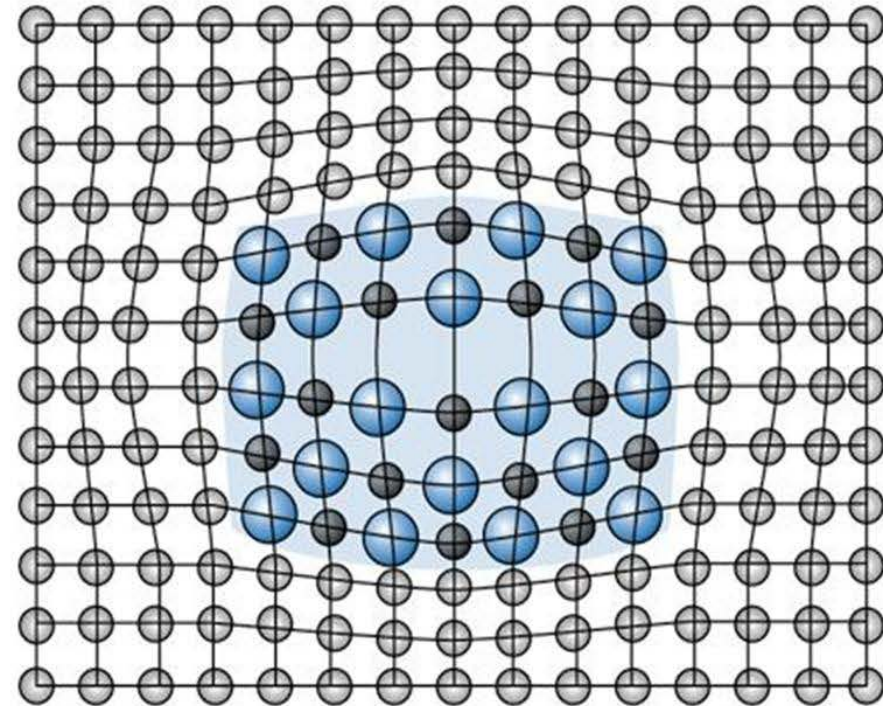
Single crystal of MnS, space group  $Fm\bar{3}m$ , FCC crystal structure embedded in Alcatraz rotor steel

# Coherent vs. Incoherent

- Which do you think would be better at sinking defects? Stopping dislocations?



Incoherent inclusion



Coherent inclusion

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# Switching Gears: Structural Material Properties

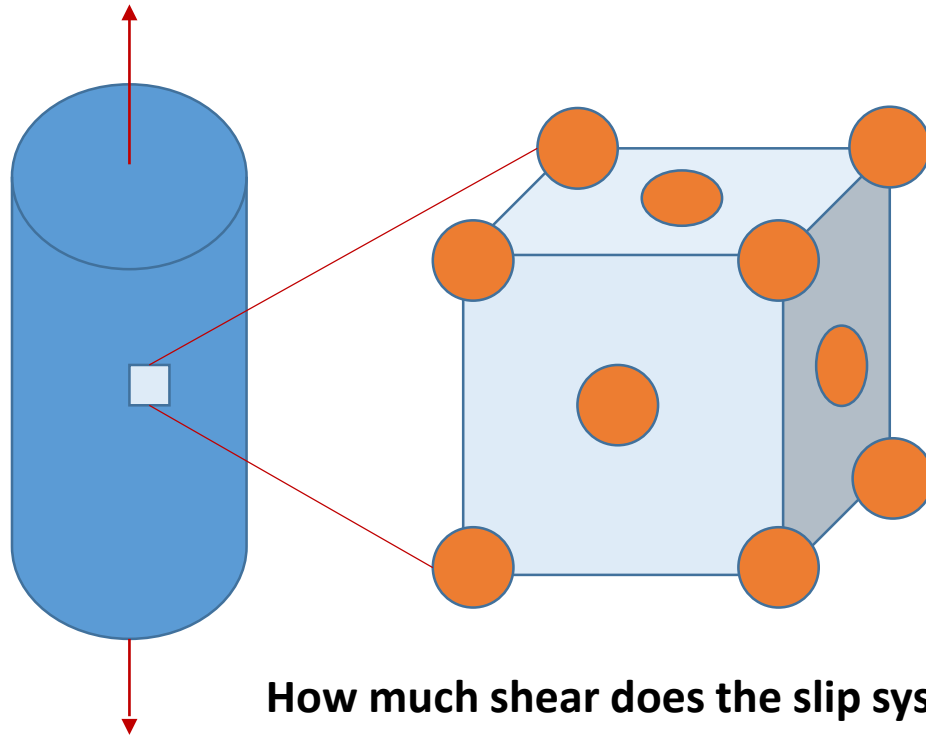
---

- Goals:
  - Understand true vs. engineering stress & strain
  - Quantify and differentiate between hardness, toughness, strength, ductility, stiffness
  - Know how to measure these properties
  - Resolve stresses onto slip systems
  - Predict the differences in mechanical response between single, dual, and polycrystalline materials

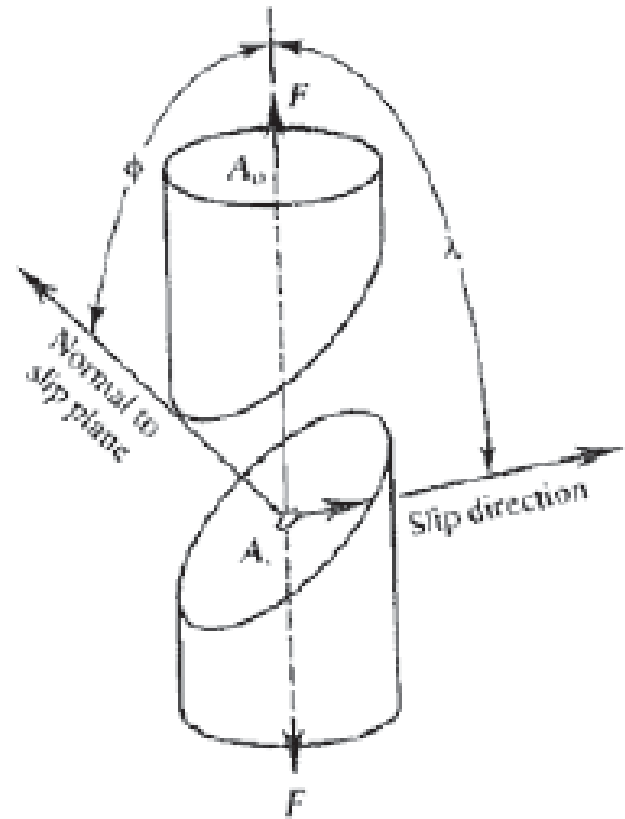
Images from now on are from T. H. Courtney, *Mechanical Behavior of Materials* unless otherwise noted

# Resolved Shear Stress

- Consider a single crystal bar of FCC material, tensioned in the  $[001]$  direction:



**How much shear does the slip system**



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# Resolved Shear Stress

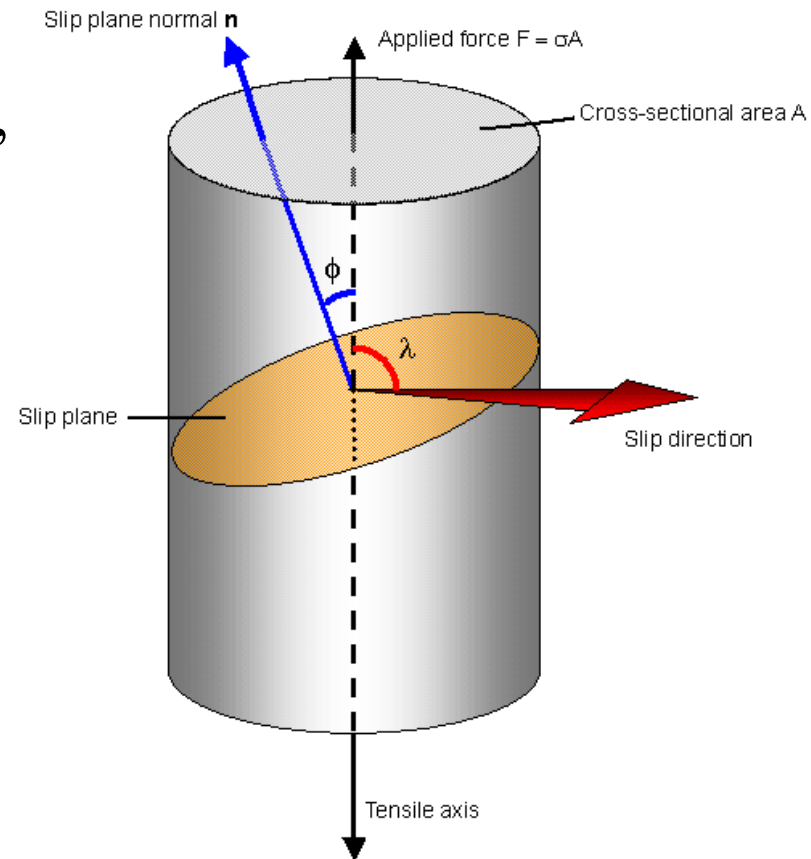
<http://www.doitpoms.ac.uk/tlplib/slip/printall.php>

- Project force onto the tilted plane containing the slip system, to get the stress

$$\sigma_{slip} = \frac{F}{A_{slip}} = \frac{F}{\frac{A_0}{\cos \theta}} = \sigma \cos \theta$$

- Also project shear movement in direction of slip

$$\tau = \sigma \cos \lambda$$



Courtesy of University of Cambridge. Used with permission.

# Resolved Shear Stress

---

- The total shear stress becomes:

$$\tau = \sigma \cos \lambda \cos \theta = \frac{\sigma}{m}$$

$$m = \frac{1}{\cos \lambda \cos \theta}$$

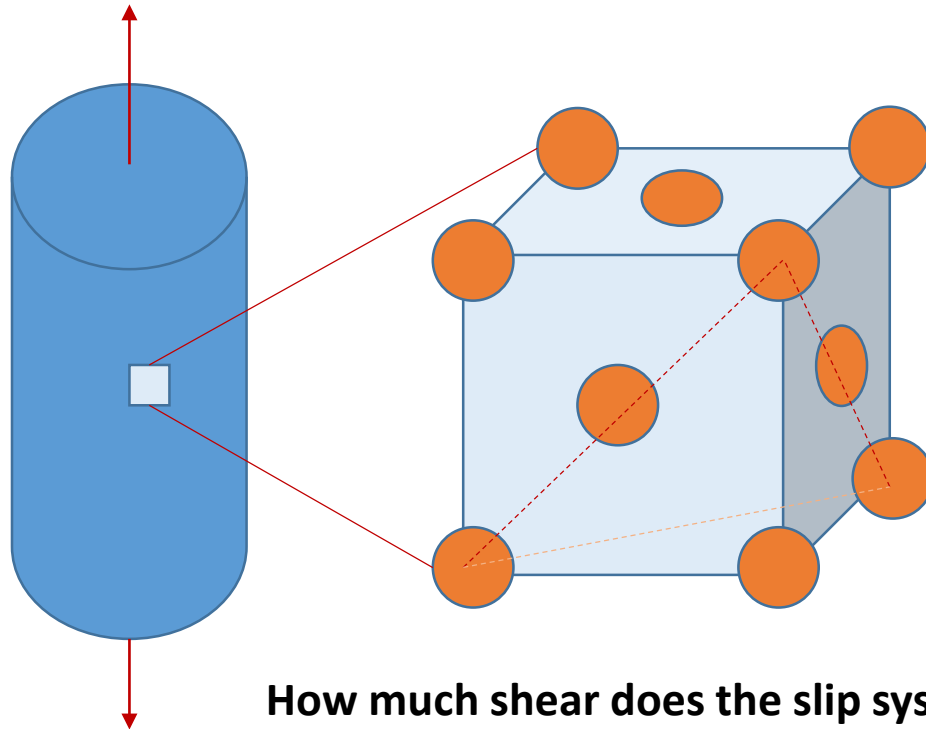
Schmid factor



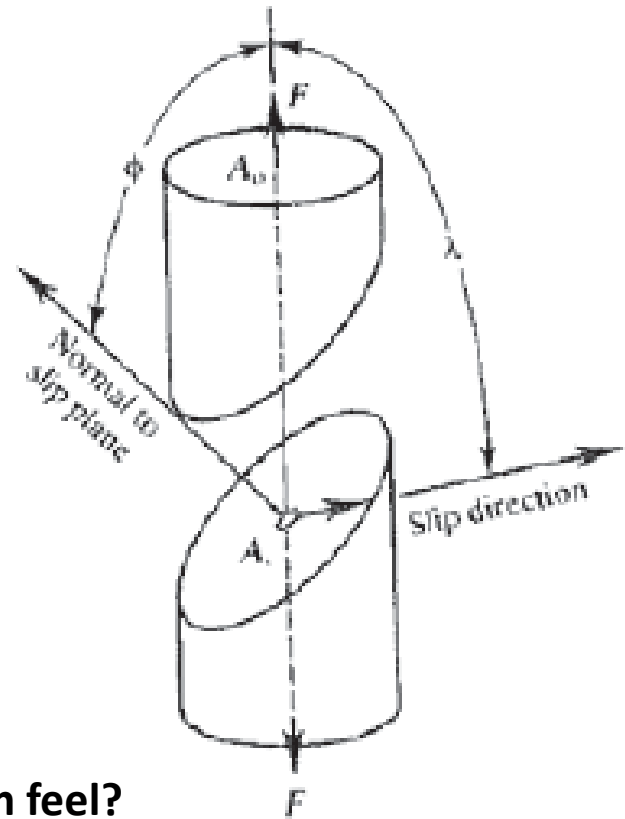
- Effectively reduces applies stress felt on a slip plane

# Resolved Shear Stress

- Consider a single crystal bar of FCC material, tensioned in the  $[001]$  direction:



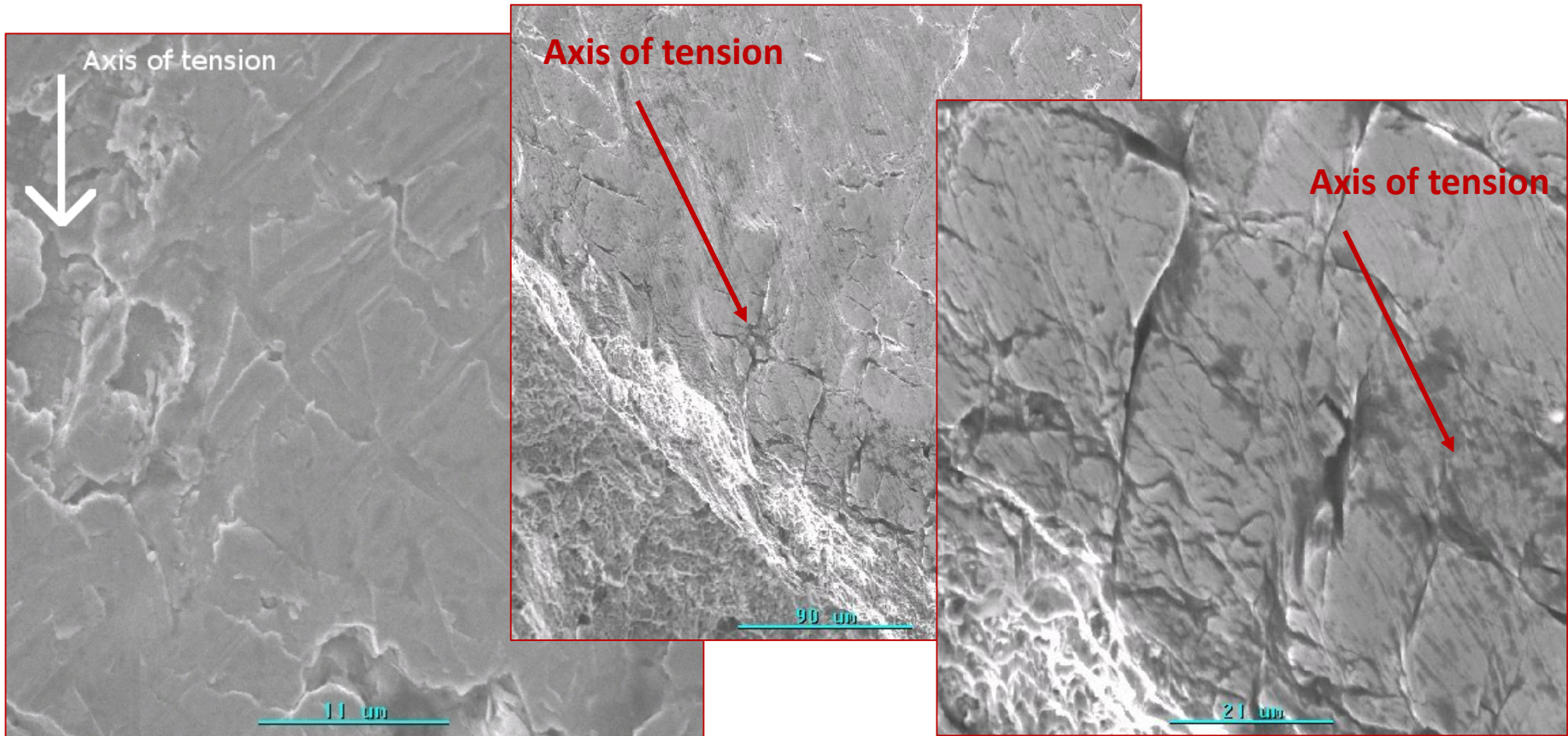
**How much shear does the slip system feel?**



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# Examples of Shear & Slip

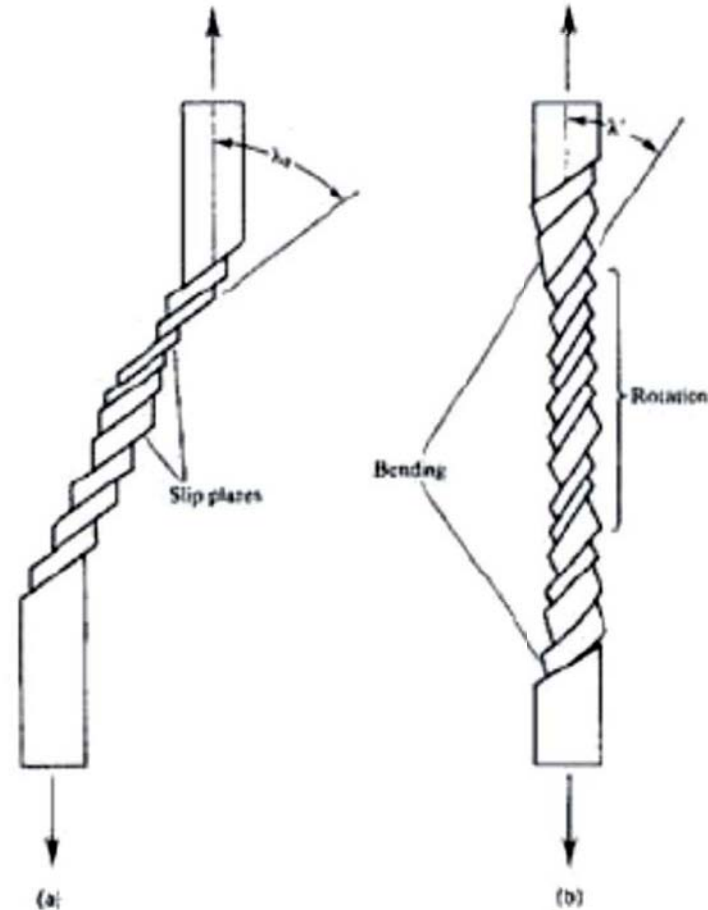
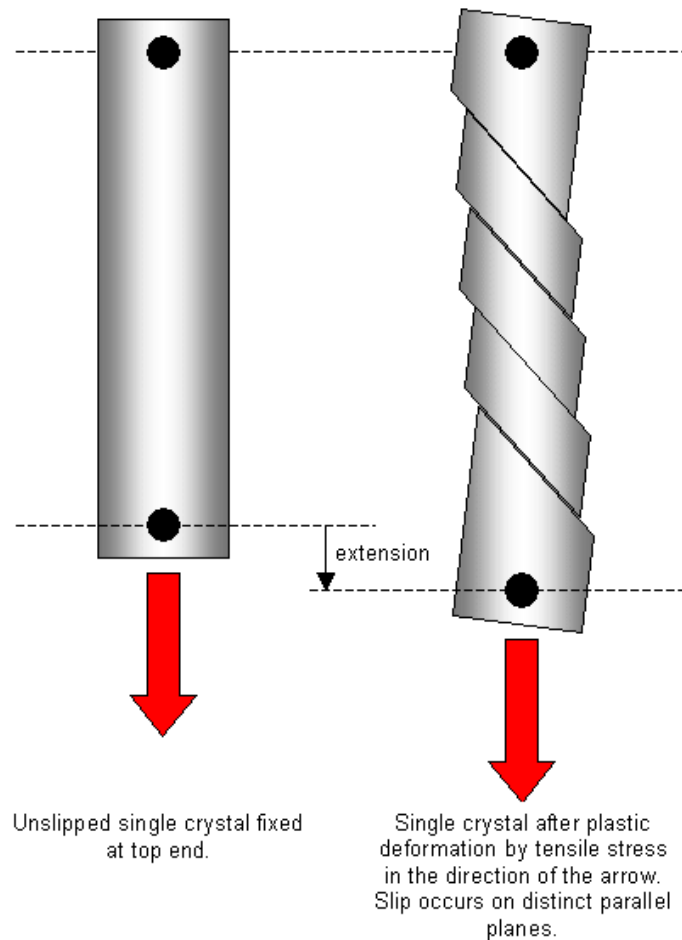
- Alcator C-Mod rotor steel in uniaxial tension:



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# Evidence of Slip Systems

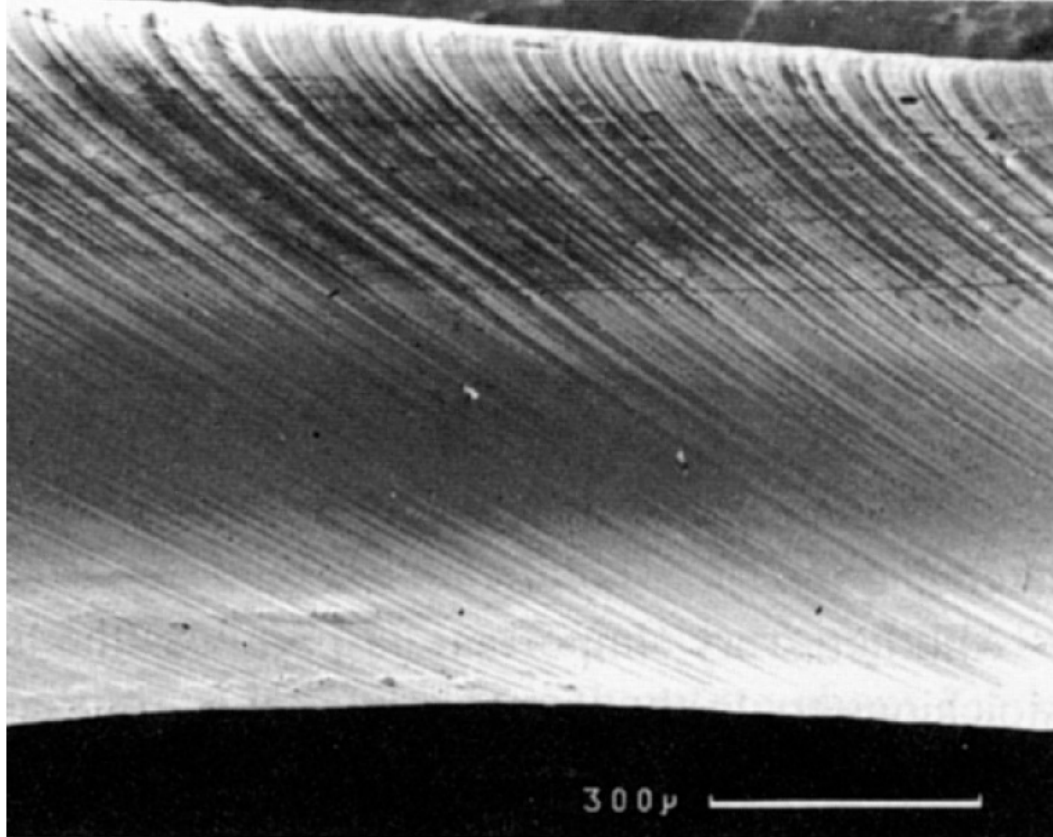
<http://www.doitpoms.ac.uk/tlplib/slip/printall.php>



Courtesy of University of Cambridge. Used with permission.

# Evidence of Slip Systems

[http://www.doitpoms.ac.uk/tlplib/miller\\_indices/printall.php](http://www.doitpoms.ac.uk/tlplib/miller_indices/printall.php)

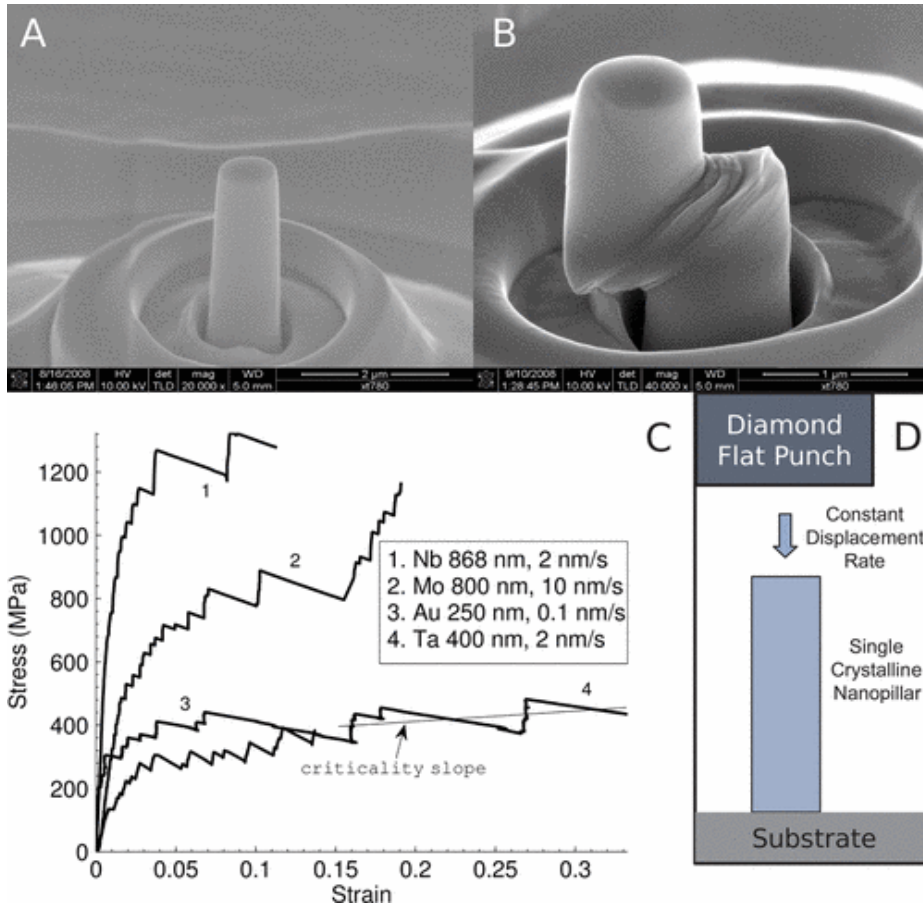


Courtesy of University of Cambridge. Used with permission.

A scanning electron micrograph of a single crystal of cadmium deforming by dislocation slip on 100 planes, forming steps on the surface

# Evidence of Slip Systems

N. Friedman et al. Phys. Rev. Lett. 109, 095507 (2012)



- Nanopillar compression tests using a diamond flat punch
- Clear 45 degree angles observed
- Slip systems activated by *shear*

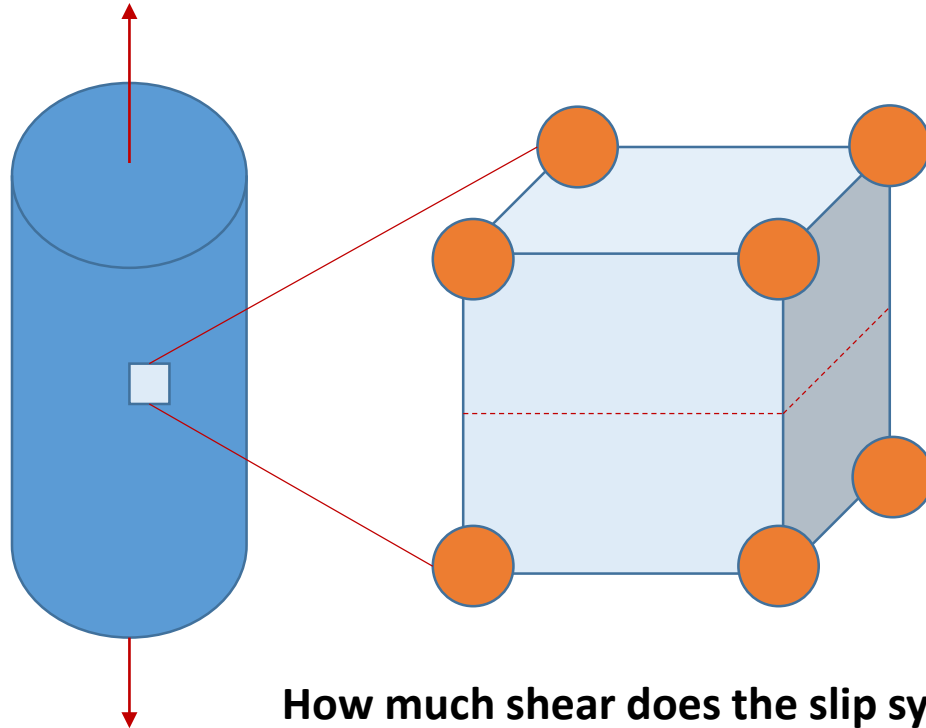
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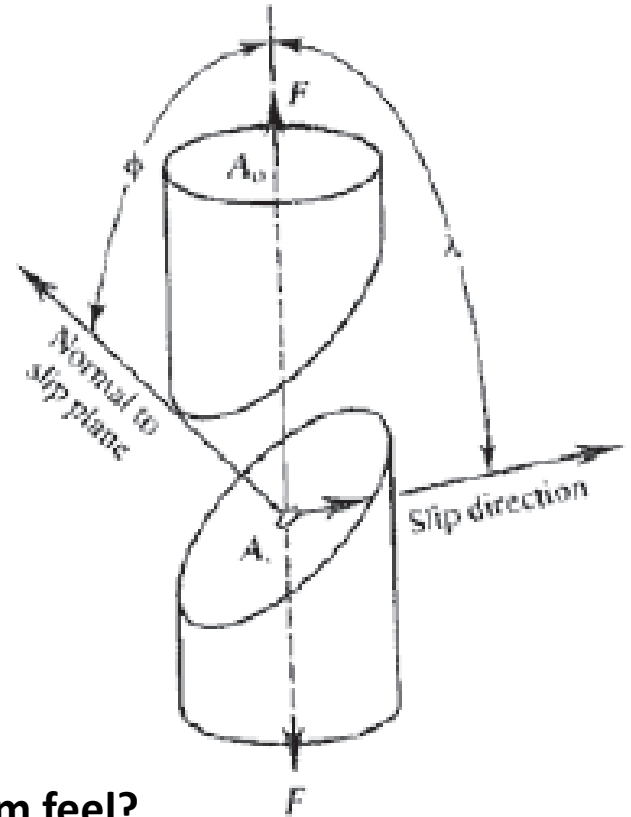


# Resolved Shear Stress

- Consider a single crystal bar of SC material, tensioned in the  $[001]$  direction:



**How much shear does the slip system feel?**



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# Resolved Shear Stress

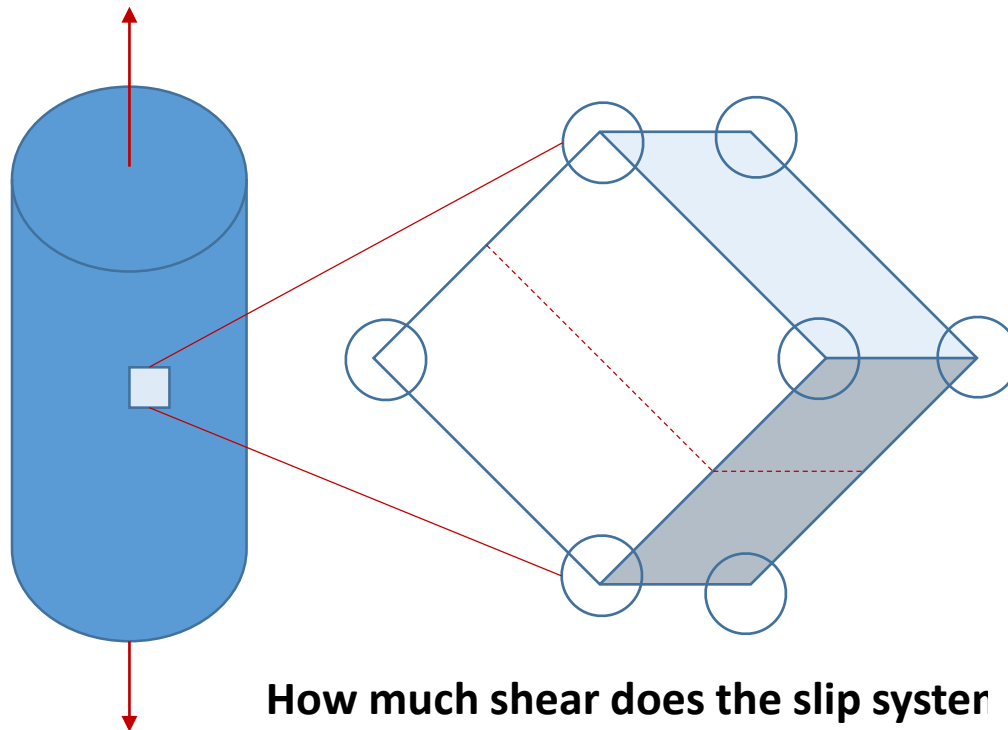
- Consider a single crystal bar of SC material, tensioned in the  $[001]$  direction:

Slip Plane	$\phi$ ( $^\circ$ ) $-\cos \phi$	Slip Direction	$\lambda$ ( $^\circ$ ) $-\cos \lambda$	Schmid Factor
(100)	90-0.00	[010]	0-1.00	0
		[001]	90-0.00	0
(010)	0-1.00	[100]	90-0.00	0
		[001]	90-0.00	0
(001)	90-0.00	[100]	90-0.00	0
		[010]	0-1.00	0

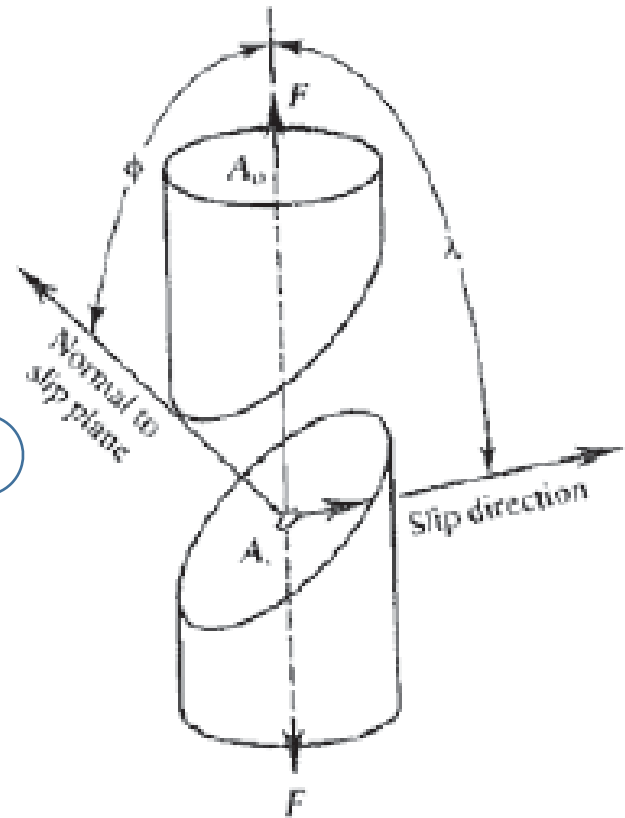
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# Resolved Shear Stress

- Consider a single crystal bar of SC material, tensioned in the  $[011]$  direction:



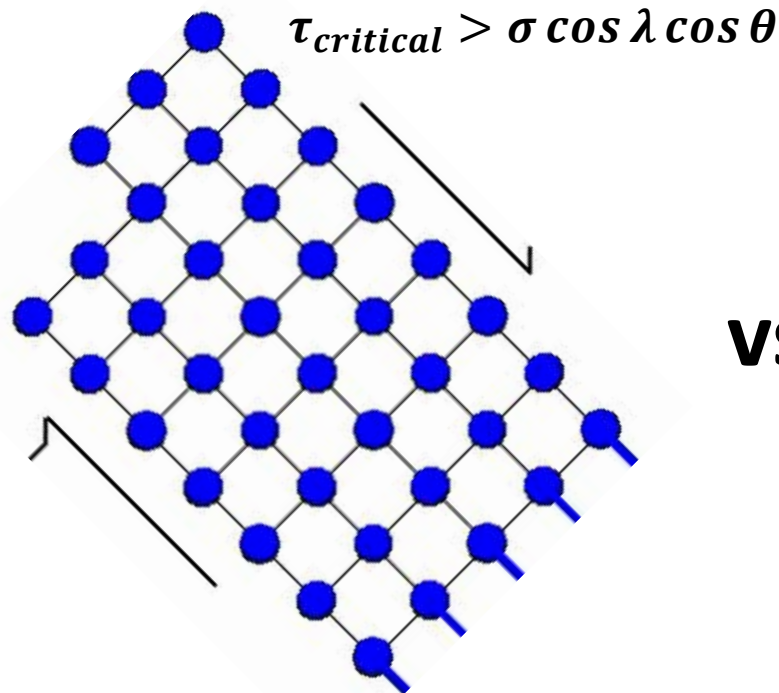
**How much shear does the slip system**



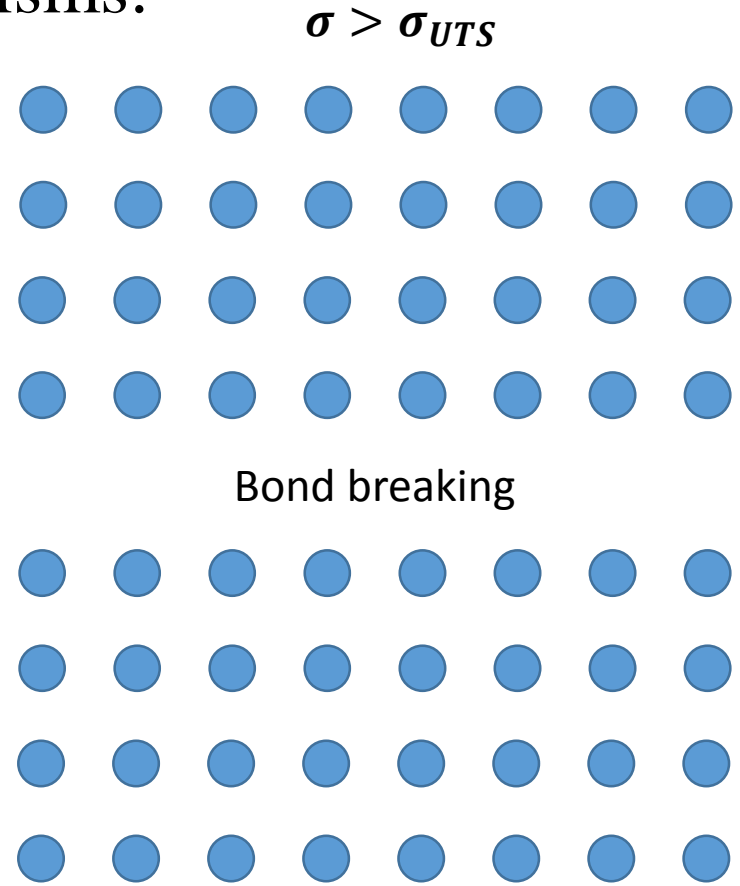
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# Will It Slip or Break?

- Balance between two mechanisms:



**VS.**



# Critical Resolved Shear Stress ( $\tau_{CRSS}$ )

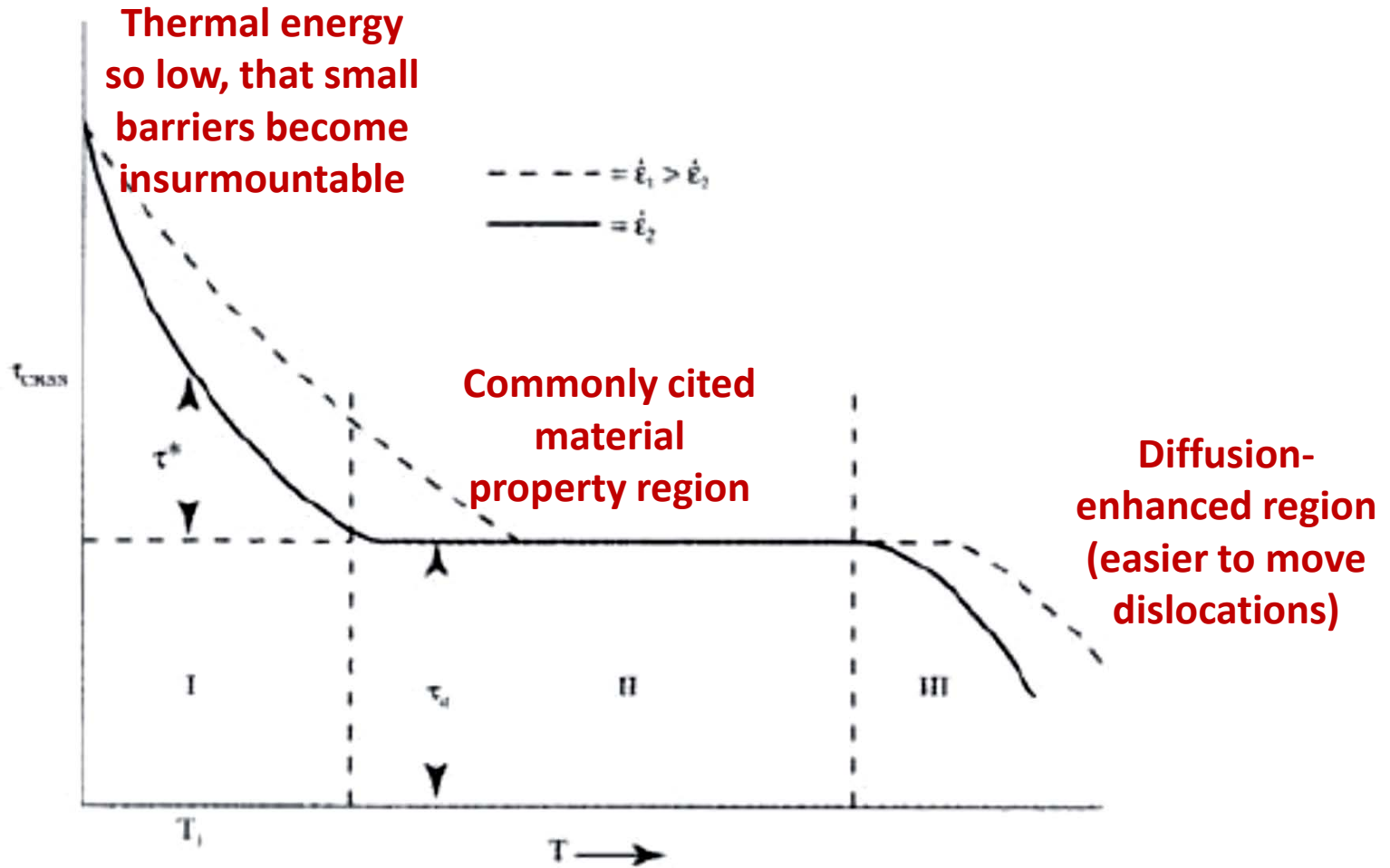
---

- Shear stress that is enough to get dislocations moving (plastic deformation)
- Related to the *yield stress* ( $\sigma_y$ ), the stress where plastic deformation starts:

$$\sigma_y = m\tau_{CRSS}$$

- NOTE:  $\sigma_y$  has crystallographic dependence in single crystals! What about polycrystals?

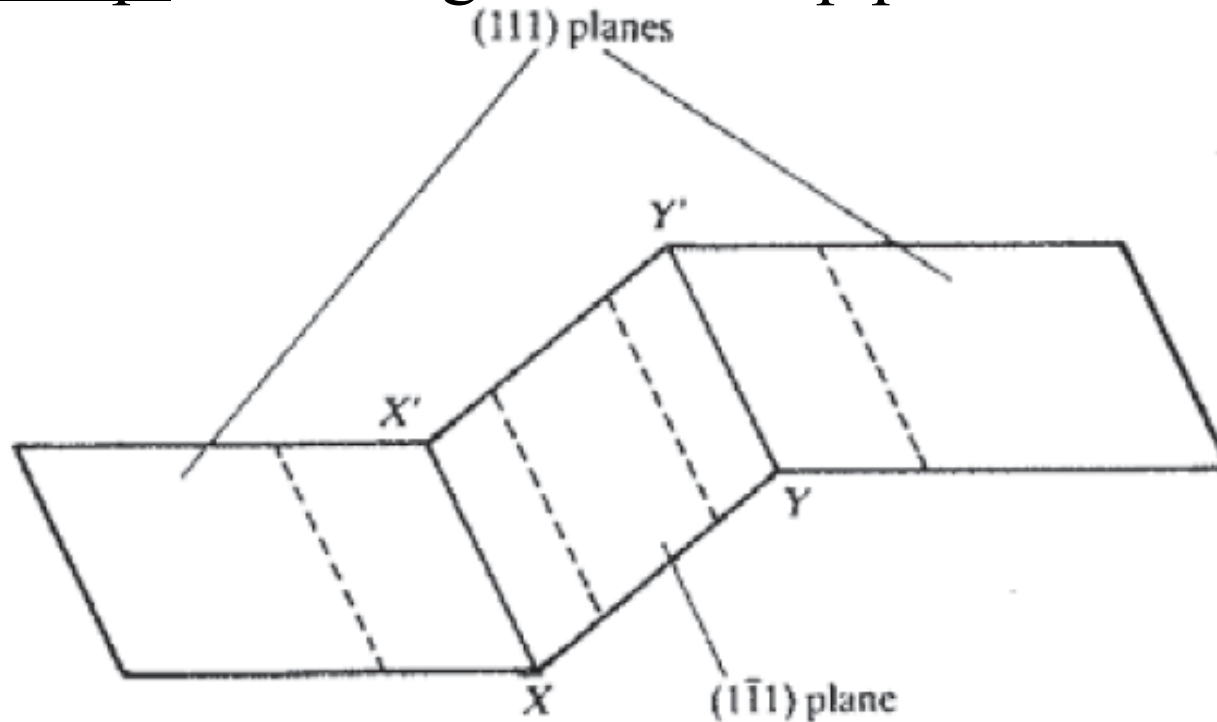
# $\tau_{CRSS}$ vs. Temperature



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# What Happens When Dislocations Get Stuck?

- Cross slip: switching to other slip planes



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- Resolved shear stress must be high enough!

# Stress vs. Strain

---

- Stress: Force over area
- Engineering stress: Force divided by *original* area
- True stress: Force divided by *actual* area as it *changes*

$$\sigma = \frac{F}{A_0} \qquad \sigma_t = \frac{F}{A(t)} = \frac{F}{A_0} \frac{A_0}{A(t)} = \sigma \frac{A_0}{A(t)}$$

- Conserve volume during stretching:  $V_0 = V(t)$



# Stress vs. Strain

---

$$\sigma = \frac{F}{A_0} \quad \sigma_t = \frac{F}{A(t)} = \frac{F}{A_0} \frac{A_0}{A(t)} = \sigma \frac{A_0}{A(t)}$$

- Conserve volume during stretching:  $V_0 = V(t)$

$$V_0 = A_0 L_0 = V(t) = A(t) L(t); \quad \frac{A(t)}{A_0} = \frac{L_0}{L(t)}$$

$$\sigma_t = \sigma \frac{A_0}{A(t)} = \sigma \frac{L(t)}{L_0} = \sigma \frac{L_0 + \delta L}{L_0} = \sigma \left( 1 + \frac{\delta L}{L_0} \right)$$

Engineering strain ( $\epsilon$ )



# True vs. Engineering Strain

---

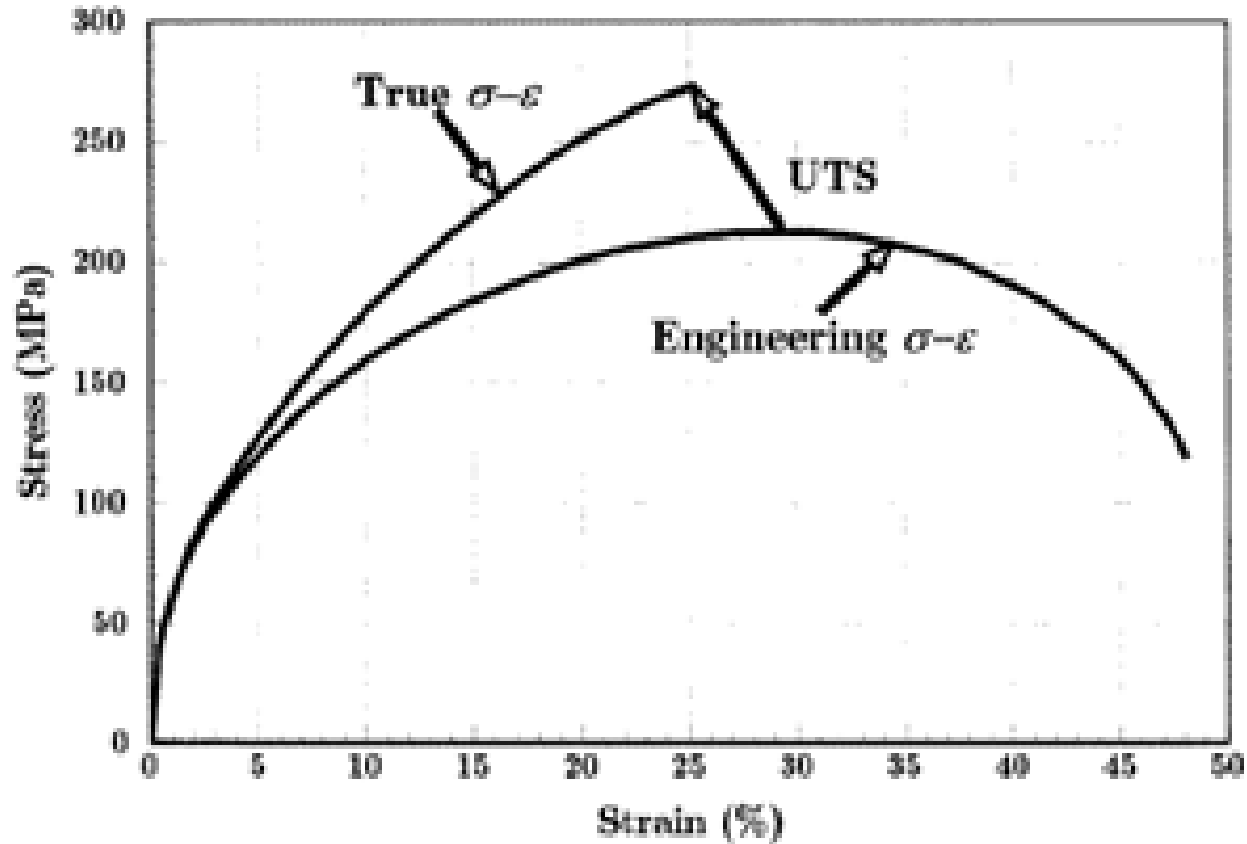
- Engineering strain ( $\epsilon$ ):  $\frac{\delta L}{L_0}$  (from *original* length)
- True strain ( $\epsilon_T$ ): Instantaneous increase in length:

$$\epsilon_T = \int_{L_0}^{L(t)} \frac{dL}{L} = \ln L(t) - \ln L_0 = \ln \left[ \frac{L(t)}{L_0} \right]$$

$$\epsilon_T = \ln \left[ \frac{L_0 + \delta L}{L_0} \right] = \ln[1 + \epsilon]$$

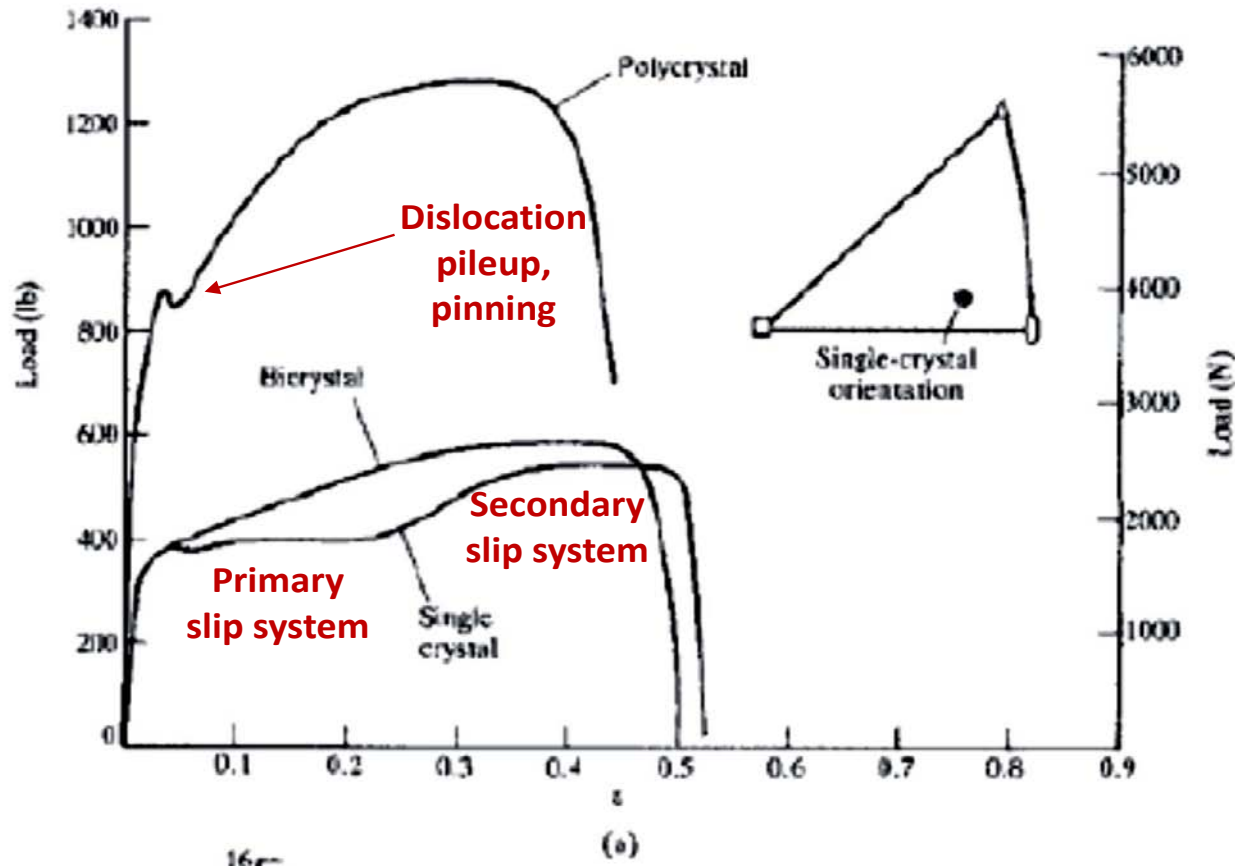
# Stress-Strain Curves

<http://keytometals.com/page.aspx?ID=CheckArticle&site=kts&NM=42>



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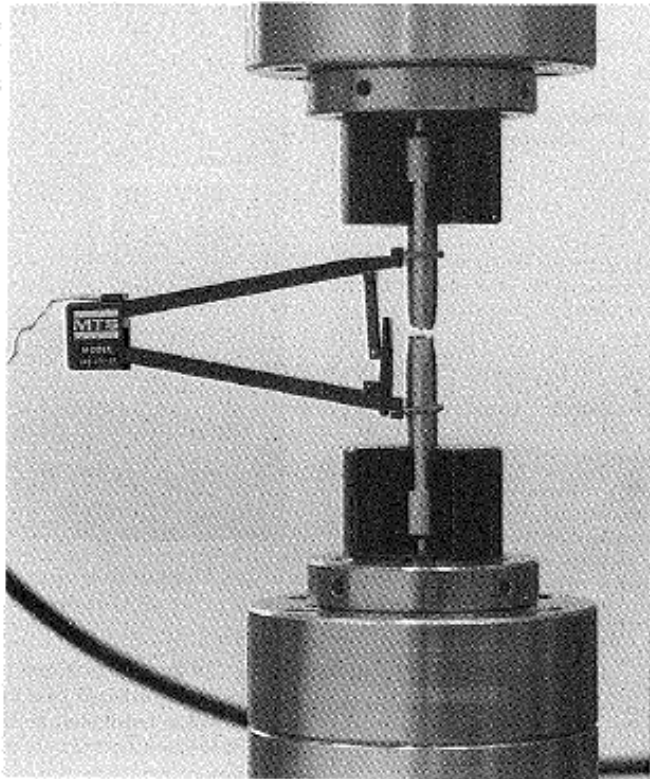
# Single, Dual, and Polycrystals



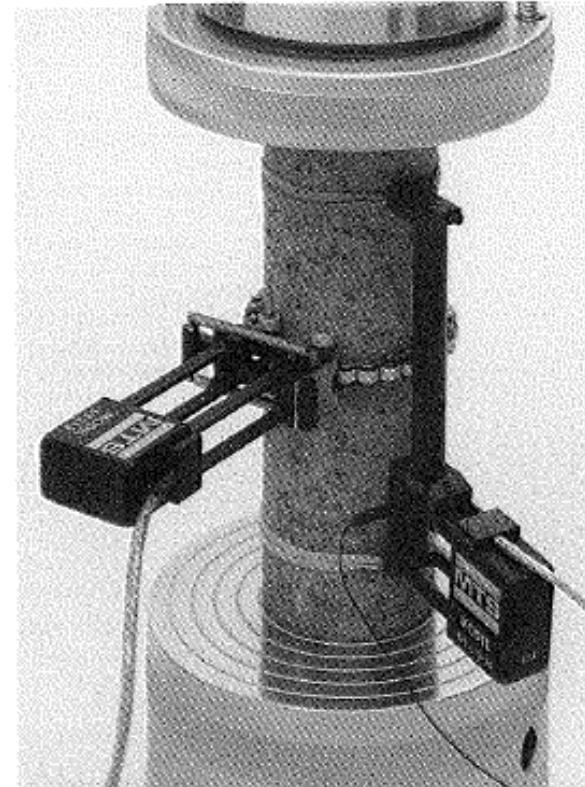
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# Measuring Stress-Strain

J. M. Gere, "Mechanics of Materials," pp. 12, 14



**Uniaxial tensile tester, with extensometer for measuring strain**



**Uniaxial compression tester, with extensometer and diameter measurement**

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# Dislocations and Defects

E. Bitzek and P. Gumbsch, Dynamic aspects of dislocation motion: atomistic simulations, *Materials Science and Engineering A*, 400-401 (2005), pp. 40-44

---

- Defects can slow down (pin) dislocations



A video is played in class to demonstrate the concept.

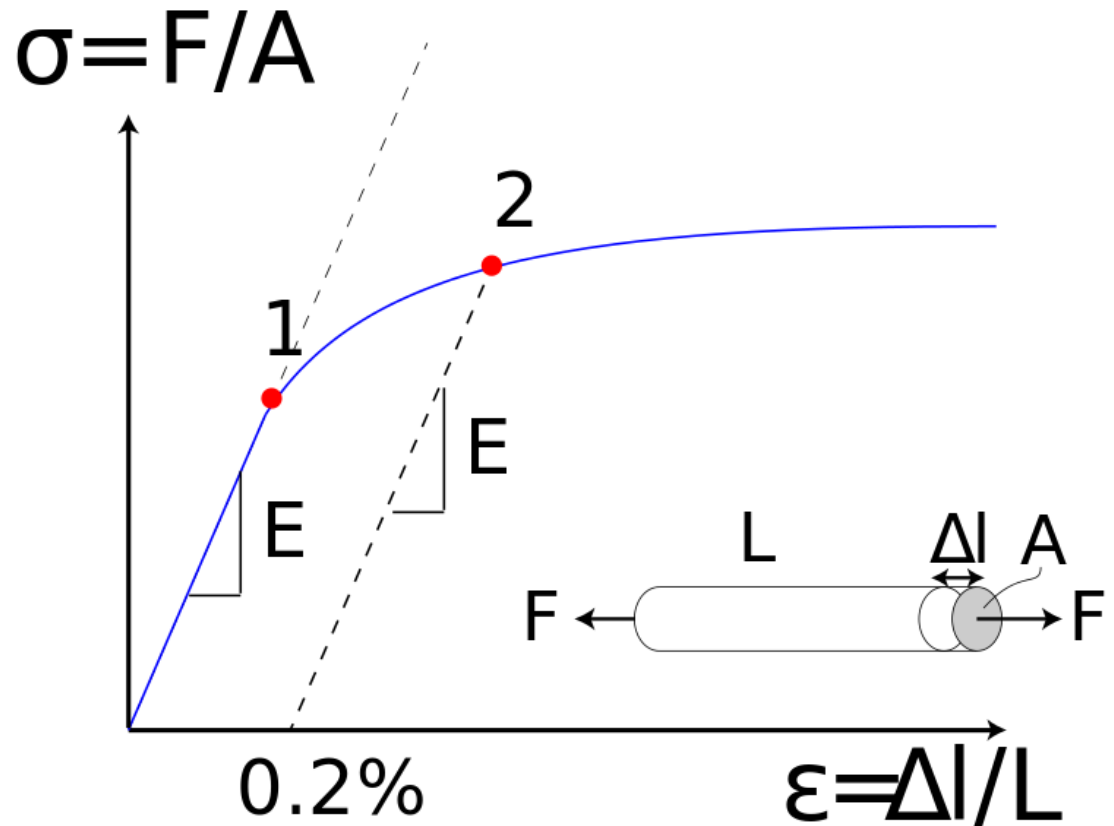
# Reviewing Material Properties

---

- Find the following on a stress-strain diagram:
  - Toughness
  - Strength
  - Ductility
  - Stiffness
- Perhaps define them first...

# Young's Modulus (Stiffness, E)

Measures elastic deformation vs. stress



Source: Wikimedia Commons

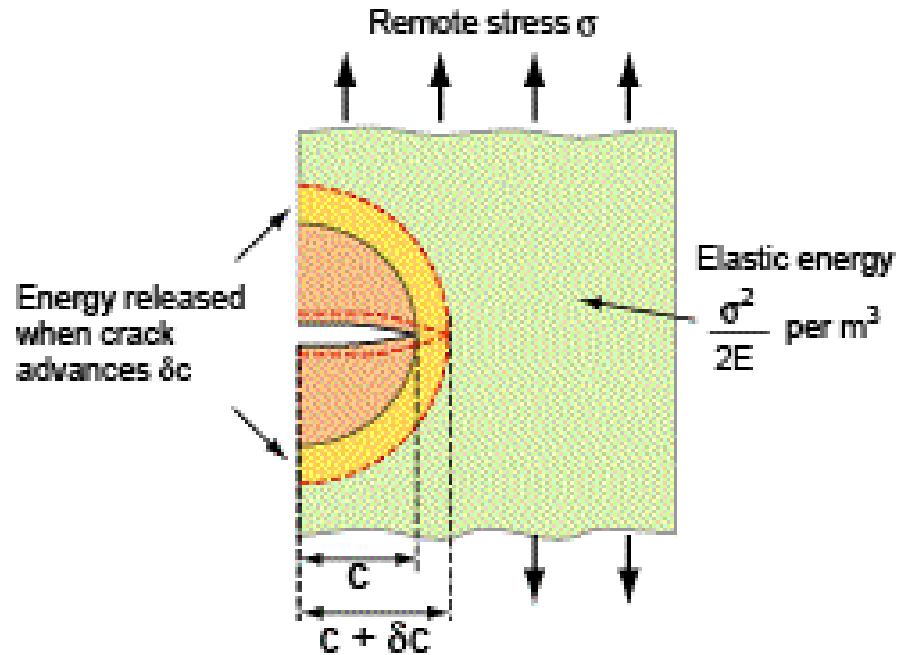
Image courtesy of [BenBritton](#) on Wikimedia. License: CC-BY-SA. This content is excluded from our Creative Commons license. For more information, see <http://ocw.mit.edu/help/faq-fair-use/>.



# Toughness ( $G_c$ )

- Measures the energy it takes to separate a material

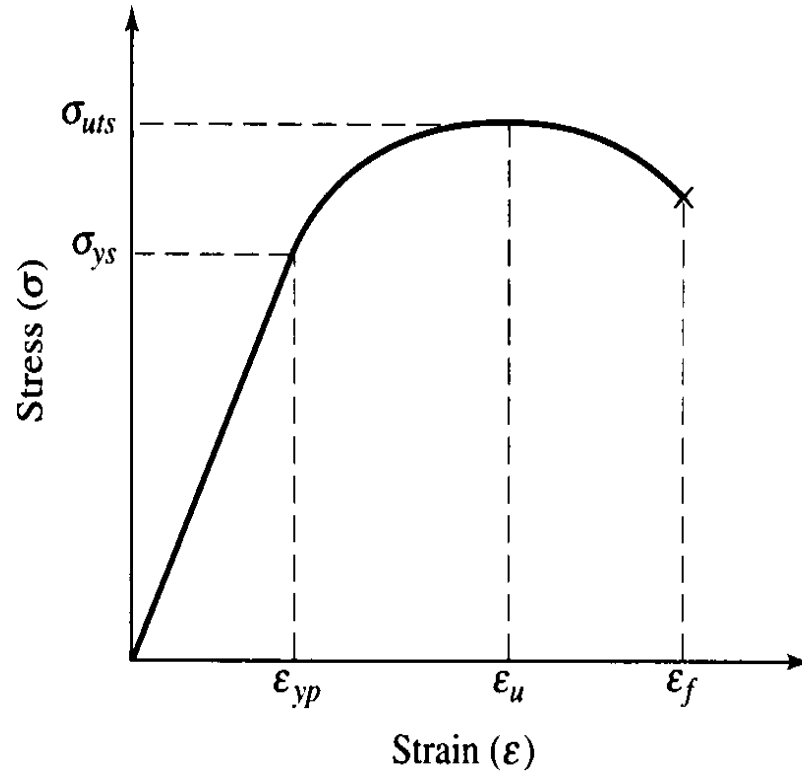
$$K_{Ic} = \sqrt{EG_c}$$



Source: [inventor.grantadesign.com](http://inventor.grantadesign.com)

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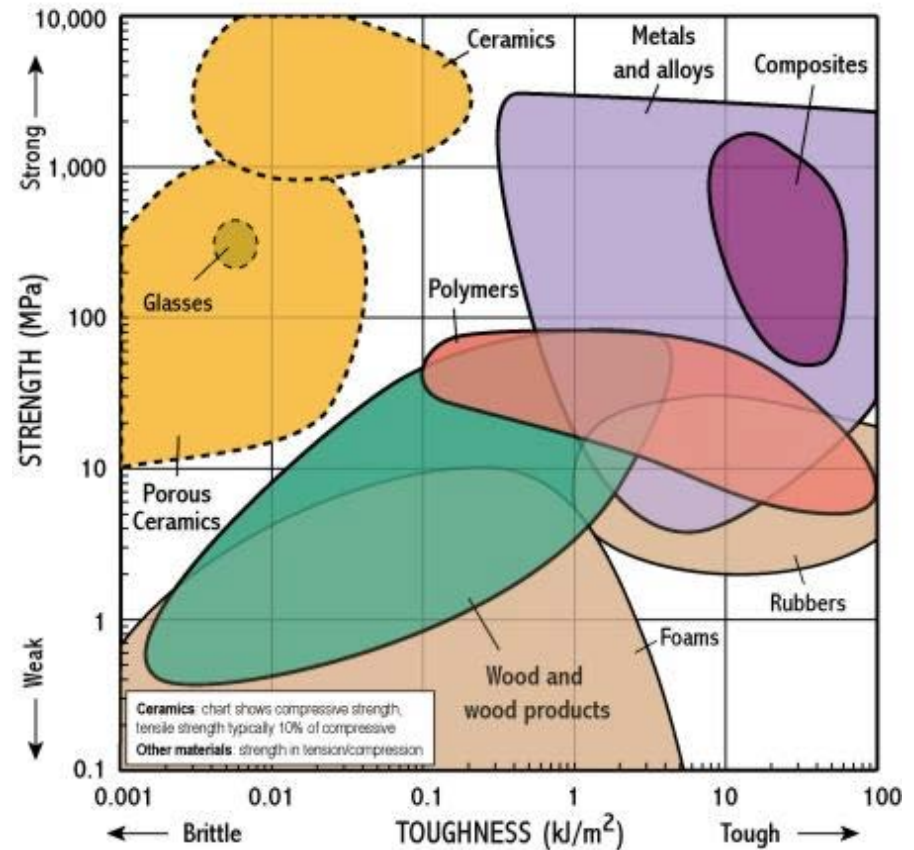
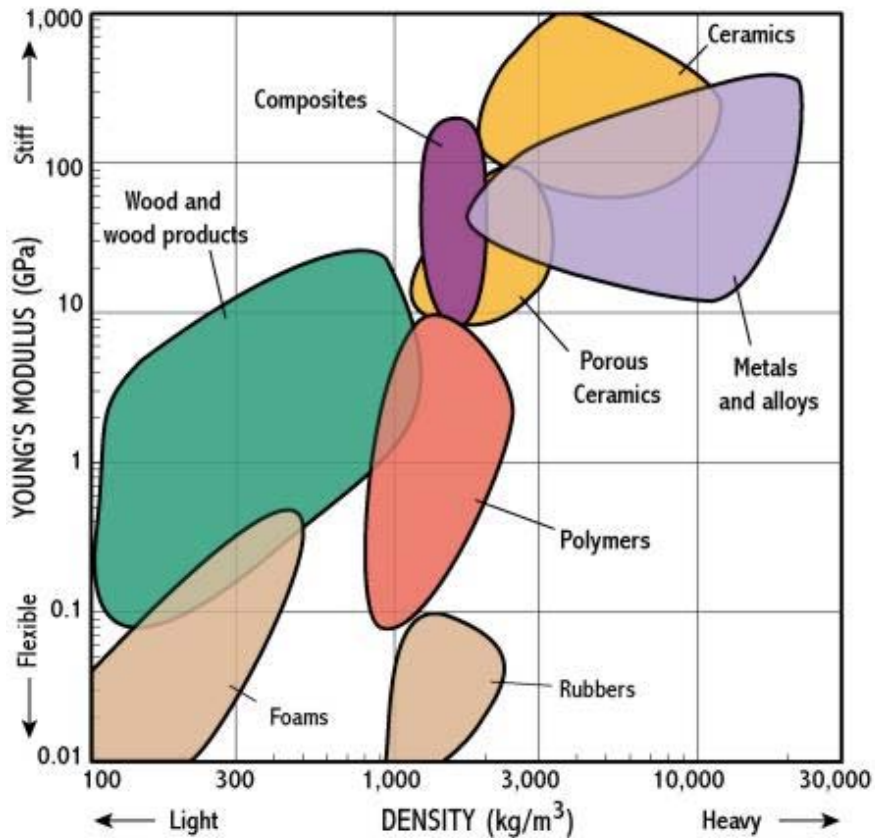
# Material Properties on Stress-Strain Diagram



Courtesy of [Ben Best](http://www.benbest.com). Used with permission.

<http://www.benbest.com/cryonics/lessons.html>

# Materials Selection Charts



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[http://www-g.eng.cam.ac.uk/125/now/mfs/tutorial/non\\_IE/charts.html](http://www-g.eng.cam.ac.uk/125/now/mfs/tutorial/non_IE/charts.html)

# Failure Criteria – Crack Propagation

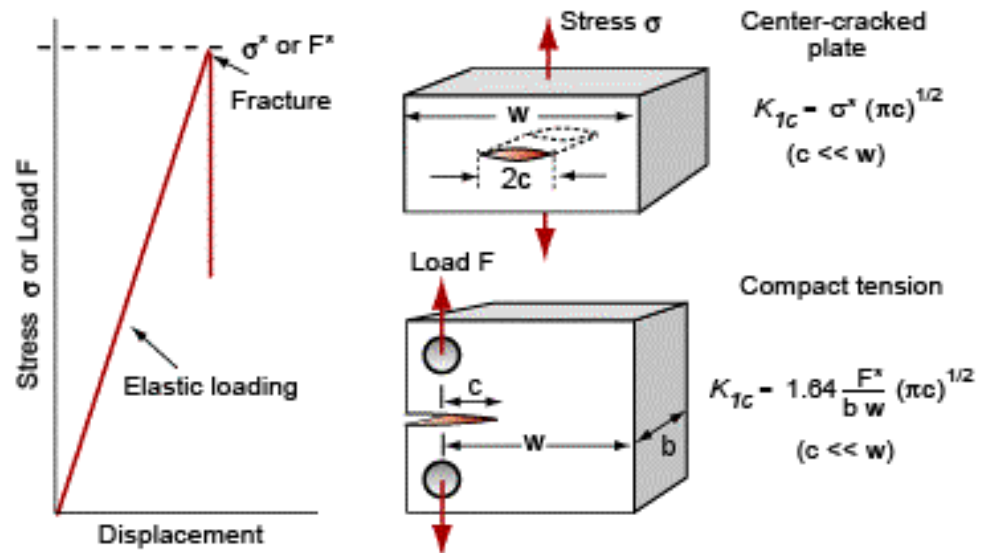
$$K_{Ic} = Y_1 \sigma^* \sqrt{\pi c} \text{ or } K_{Ic} = Y_2 \frac{F^*}{b w} \sqrt{\pi c}$$

Resistance to crack propagation

- $Y_1, Y_2$  are geometric factors near 1

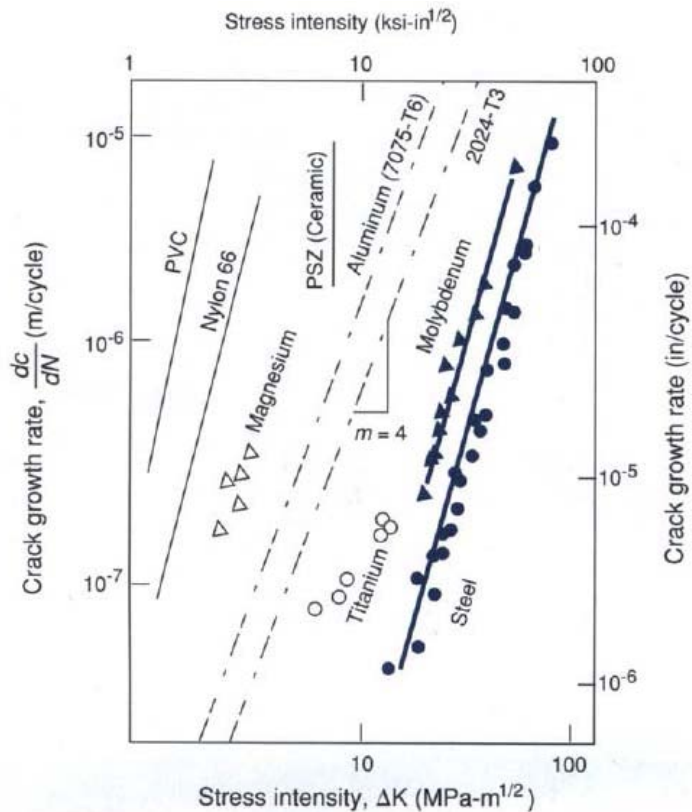
- $\sigma^*, F^*$  are critical stress and force, respectively

Source: inventor.grantadesign.com

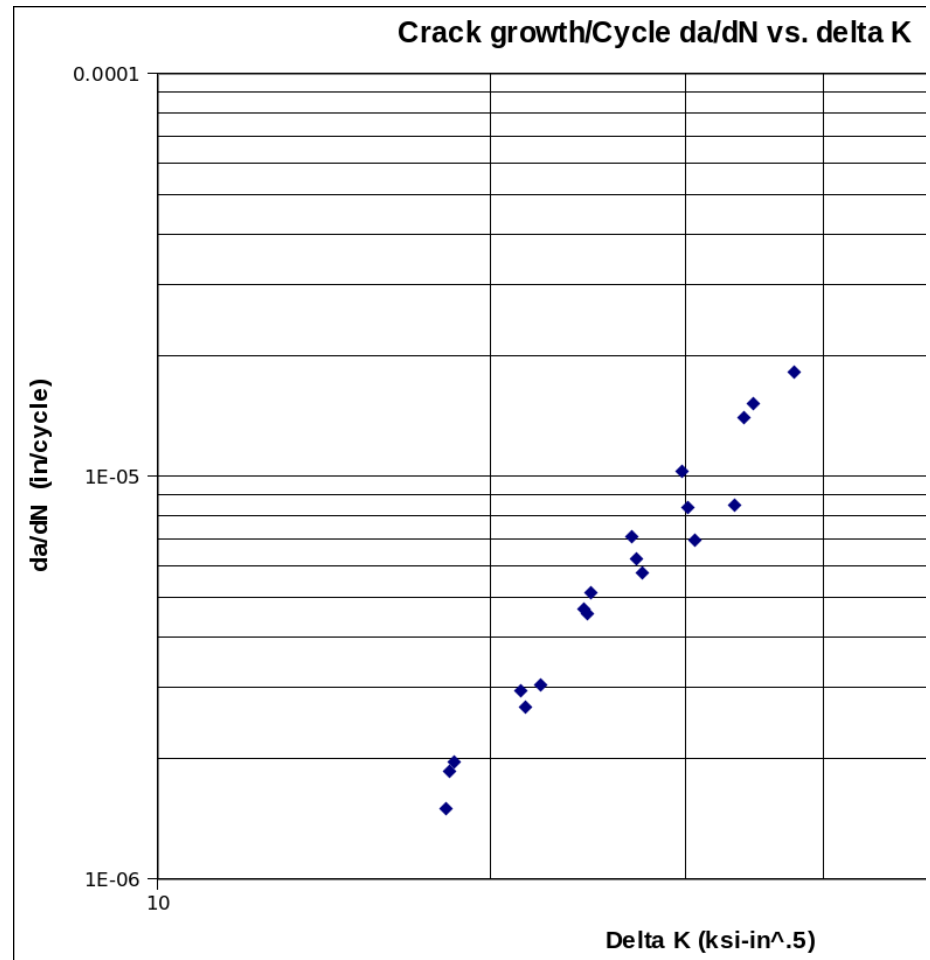


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# Fracture Toughness – Real Data from Alcatraz C-Mod

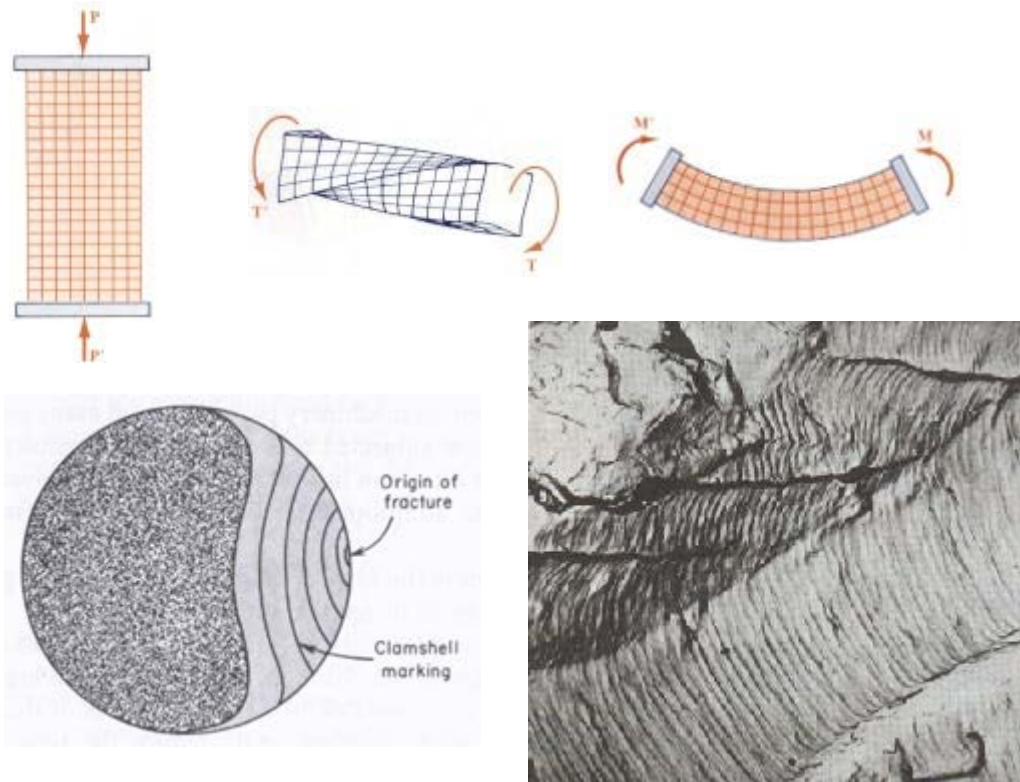


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Engineering Materials Science, Milton Ohring, Ch. 10

# Failure Criteria – Fatigue

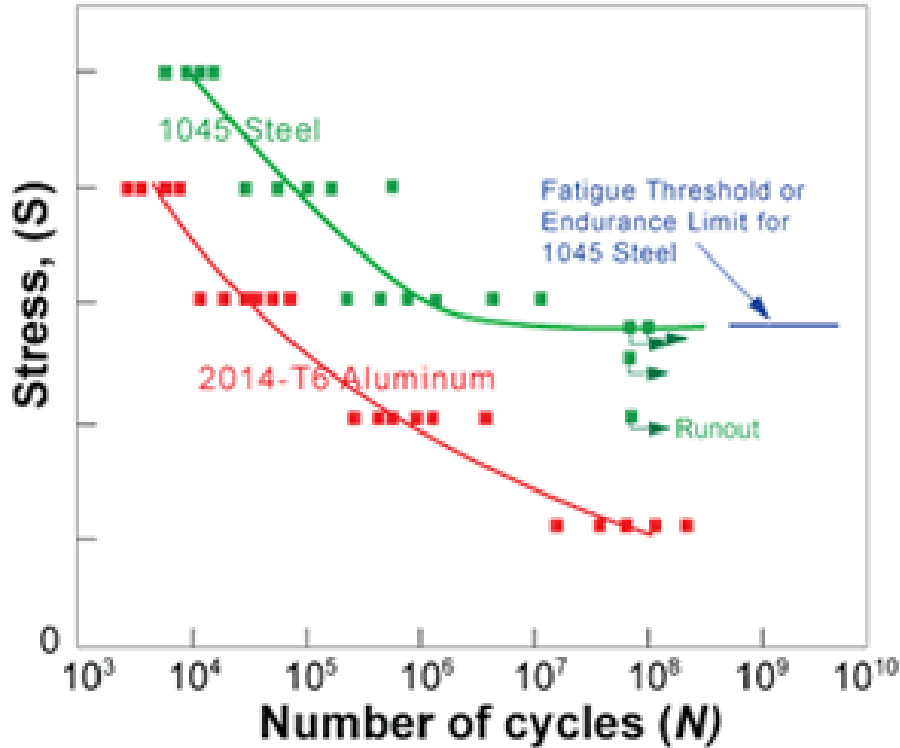


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- Repeated application of stress can cause cracks to grow
- Induced by vibrations, mechanical loading
- Telltale “fatigue striations”
- **Where do these come from?**

Source: [www.sv.vt.edu/classes/MSE2094\\_NoteBook/97ClassProj/anal/kelly/fatigue.html](http://www.sv.vt.edu/classes/MSE2094_NoteBook/97ClassProj/anal/kelly/fatigue.html)

# Failure Criteria – Fatigue

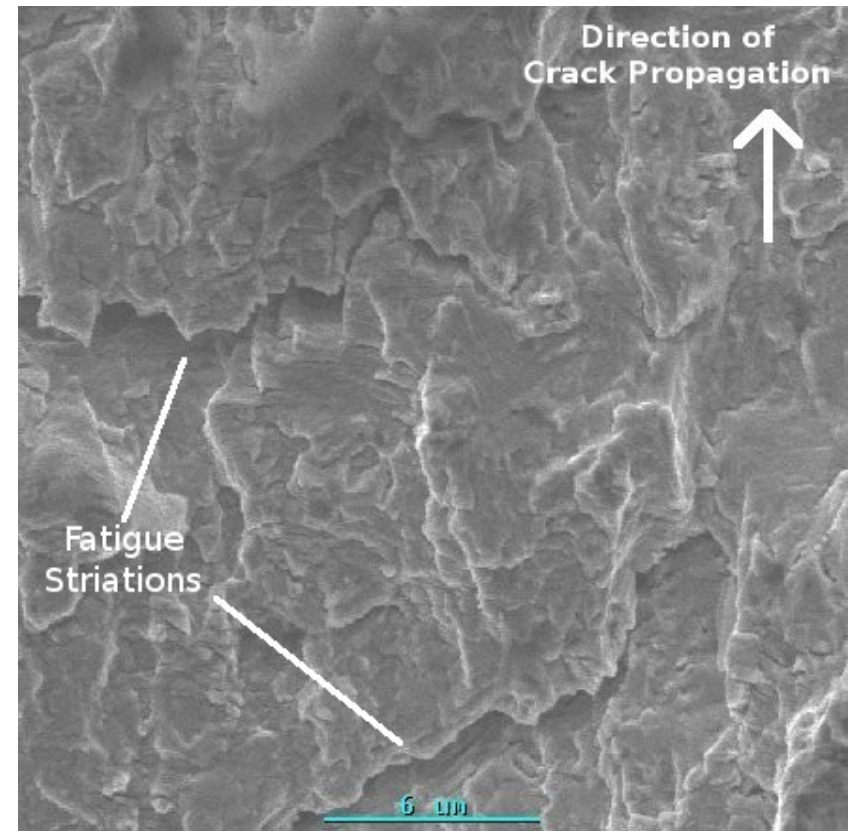
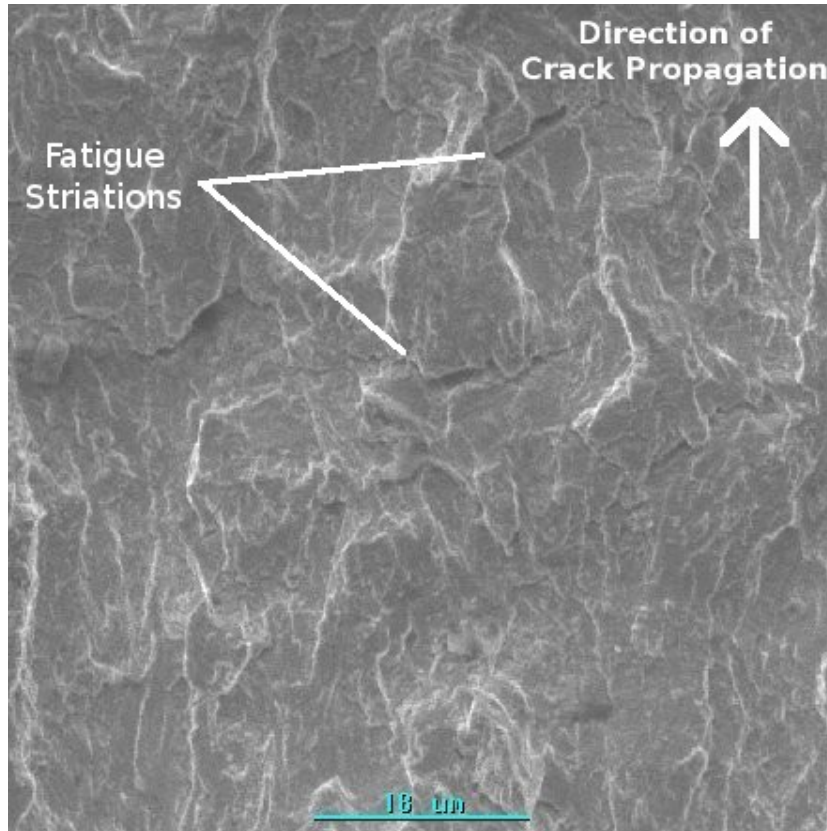


This image is in the public domain.

- Stress (S) vs. number of cycles (N)
- Lower limit of stress (where N is infinite) is the “safe zone”
- **Why do these limits exist?**

Source: [www.nde-ed.org/EducationResources/CommunityCollege/Materials/Mechanical/S-NFatigue.htm](http://www.nde-ed.org/EducationResources/CommunityCollege/Materials/Mechanical/S-NFatigue.htm)

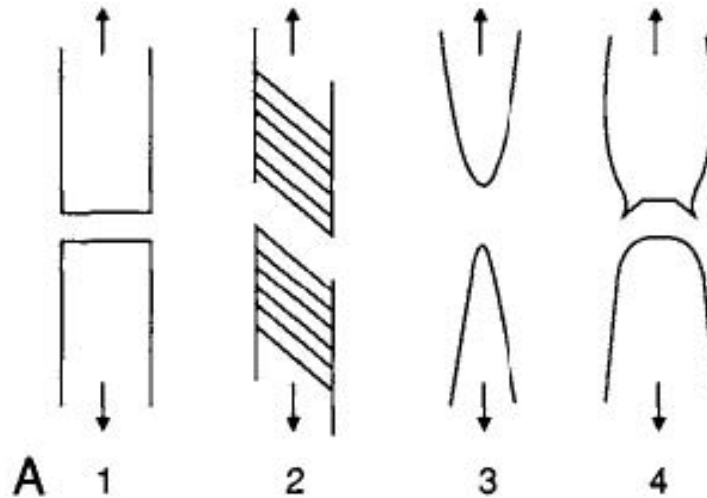
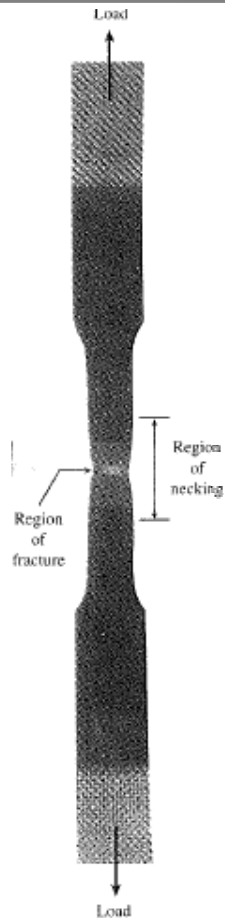
# Fatigue Striations in Alcatraz C-Mod Rotor



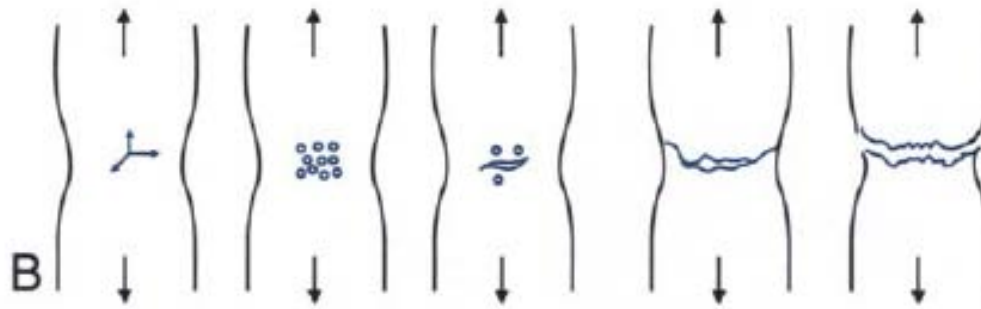
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# Failure Mechanisms in Tension



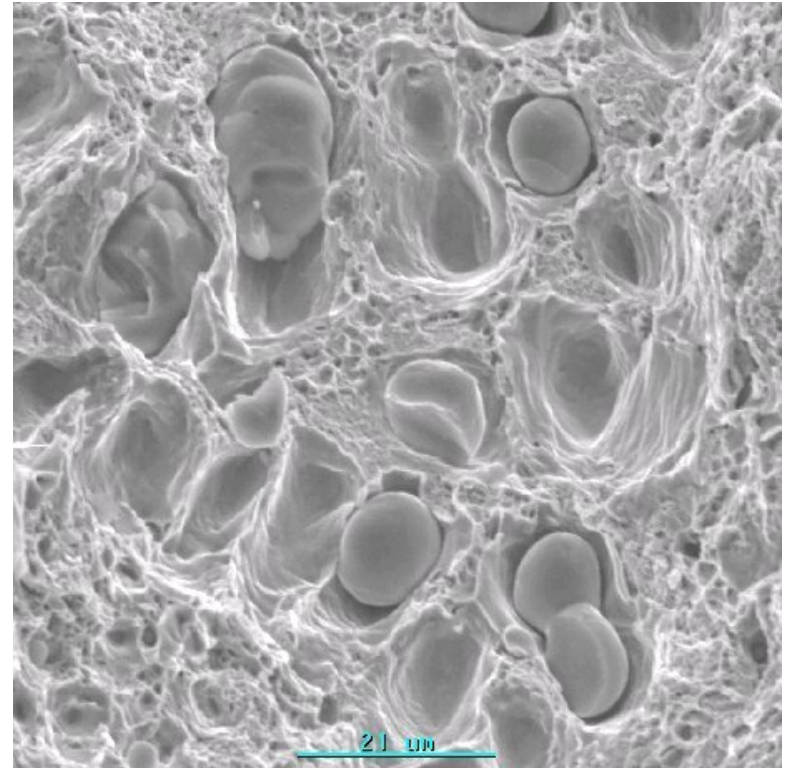
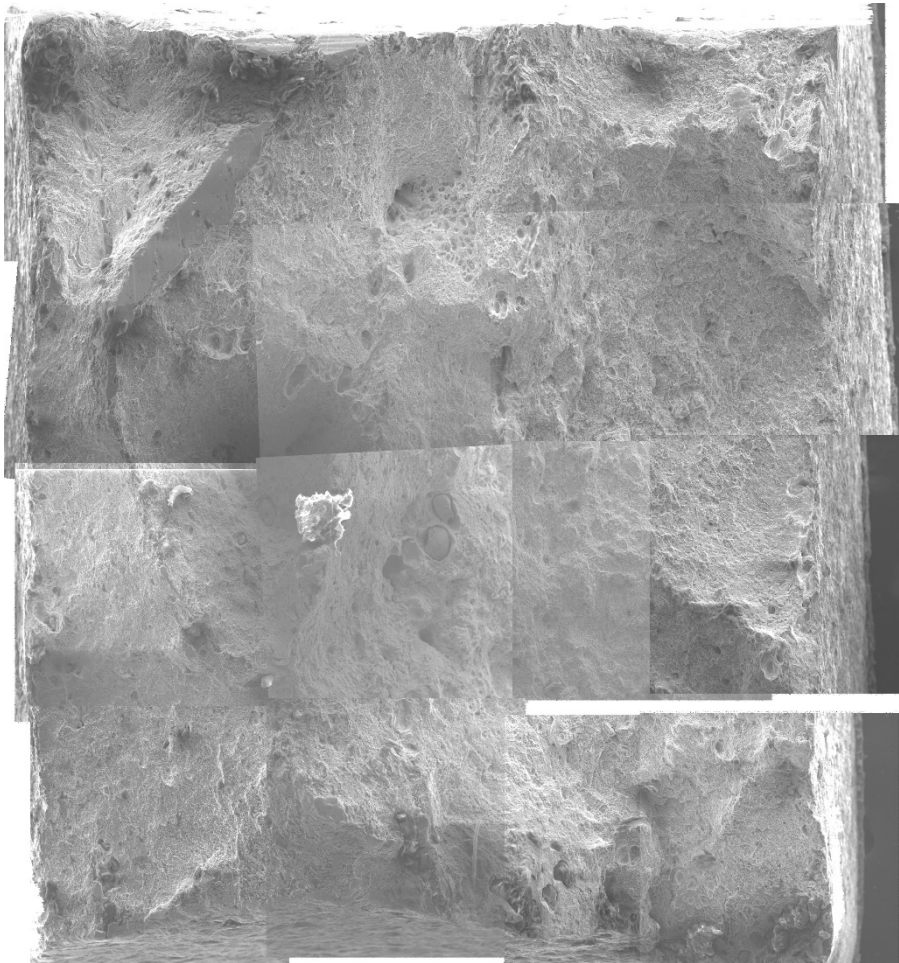
1. Brittle fracture
2. Single crystal slip bands
3. Ideal ductile fracture (full elongation)
4. Realistic cup-and-cone fracture



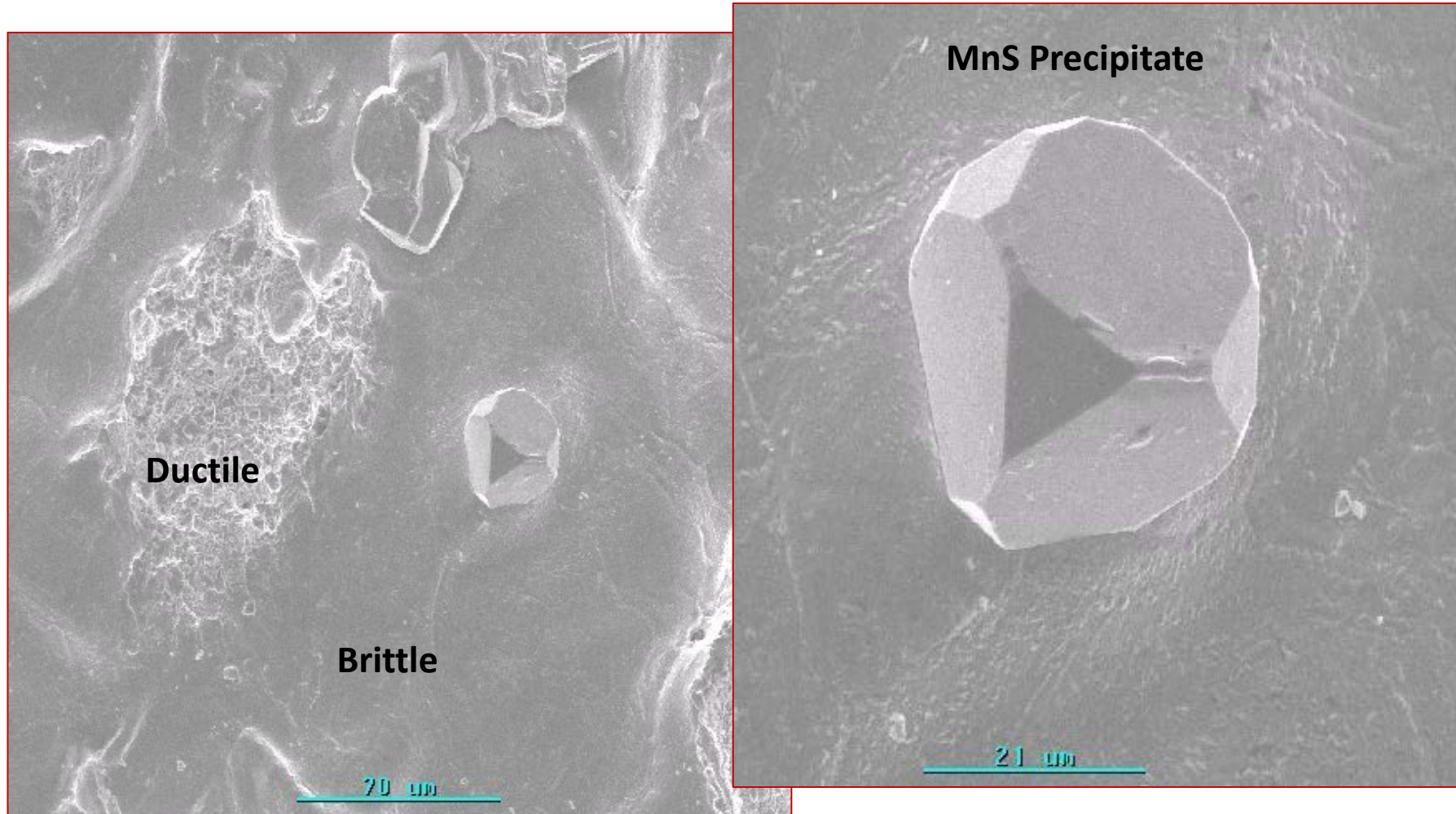
**Stages of cup-and-cone fracture formation in ductile materials**

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# Examples of Cup-and-Cone Fracture in Alcator C-Mod

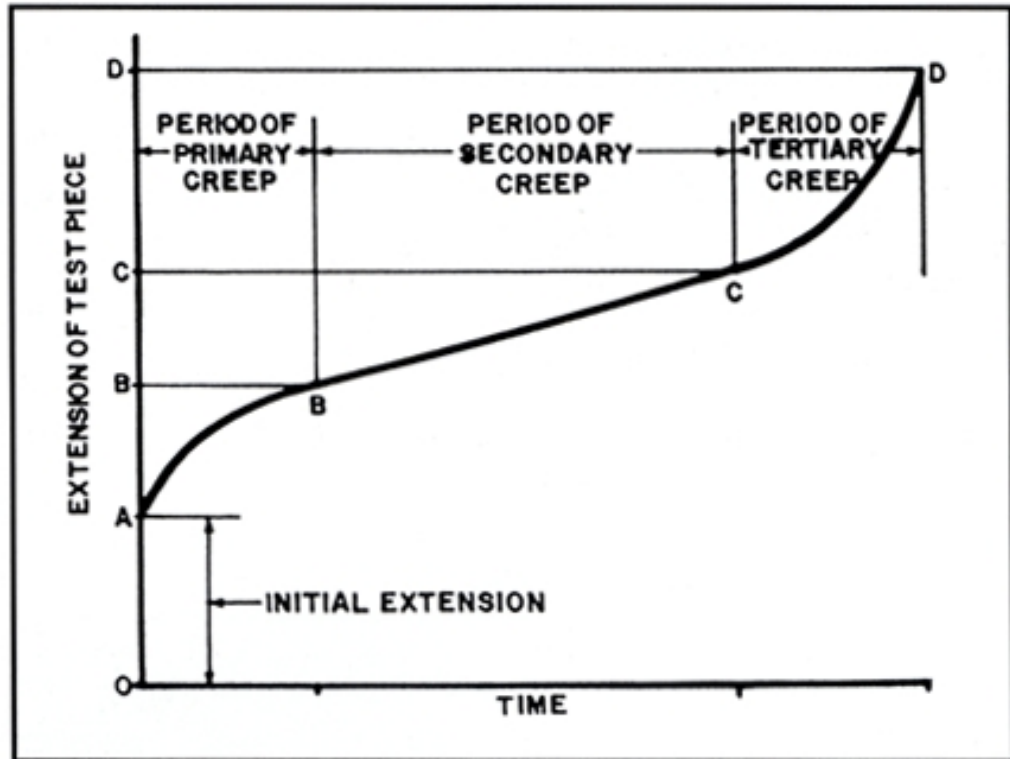
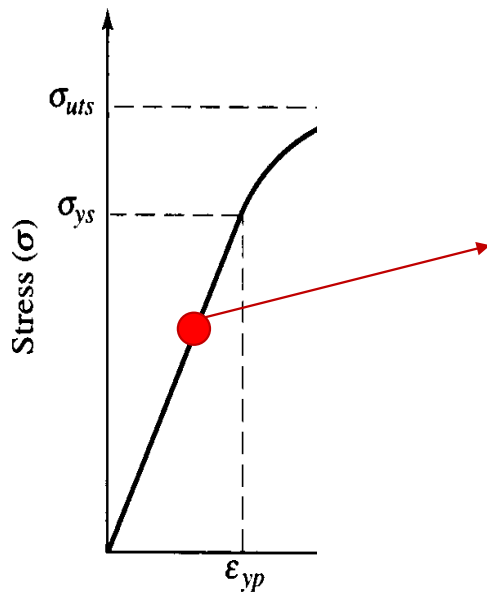


# Brittle & Ductile Fracture, Side by Side



# Creep – Plastic Deformation Below Yield Stress

- Imagine stretching a bar of metal within the elastic region



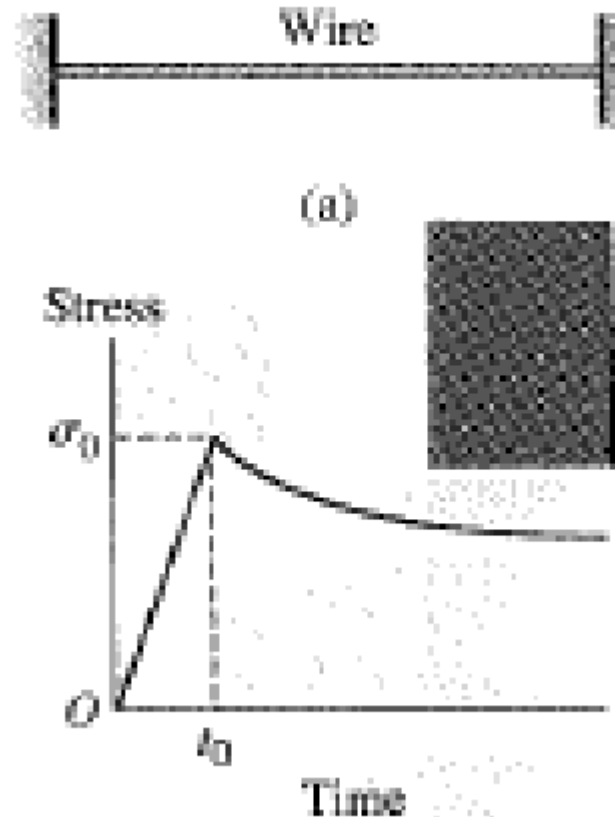
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<http://www.nationalboard.org/Index.aspx?pageID=181>

# Creep – Stress vs. Time

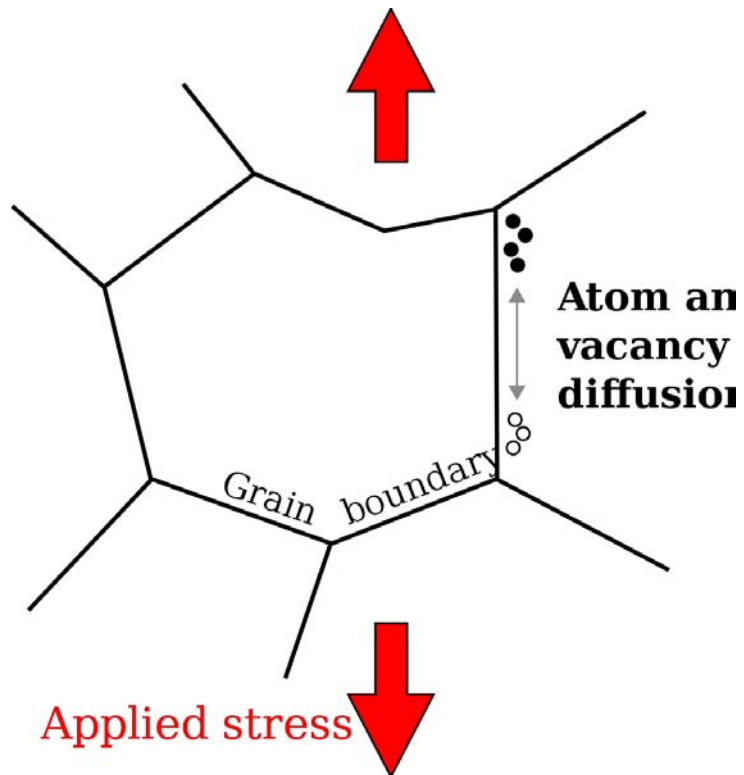
J. M. Gere, “Mechanics of Materials,” pp. 22

- Stress increased elastically to  $\sigma_0$
- Held for long time
- Stress at constant strain decreases due to *creep*



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# Creep Mechanisms



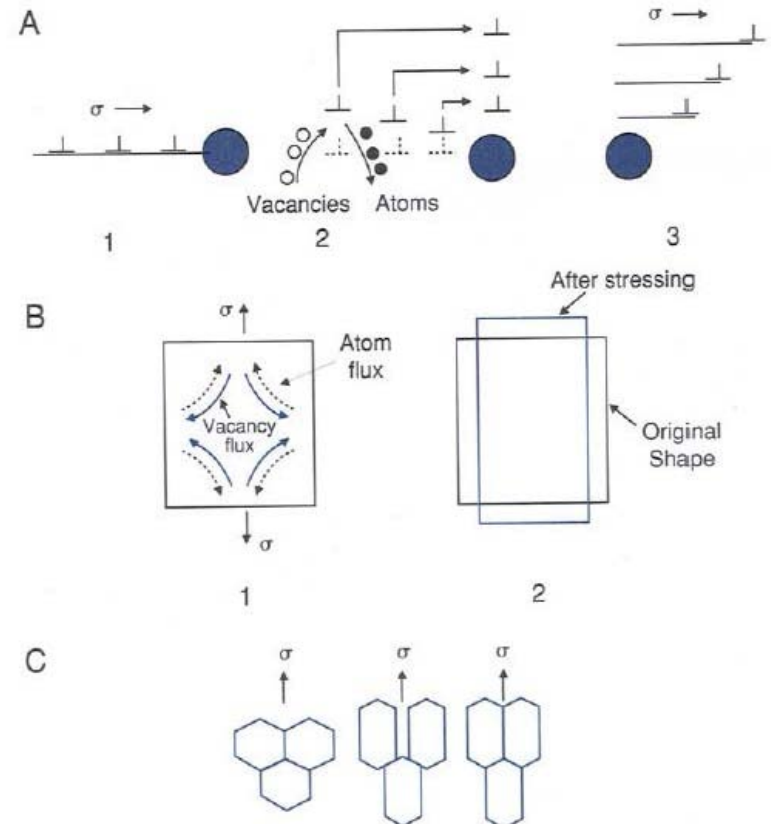
This image is in the public domain.

Source: Wikimedia Commons

- Plastic flow under constant stress
- Tension, gravity...
- Happens well below yield stress
- Multiple modes (Coble, Nabarro-Herring...)

# Creep Mechanisms

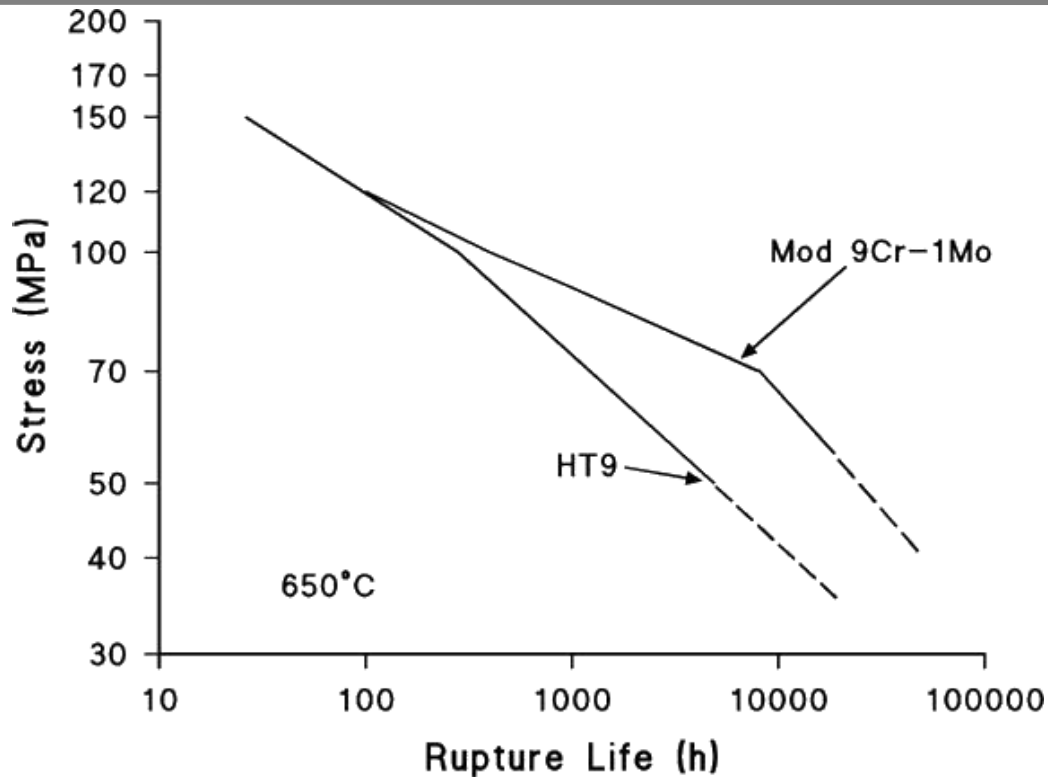
- Dislocation climb
  - Follows power law
- Nabarro-Herring (diffusional)
  - Vacancy movement
- Coble
  - Grain boundary movement



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Engineering Materials Science, *Milton Ohring*, Ch. 10

# Failure Criterion – Creep Lifetime



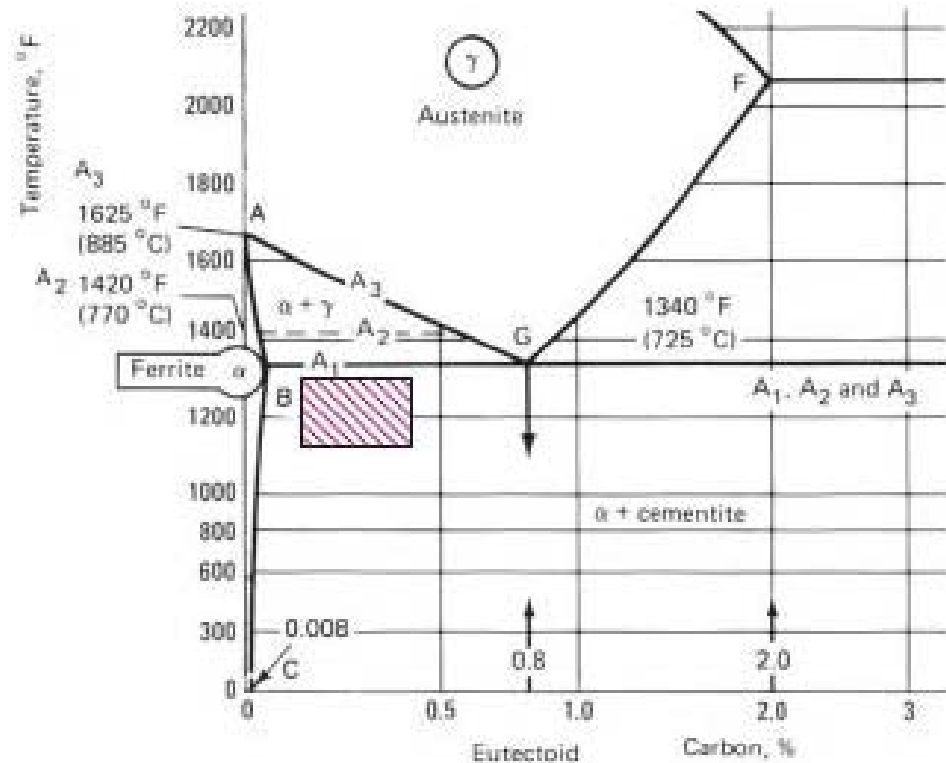
- Creep rupture lifetime can limit usefulness of part
- Example: Alloys HT9, T91 in high temperature service conditions

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Source: Klueh, R. L., and A. T. Nelson. "Ferritic / Martensitic Steels for Next-generation Reactors." *Journal of Nuclear Materials* 371, no. 1-3 (2007): 37-52.

Source: R.L. Klueh, A.T. Nelson. *J. Nucl. Mater.*, 371(1-3):37-52 (2007).



# Creep Failure by Time at Temperature and Pressure



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**Creep failure of alloy T91 due to improper heat treatment, heated above A1 temperature. In T. Totemeier, "Experience with Grade 91 Steel in the Fossil Power Industry." Presentation, ALSTOM, Feb. 2009.**

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## 22.14 Materials in Nuclear Engineering

Spring 2015

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