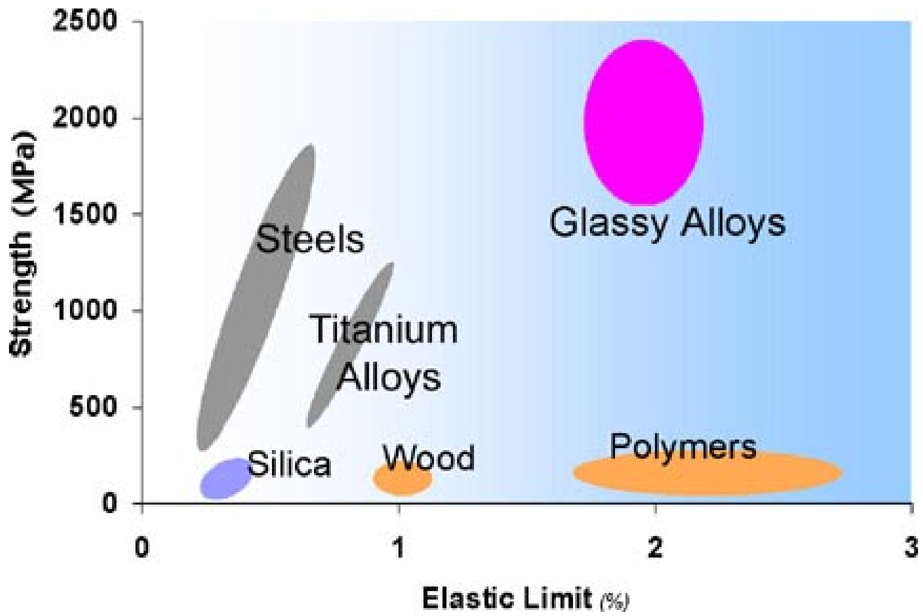
Material Mystery of the Day – Bulk Metallic Glasses

- Most metals are crystalline – have regular, repeating arrays of atoms.
- Amorphous metals – bulk metallic glasses – do not.
  - How to get this structure?
    - Create alloys with many atoms of different sizes.
    - Quench metals *extremely* quickly so that atoms (10^6 K/s) don't have time to diffuse to equilibrium positions.
- First amorphous alloy ~1960, Caltech – $Au_{75}Si_{25}$
- Northwestern – 2018: AI to identify new candidate materials!



Material Mystery of the Day – Bulk Metallic Glasses

- Questions:
  - Would this show up on the equilibrium phase diagram?
  - **Why are bulk metallic glasses are often *stronger*, than crystalline metals?**
  - How do you think a stress strain-curve for an amorphous metal might.
  - Stress-strain curve?
  - **Applications?**

https://www.youtube.com/watch?v=WbPpgQtv7Xc

Mechanical Properties cont., Plasticity

Dr. Jonathan Emery

Cook 3035 — jonathan.emery@northwestern.edu

ANNOUNCEMENTS — May 19th, 2020

Lecture Topic -Finish Mechanical Properties/Stress-strain curves
-Plastic Deformation

Logistics -P-set/Quiz D8 next **Wednesday**

Reading Chap. 7.1—7.6, (7.8-7.12)

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Outline

- Analysis of Stress-strain Curves
  - Young's modulus
  - Yield strength
  - Ultimate tensile strength
  - Ductility
  - Resilience
  - Toughness

- The physical mechanism behind plasticity is the permanent motion of atoms. This is embodied through dislocation (e.g., edge and screw) motion.

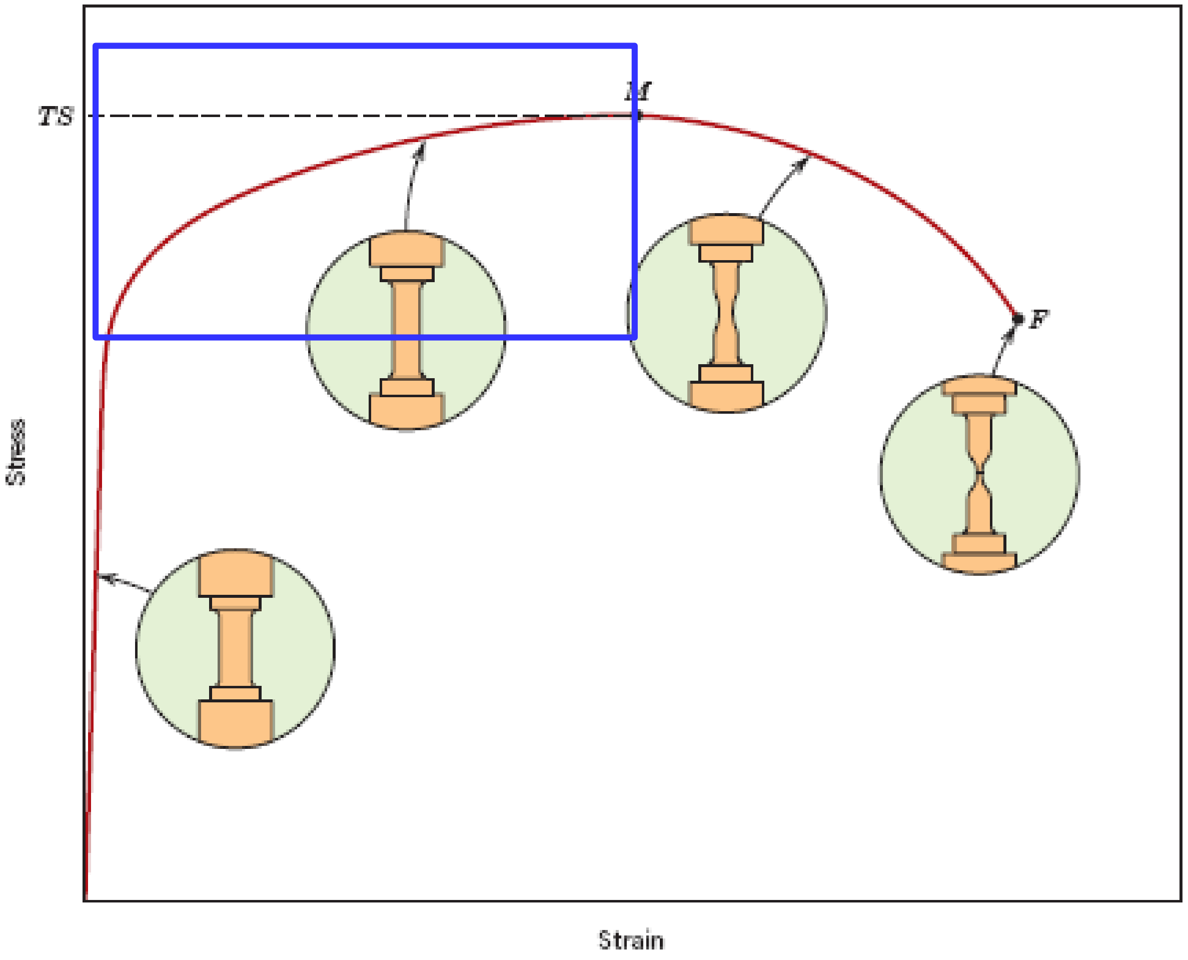
- Edge and screw dislocations can be quantified using Burger's circuits to acquire a Burger's vector, which has a direction and magnitude.

- Slip will occur along preferred planes in crystals – the lowest energy barriers are along close-packed direction within close-packed planes.

Plastic Deformation [VL]

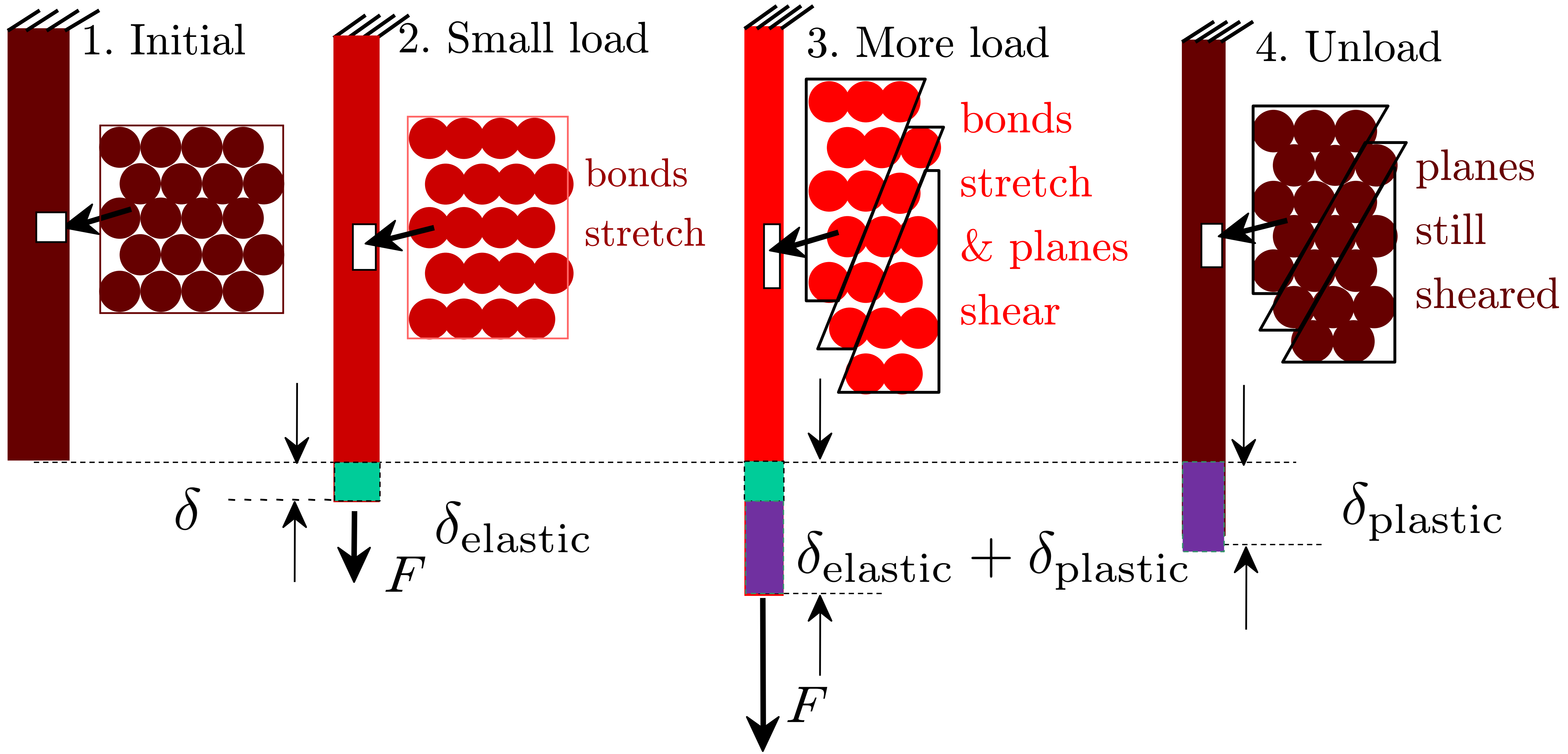
- Typical metals deform elastically up to a strain of ε ~0.005, or 0.5%
-
- Beyond this yield point, permanent, non-recoverable (plastic) deformation occurs.

- Plastic deformation implies *breaking* of bonds.



Continue with more in-depth discussion on plastic deformation mechanisms next time.

Atomic-Level Plastic Deformation [VL]



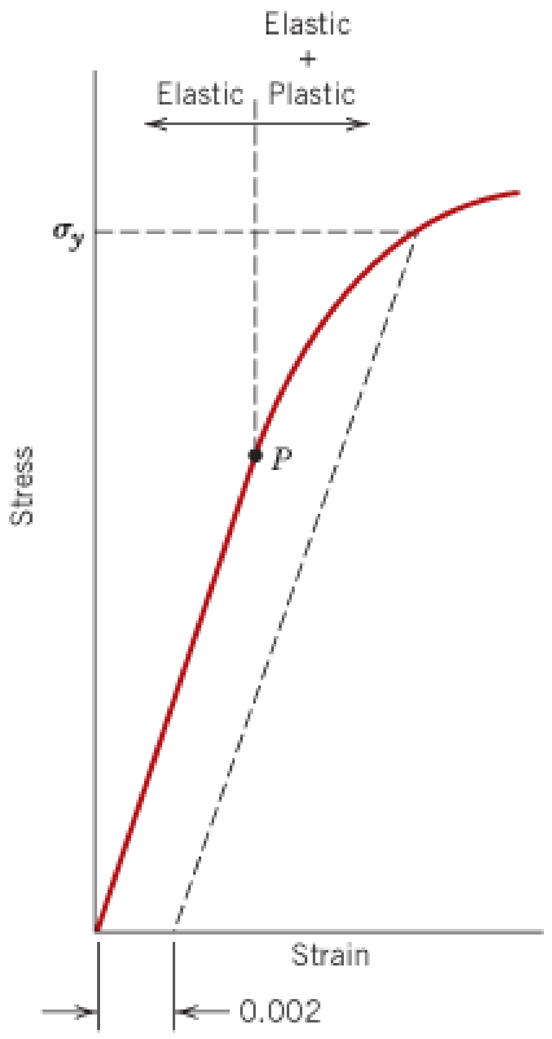
Yield Strength, σ_y [VL]

- Yield strength (σ_y) is the stress at which measurable plastic deformation has occurred.

- Use $\varepsilon = 0.002$ strain offset method.

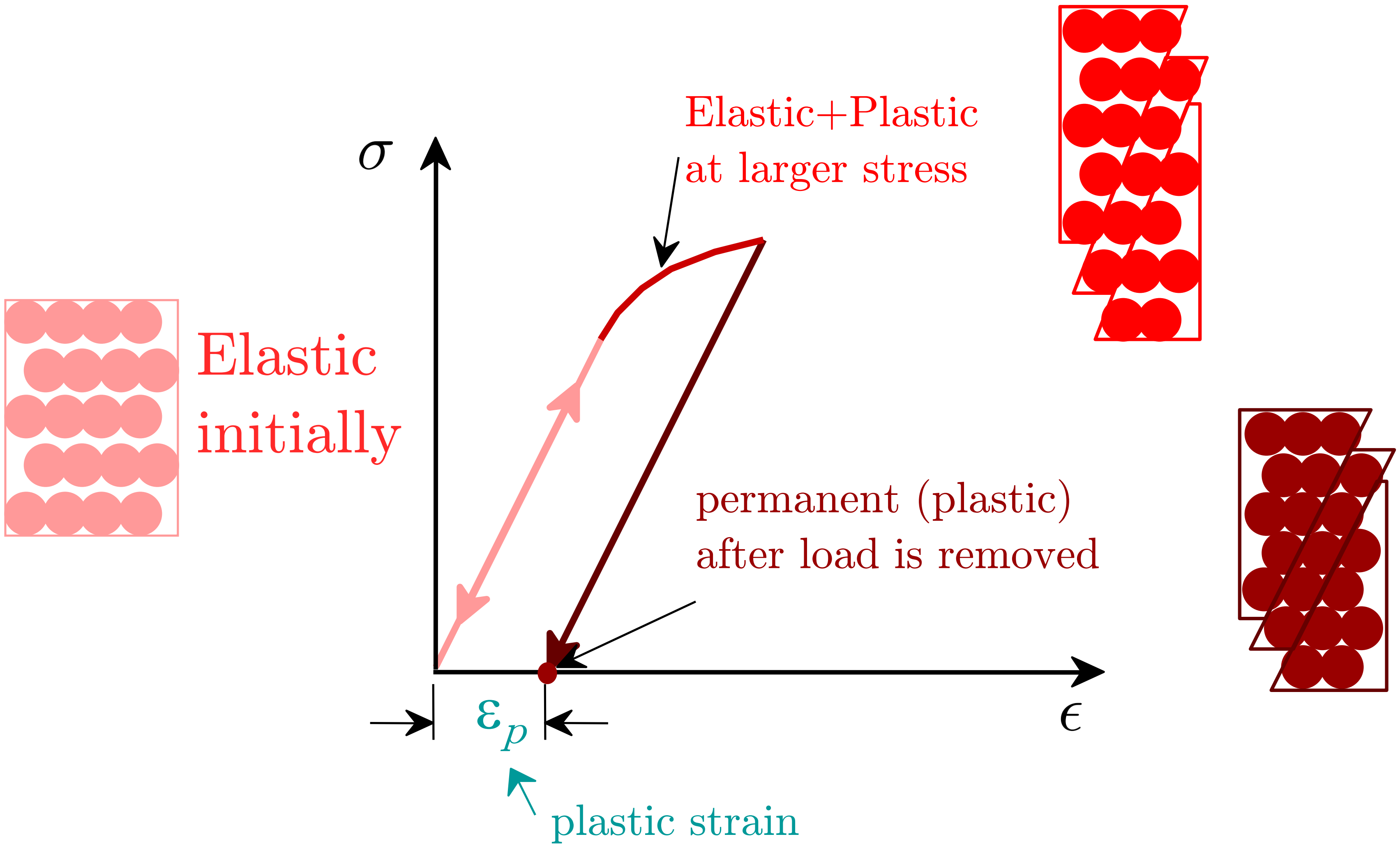
Characteristic stress-strain curves:
- Gradual elastic-plastic (most metals) deformation is often considered “failure” in engineering design.

1. Proportionality limit
2. Offset Yield Strength ($\varepsilon = 0.002$ or 0.2%)



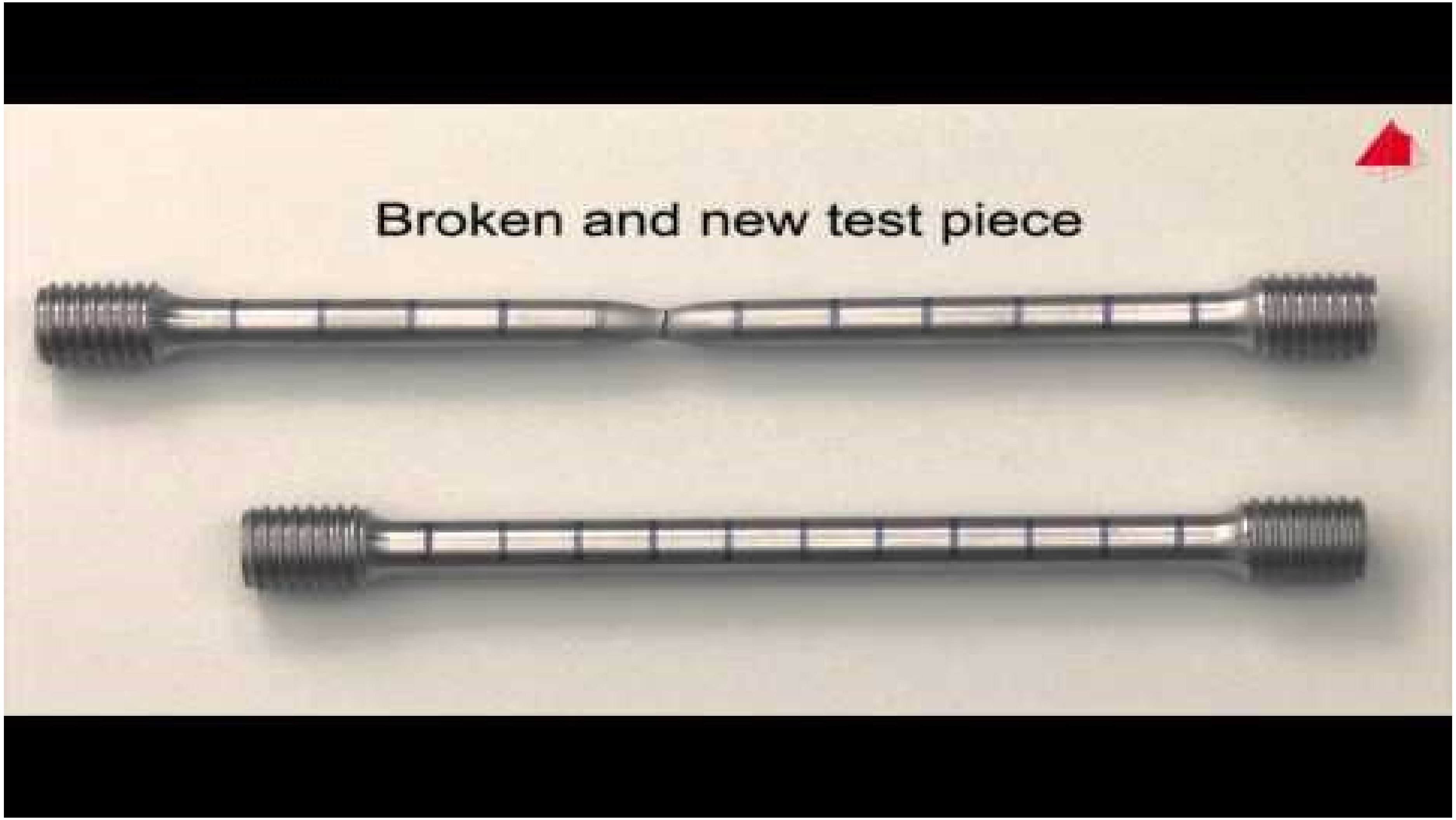
Elastic Recovery After Plastic Deformation (Video Lecture)

- Simple tension test:



Tensile Test

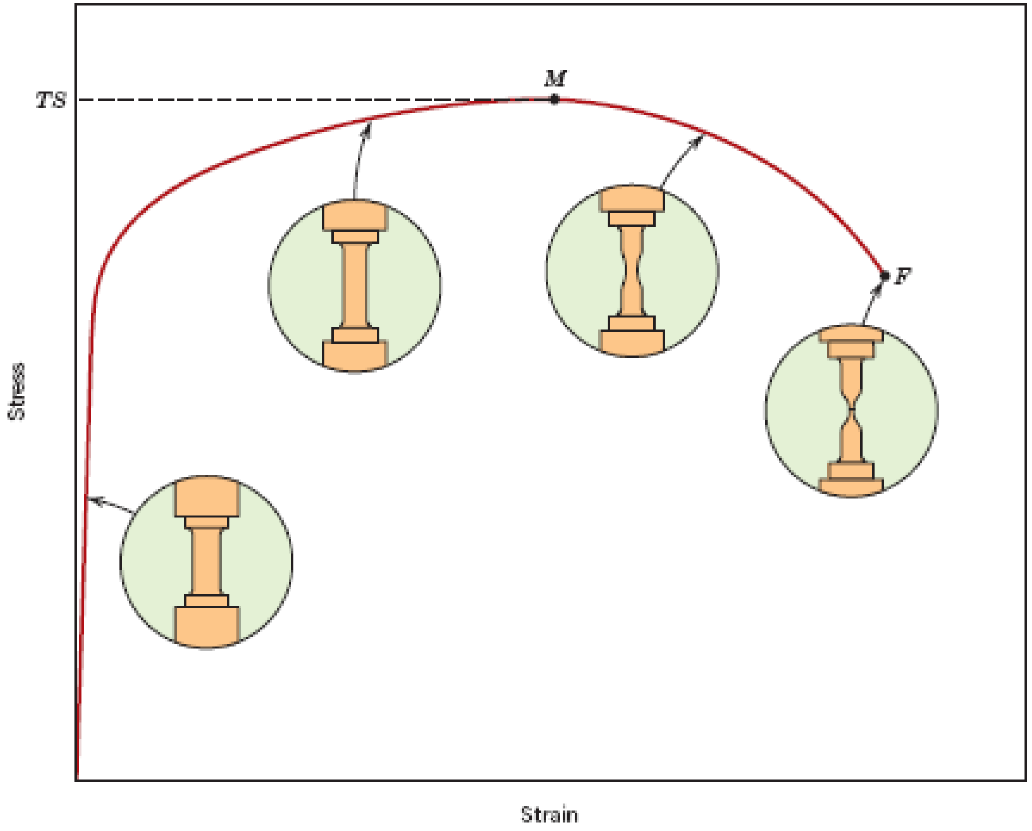
6:00-end



Tensile Strength [VL]

- Maximum stress on engineering stress-strain curve.
- Maximum stress applied on a structure in tension
- Failure will occur if this stress is maintained

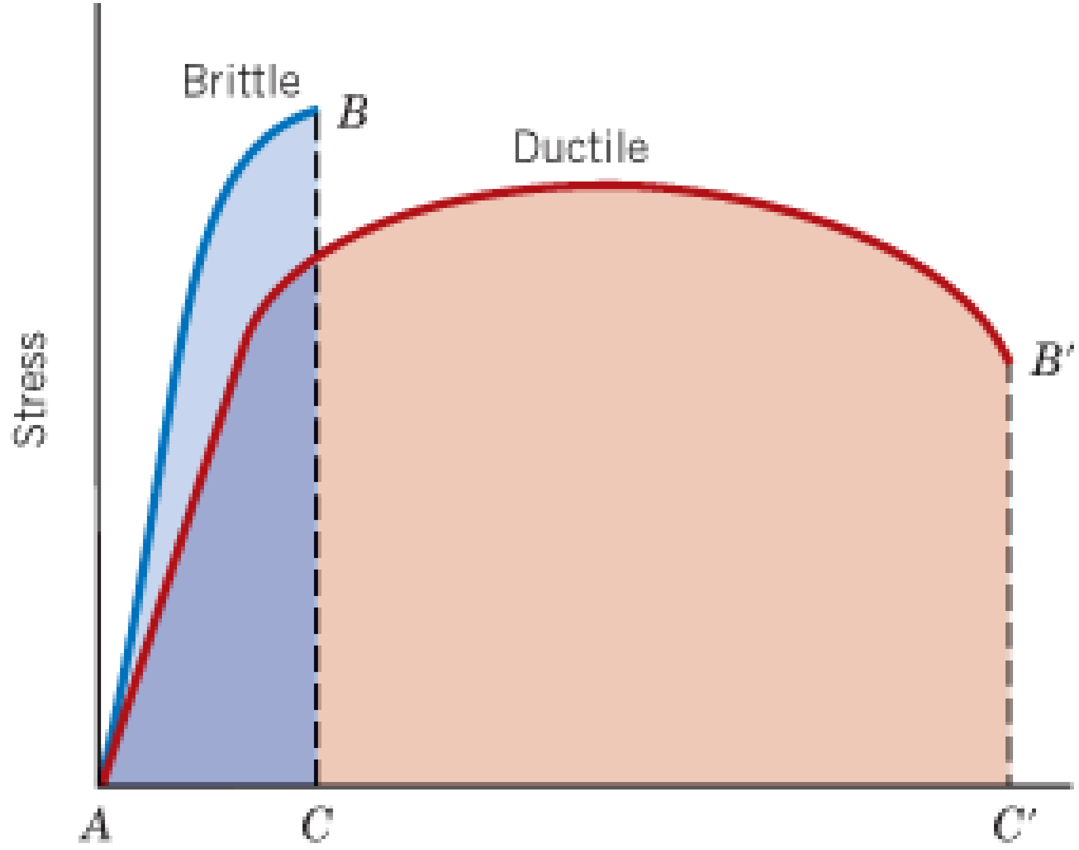
Tensile Strength (TS)



Ductility [VL]

- How much can a material deform before fracture?
- %EL at fracture.

$$\%EL = 100 \times (\frac{l_f - l_0}{l_0})$$



$C \rightarrow \%EL_B$ $\quad$ $C' = \%EL_{B'}$

Ductility

- Degree of plastic deformation that can be sustained before fracture
- Influences "workability" of material

Table 6.2 Typical Mechanical Properties of Several Metals and Alloys in an Annealed State

Metal Alloy	*Yield Strength, MPa (ksi)*	*Tensile Strength, MPa (ksi)*	*Ductility, %EL [in 50 mm (2 in.)]*
Aluminum	35 (5)	90 (13)	40
Copper	69 (10)	200 (29)	45
Brass (70Cu-30Zn)	75 (11)	300 (44)	68
Iron	130 (19)	262 (38)	45
Nickel	138 (20)	480 (70)	40
Steel (1020)	180 (26)	380 (55)	25
Titanium	450 (65)	520 (75)	25
Molybdenum	565 (82)	655 (95)	35

Resilience, U_r [VL]

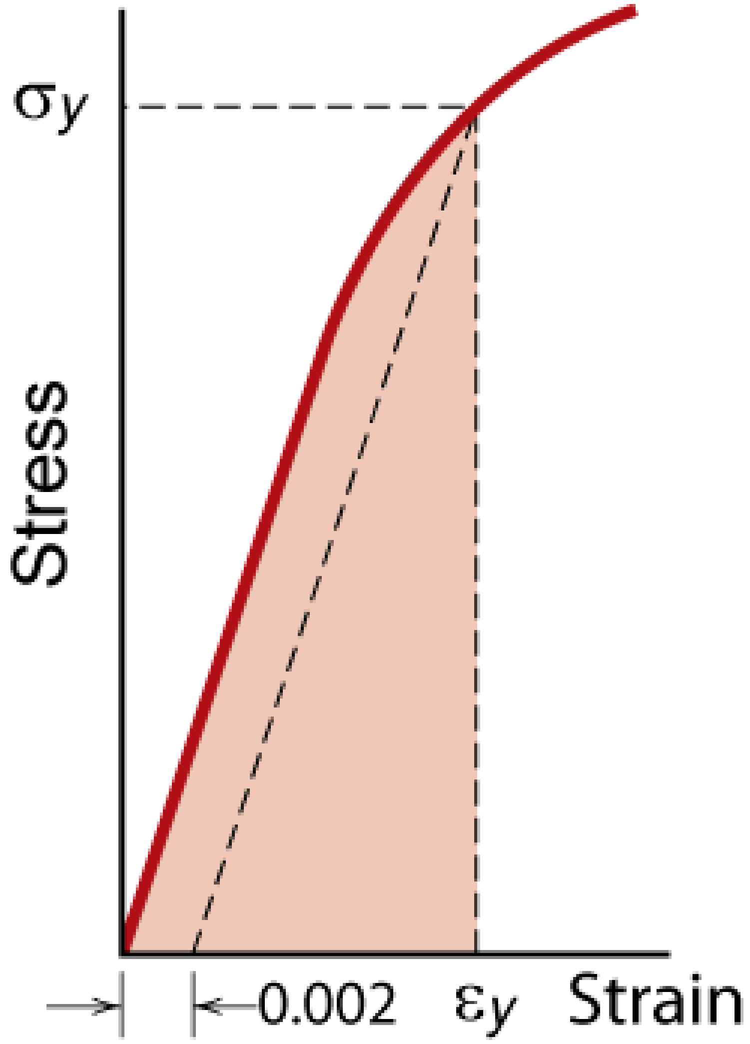
$$U_r = \int_0^{\epsilon_y} \sigma d\epsilon$$

Approximate by assuming linear elastic region:

$$U_r \approx \frac{1}{2}\sigma_y \epsilon_y$$

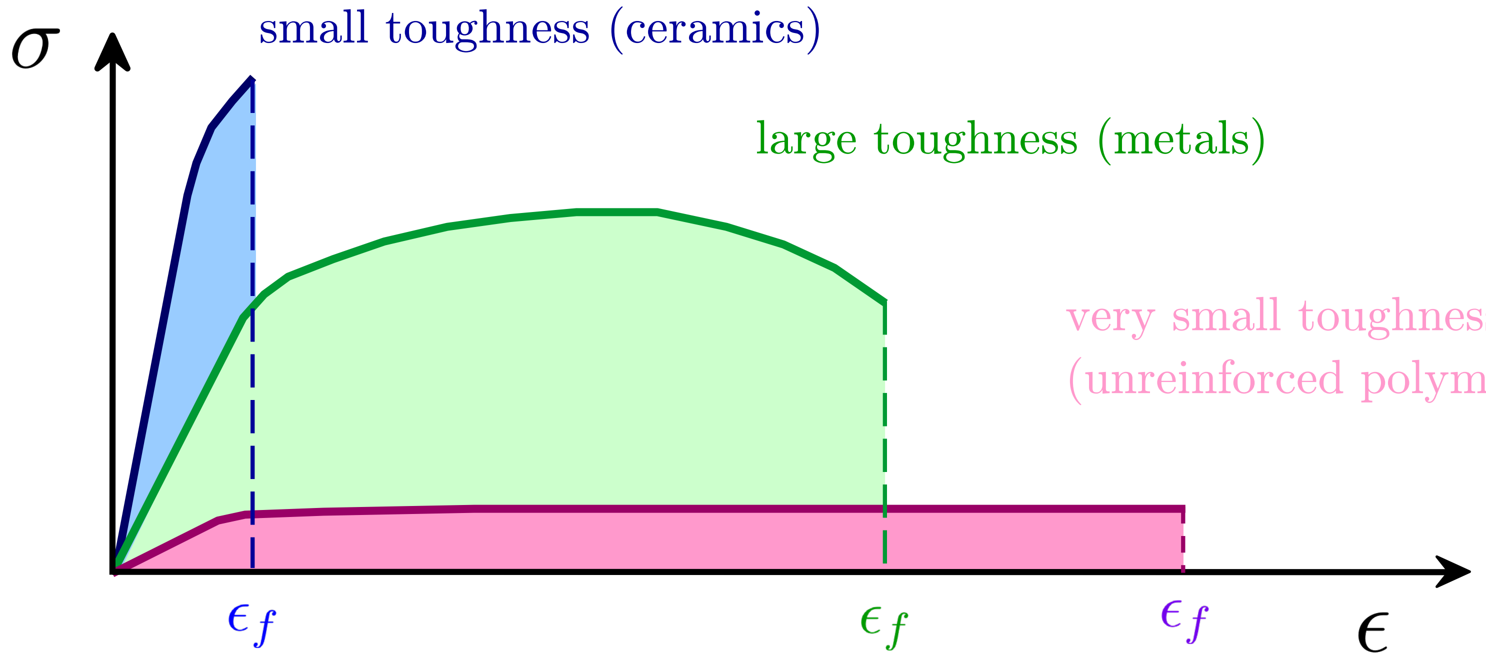
$$U_r \approx \frac{1}{2}\sigma_y \epsilon_y \approx \frac{1}{2}\sigma_y \frac{\sigma_y}{E} = \frac{\sigma_y^2}{2E}$$

- Ability of a material to store energy –
  - Apply elastic deformation
  - Retrieve energy
- Think: shooting a rubber band across the room.
- How to make the best diving board? (or spring…)



Toughness [VL]

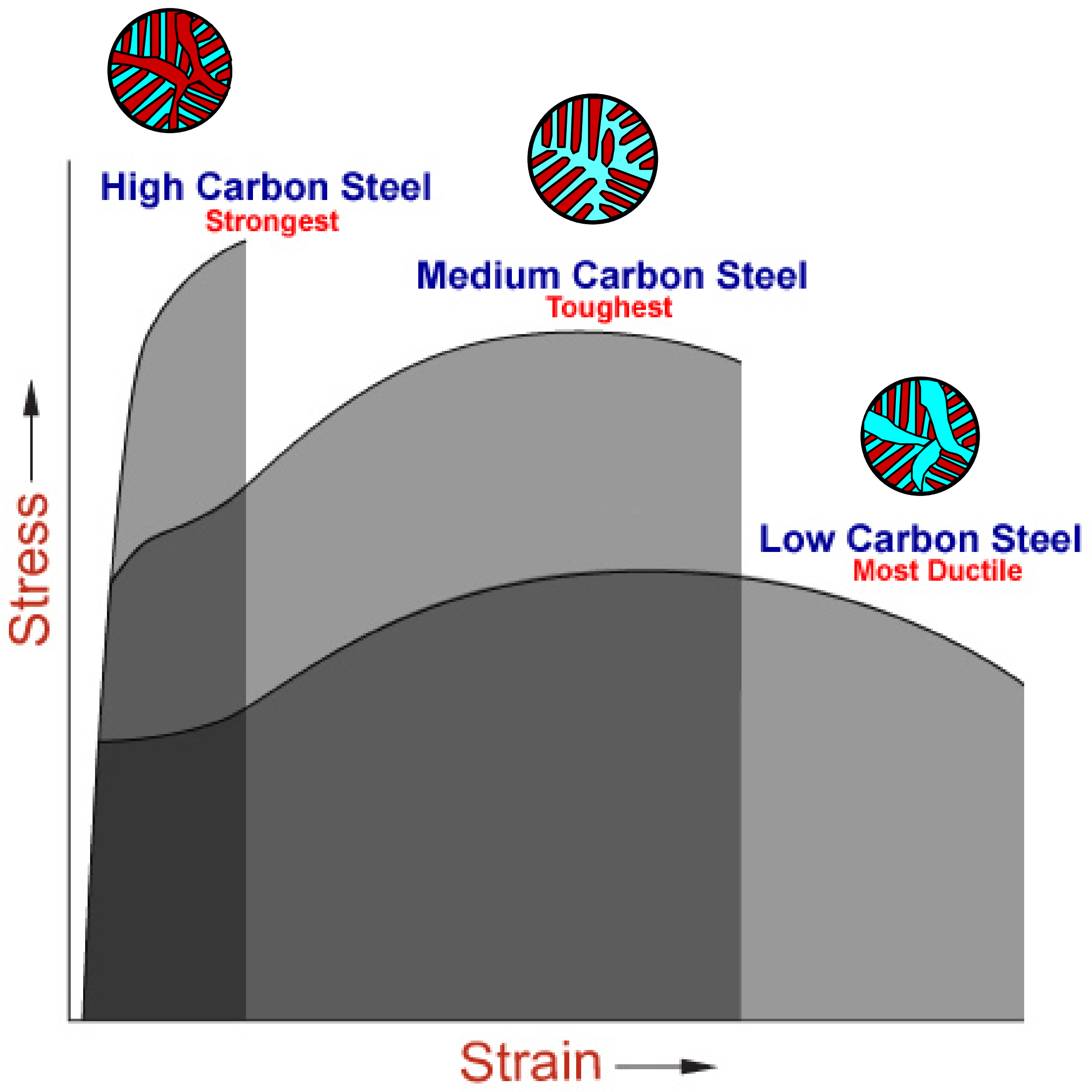
- Energy to break a unit volume of material
- Approximate by the area under the entire stress-strain curve.



$$U_t = \int_0^{\epsilon_f} \sigma d\epsilon$$

High toughness → both high tensile strength and high ductility

Comparisons of Steel



Summery: Values from the Stress-Strain Curve

- Young's modulus (E or Y): Resistance to elastic deformation:

$$E = \frac{\Delta\sigma}{\Delta\epsilon}$$

- Yield strength (σ_y): Stress at onset of plastic deformation (0.002 method).

- Ductility (%EL): Degree of deformation at fracture. Characterized by:

$$\%EL = 100 \times \left(\frac{l_f - l_0}{l_0}\right)$$

- Tensile strength (TS): Maximum engineering stress that a specimen can tolerate

- Resilience: Energy stored during elastic deformation to the yield strain.

$$U_r = \int_0^{\epsilon_y} \sigma d\epsilon$$

- Toughness: Energy absorbed prior to fracture of a material.

$$U_t = \int_0^{\epsilon_f} \sigma d\epsilon$$

Red – derived from stress strain curve, Green – derived from area under regions of the stress-strain curve.

Concept Check

Select one ore more answers for the following question: Which of the following properties ***cannot*** be found using a stress-strain curve derived from a tensile test?

A. Poisson's Ratio

B. Yield Strength

C. Tensile Strength

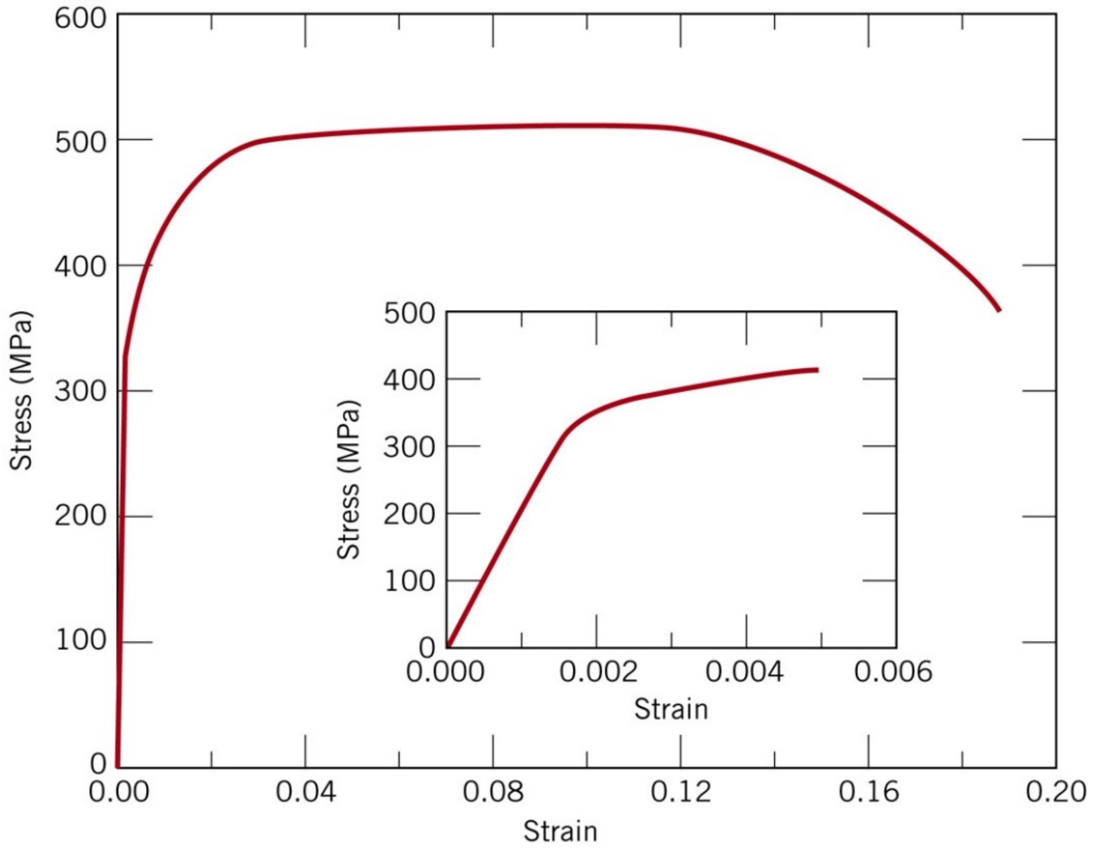
D. Toughness

E. Young's Modulus

F. Resilience

G. Shear Modulus

H. Elongation-to-fracture (ductility)



Concept Check – Solution

. ***Select one ore more answers for the following question:*** Which of the following properties ***cannot*** be found using a stress-strain curve derived from a tensile test?

A. Poisson's Ratio
B. Yield Strength
C. Tensile Strength
D. Toughness
E. Young's Modulus
F. Resilience
G. Shear Modulus
H. Elongation-to-fracture (ductility)

Solution:

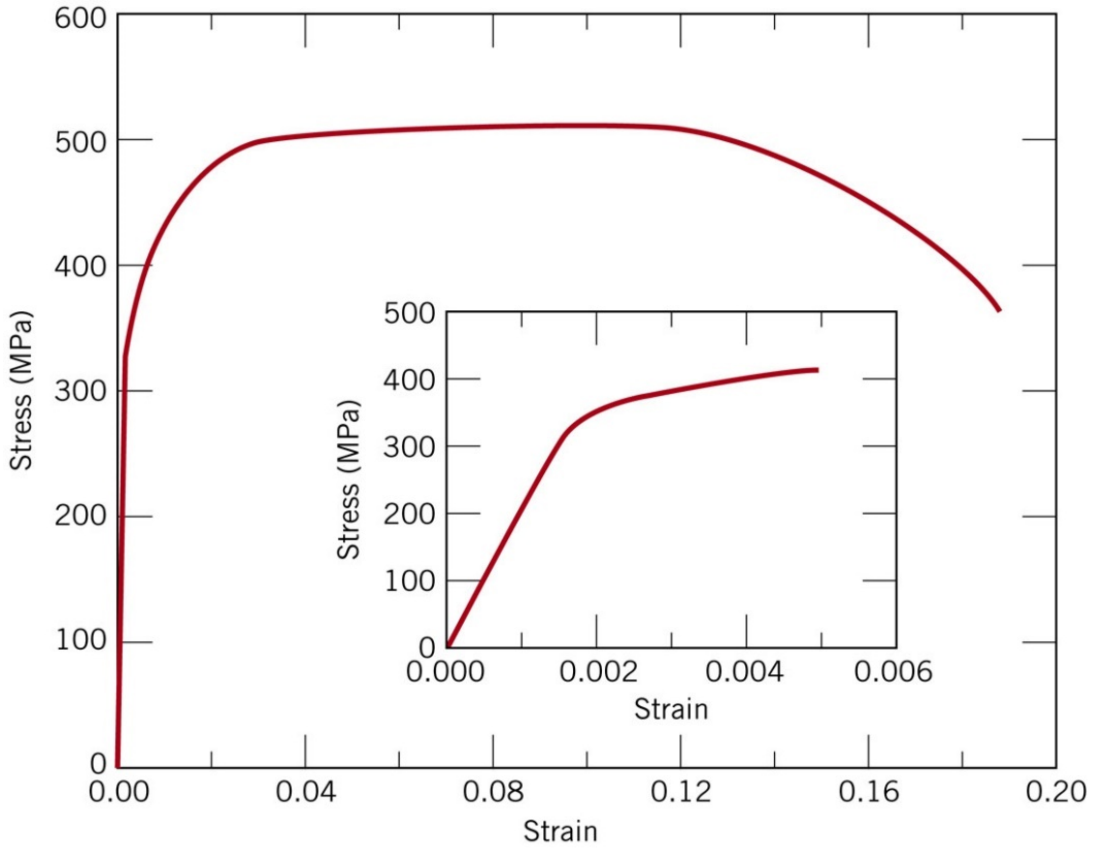
- The yield strength is found by the transition of elastic to plastic deformation (linear to sub-linear on the stress-strain curve).
- The tensile strength is the highest stress reached by the curve.
- The toughness is the integral of the stress-strain curve.
- The Young's modulus is the slope of the curve in the elastic (linear) regime.
- Ductility is derived as the strain-to-fracture.

The Poisson's ratio cannot be directly derived from the stress-strain curve, and this is a ***tensile*** test, so we can't get the shear modulus (although, with isotropic materials there is a conversion).

Concept Check

. For the stress-strain curve to the right, derive the following values:

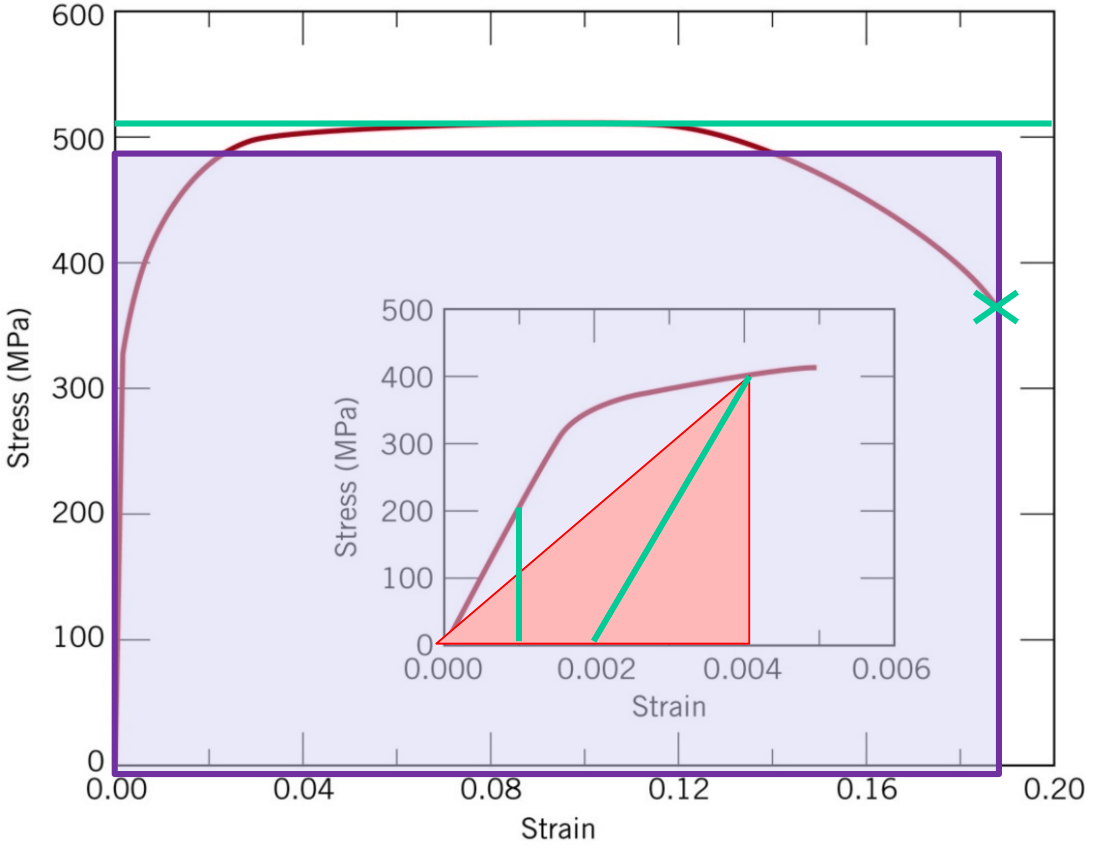
- ◇ The elastic modulus.
- ◇ The yield strength.
- ◇ The ultimate tensile strength.
- ◇ The ductility.
- ◇ The resilience.
- ◇ The fracture toughness.



Concept Check – Solution

Solution:

- The elastic modulus is $E = \frac{\Delta\sigma}{\Delta\epsilon}$ in the linear-elastic region. I'll pick the origin as one point and about $\epsilon = 0.001$ and $\sigma = 200\,\text{MPa}$ as the other: $E = \frac{200\,\text{MPa} - 0\,\text{MPa}}{0.001 - 0} = 150 \times 10^3\,\text{MPa} = 150\,\text{GPa}$.
- the yield strength using the 0.002 offset method is about 400 MPa, read from the graph.
- The tensile strength is about 510 MPa, read from the graph.
- The ductility is the total eleongation at fracture — the end of the stress-strain curve — this is about 0.19.
- The resilience is approximated well using the $U_r = \frac{1}{2}\epsilon_y\sigma_y = \frac{1}{2}400\,\text{MPa} \times 0.004 = 0.8\,\text{MPa}$.
- The toughness is the area under the entire curve. I approximated this with an area the includes a bit of area outside the curve and precludes a bit of area inside the curve. Should be pretty good. I get about $475\,\text{MPa} \times 0.1920\,\text{MPa}$.



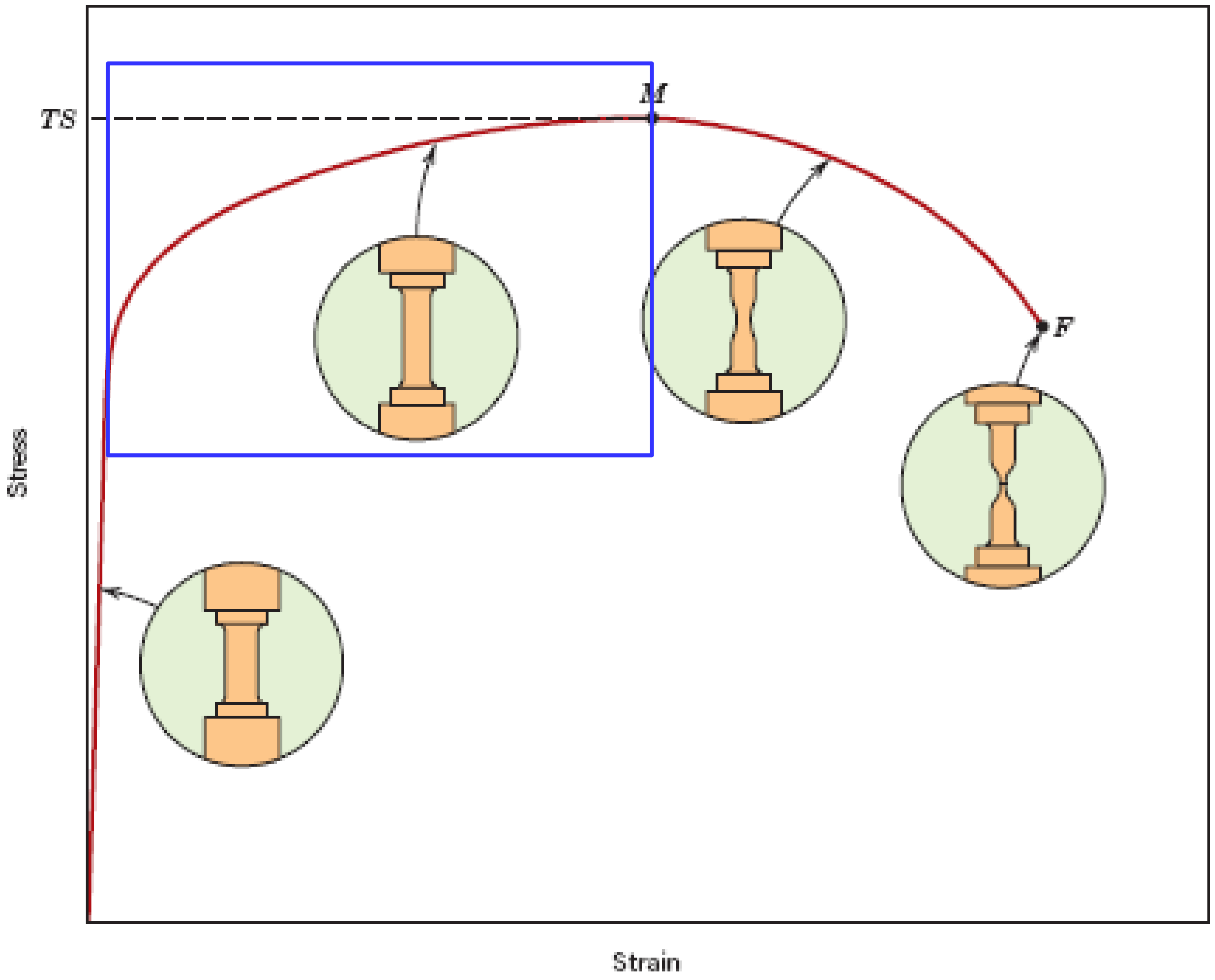
Dislocations and Plasticity

- What are the structural/mechanistic sources of plasticity?
- How does *dislocation motion* embody plasticity?
- How do other imperfections (0D, 1D and 2D) interact with dislocations to influence plasticity?
- How can we use these phenomena to strengthen materials?

L. Bragg W.M Lomer, and J. Nye, 1954., honda.com

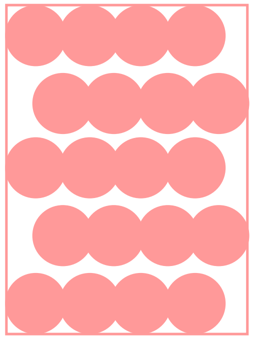
Plasticity

Plastic deformation behavior is *dominated* by the motion of dislocations (1D or line defections)

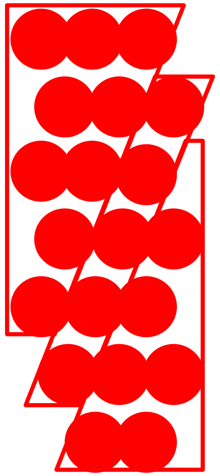


Is Our Cartoon Right?

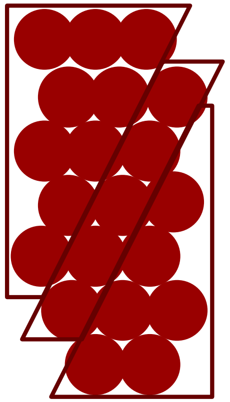
1.) Elastic Deformation



2.) “Slip”/Yield



3.) Permanent deformation



Atomic Motion in Perfect Crystal

The motion of *entire* atomic planes is *extremely* energetically expensive.

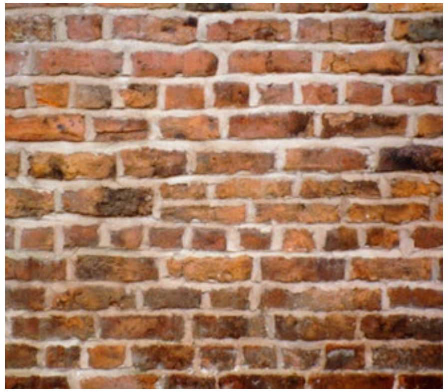
Material	τ_{theory} [10^6 N/m^2]	$\tau_{\text{exp.}}$ [10^6 N/m^2]
Ag	1.0×10^3	0.37
Al	0.9×10^3	0.78
Cu	1.4×10^3	0.49
Ni	2.6×10^3	3.20
α-Fe	2.6×10^3	27.5

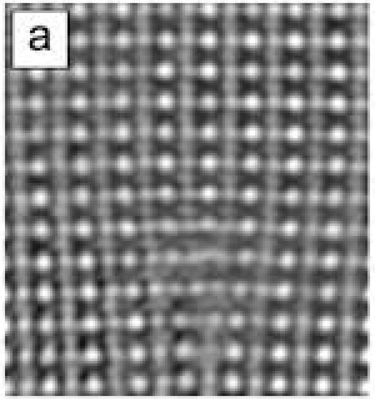
What's going on?

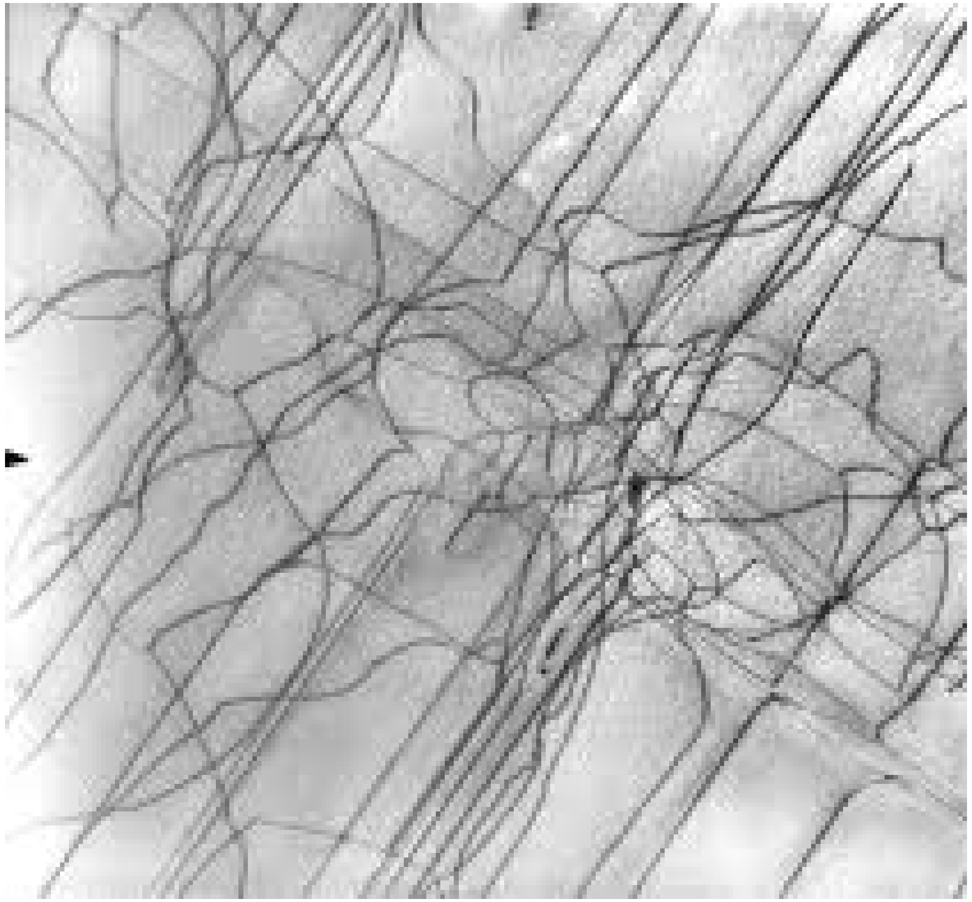
$\rightarrow$ Our model is wrong

- Perfect crystal: all atoms must slide at the same time for plastic deformation to occur.
- An *imperfect* crystal has no such limitation.
- In the 1930s, scientists develop the first aspects of the theory of *dislocation-mediated* plasticity.

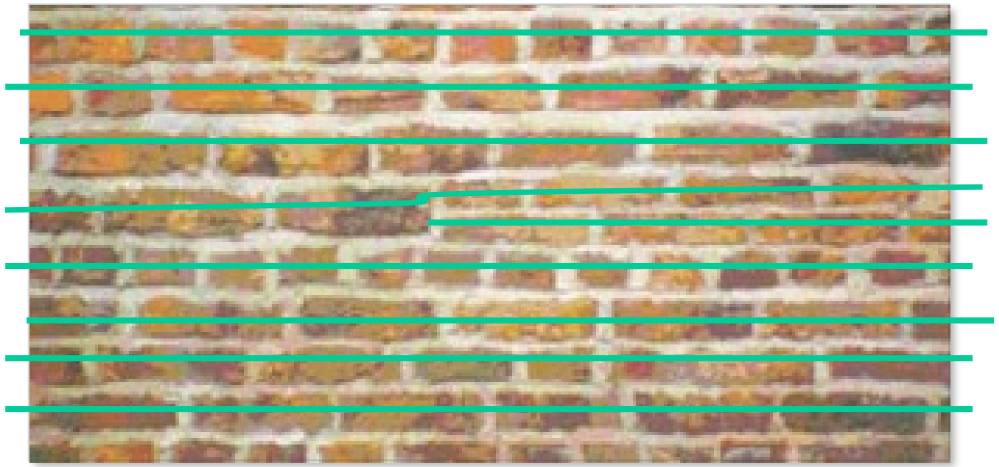
- **Dislocation Motion and Behavior**
  - **Edge dislocation**
  - **Screw dislocation**
  - **The Burgers vector**
  - Dislocation motion and slip systems (qualitative)
- Plastic Deformation in Single Crystals

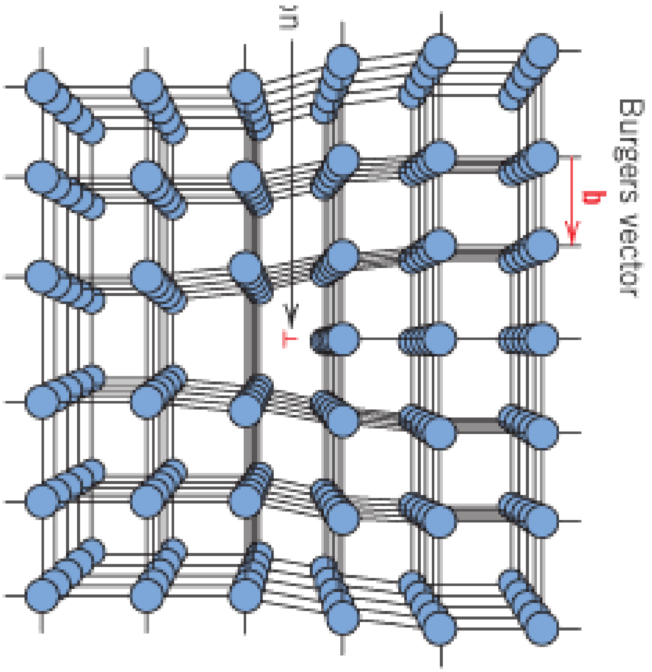






Edge Dislocation





- Dislocations
  - 1D defects around which atoms are <u>misaligned</u>
  - *Dislocation Line*: Line in the crystal around which some of the atoms are misaligned

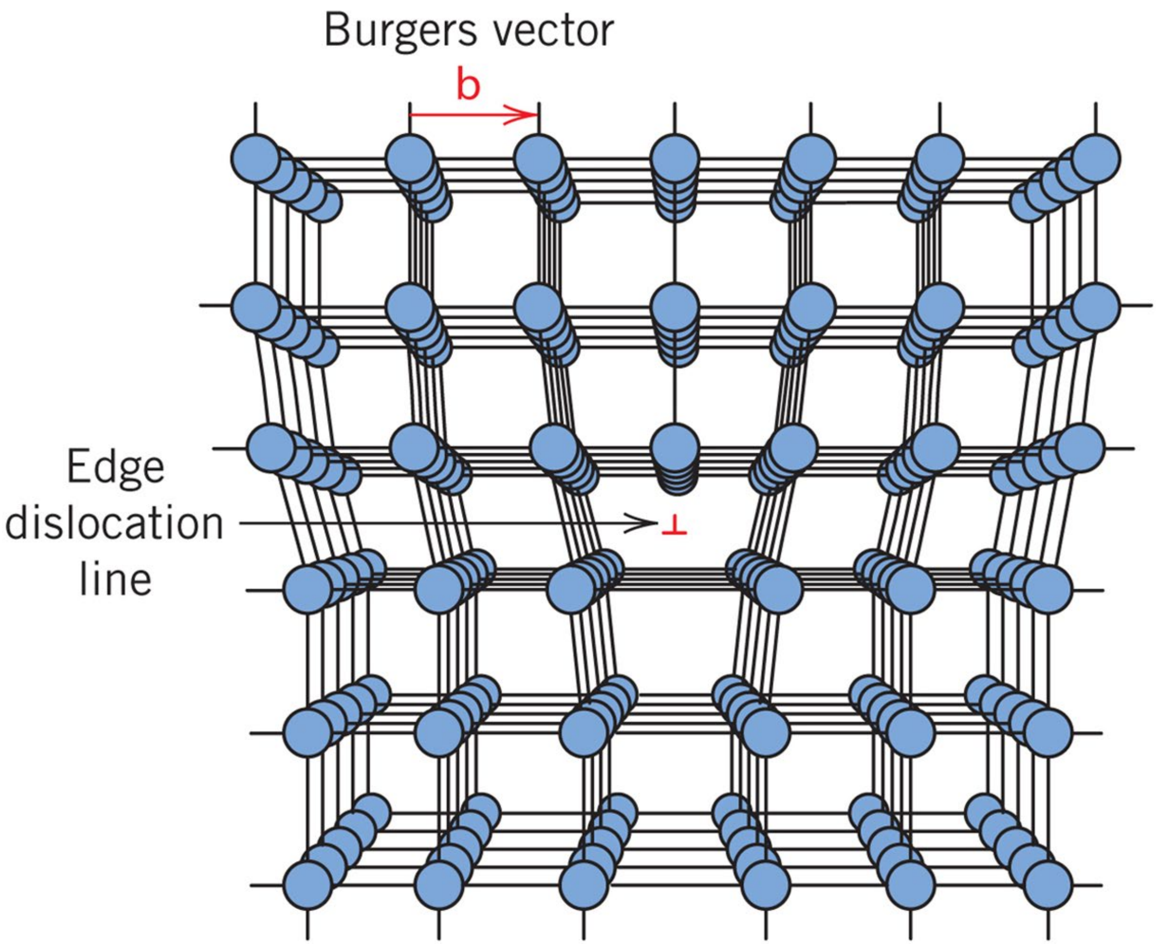
- Edge dislocation
  - Extra half-plane of atoms inserted in a crystal structure
  - ***b*** perpendicular (⊥) to dislocation ***line***

Burger's vector, ***b***: a measure of lattice distortion *wrt* magnitude and direction

Line Defects: Dislocations

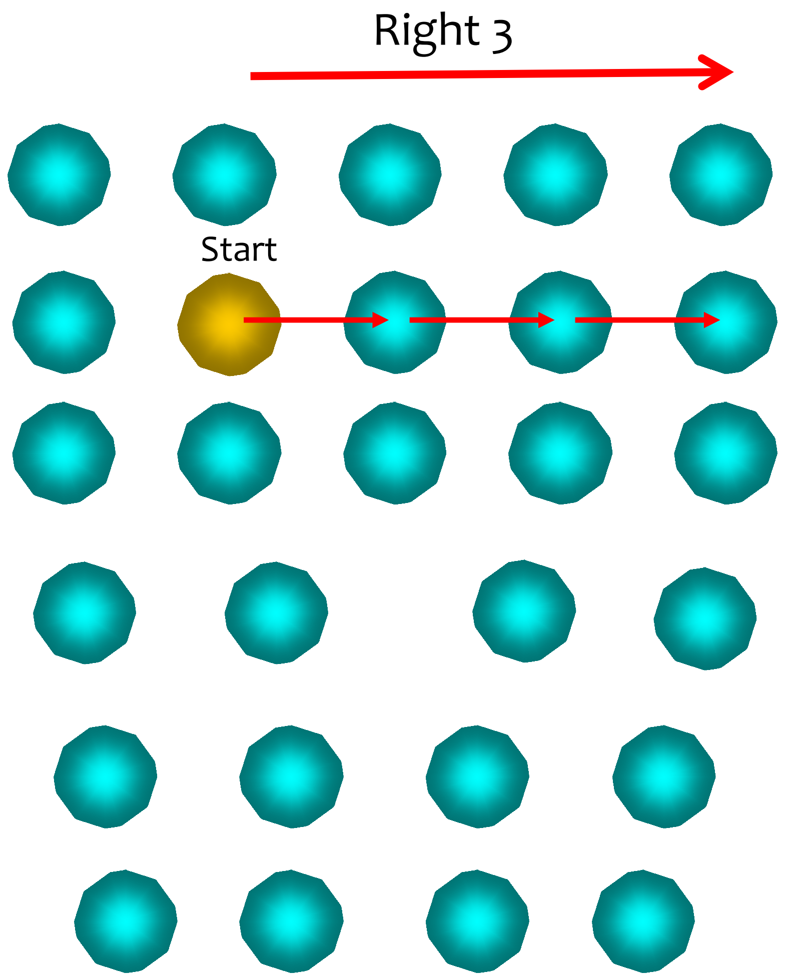
- Extra half-plane of atoms
- Terminates in the crystal body
- Local lattice distortion around dislocation core.
  - Non-ideal bond lengths
  - Strain energy

- Distortion *decreases* at large distances
  - High strain magnitudes near the dislocation core
  - Perfect crystal far away from imperfection



Defining the Burgers vector

- *Quantifies* a dislocation
- Central concept to dislocation theory
  - Describes dislocation motion
  - Quantifies lattice stress/strain
  - Quantifies dislocation energy



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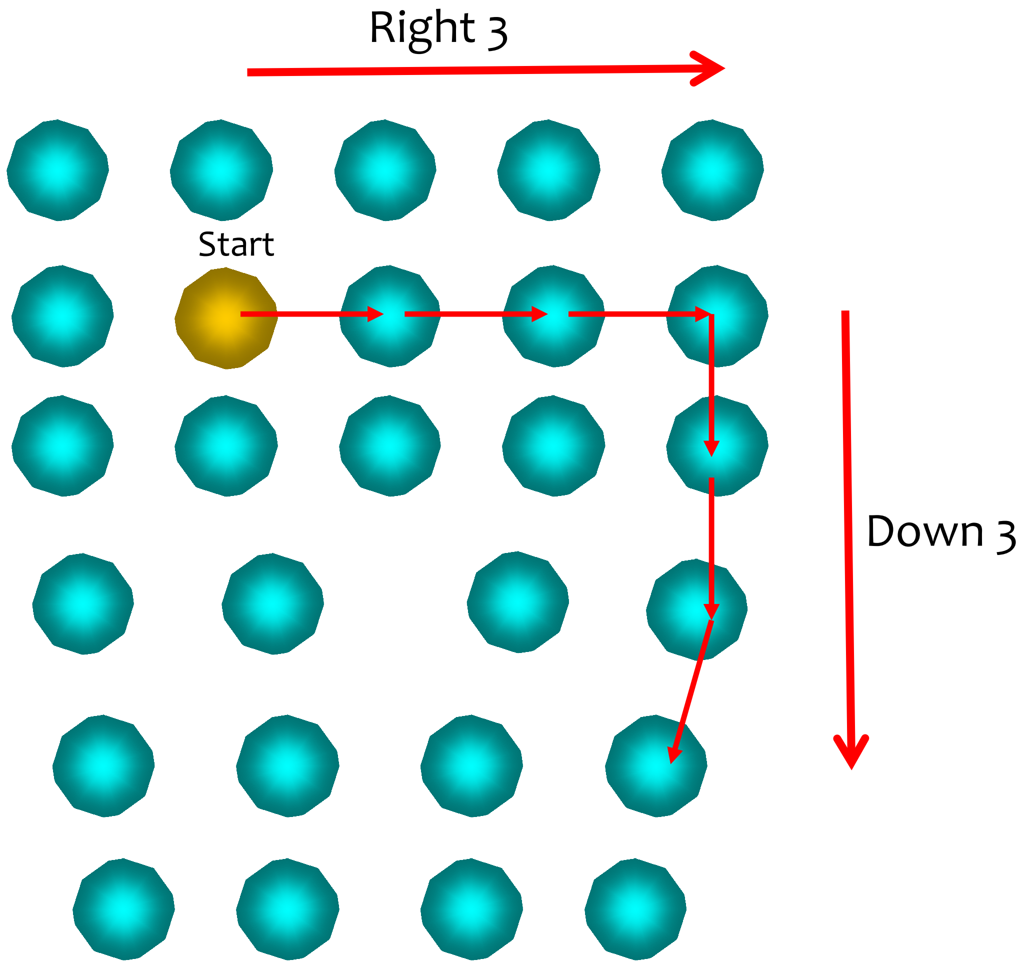

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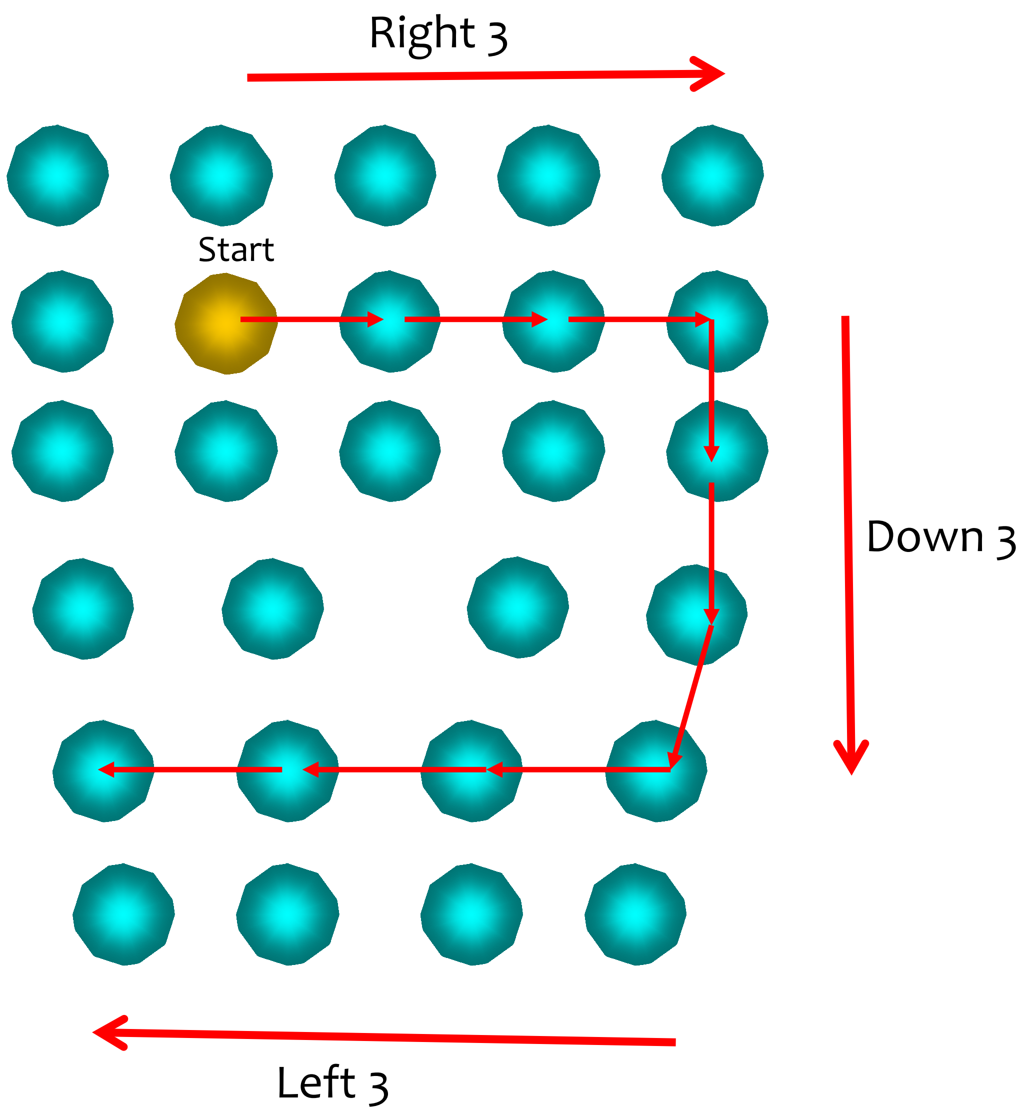

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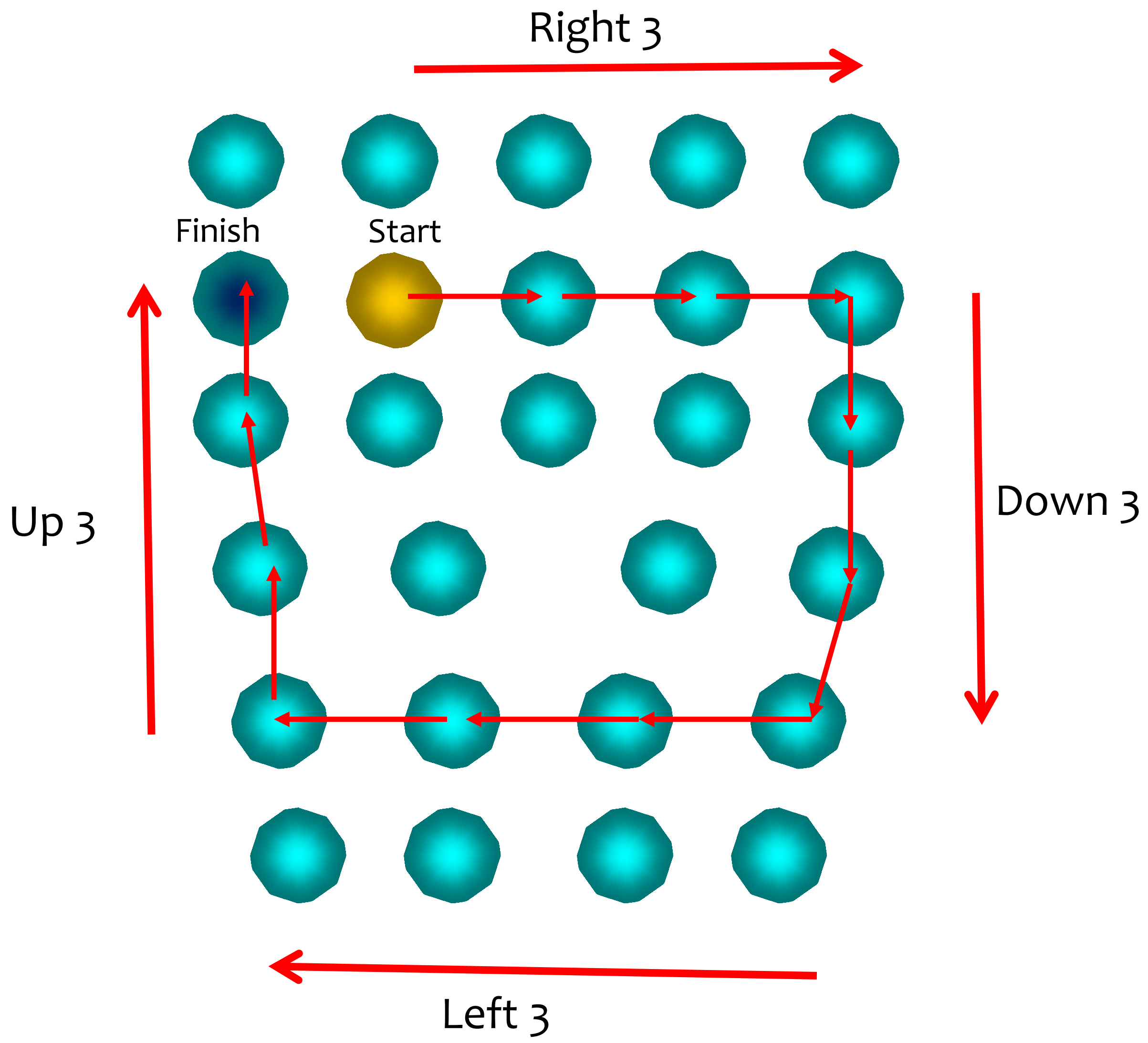
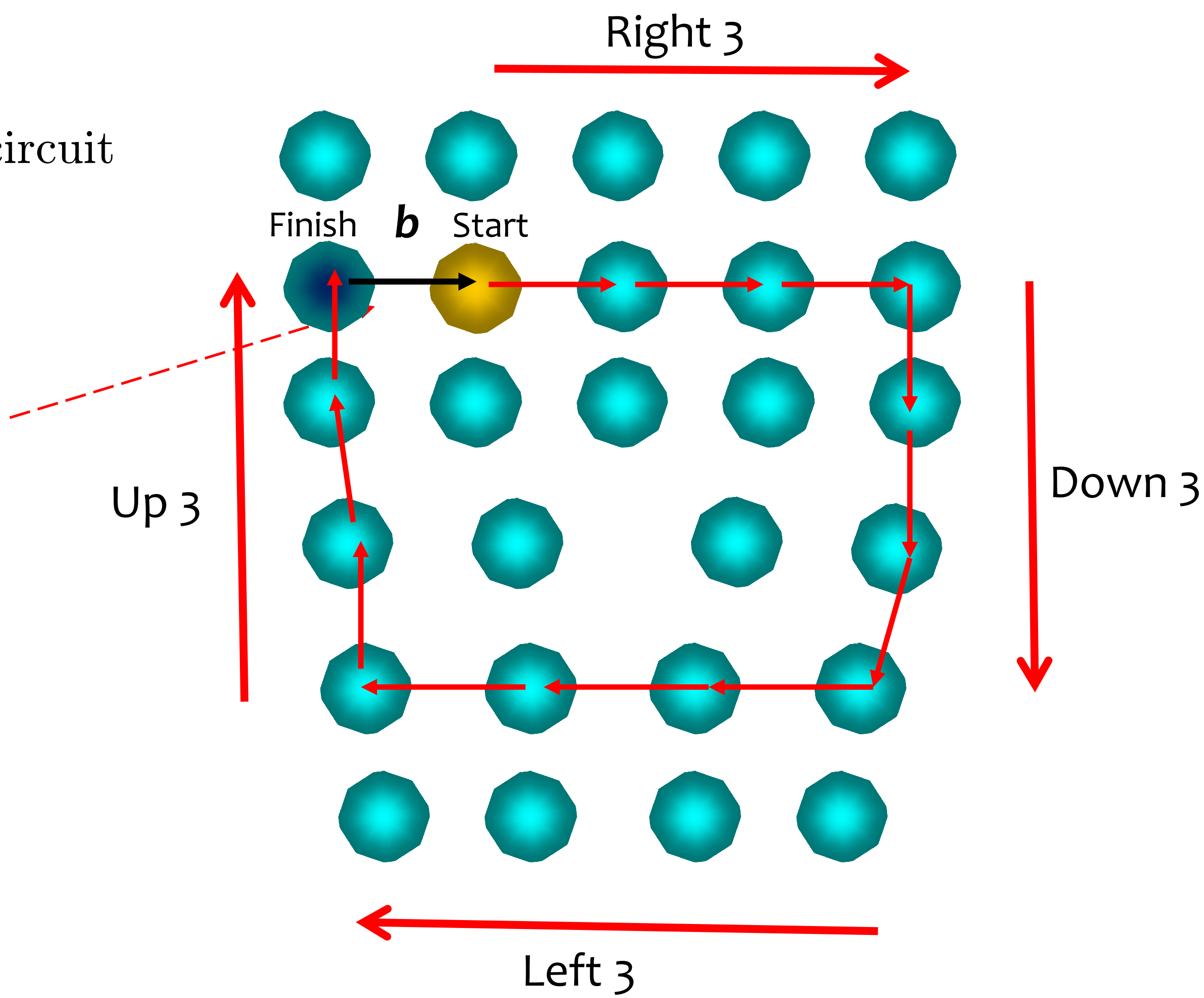


Defining the Burgers Vector

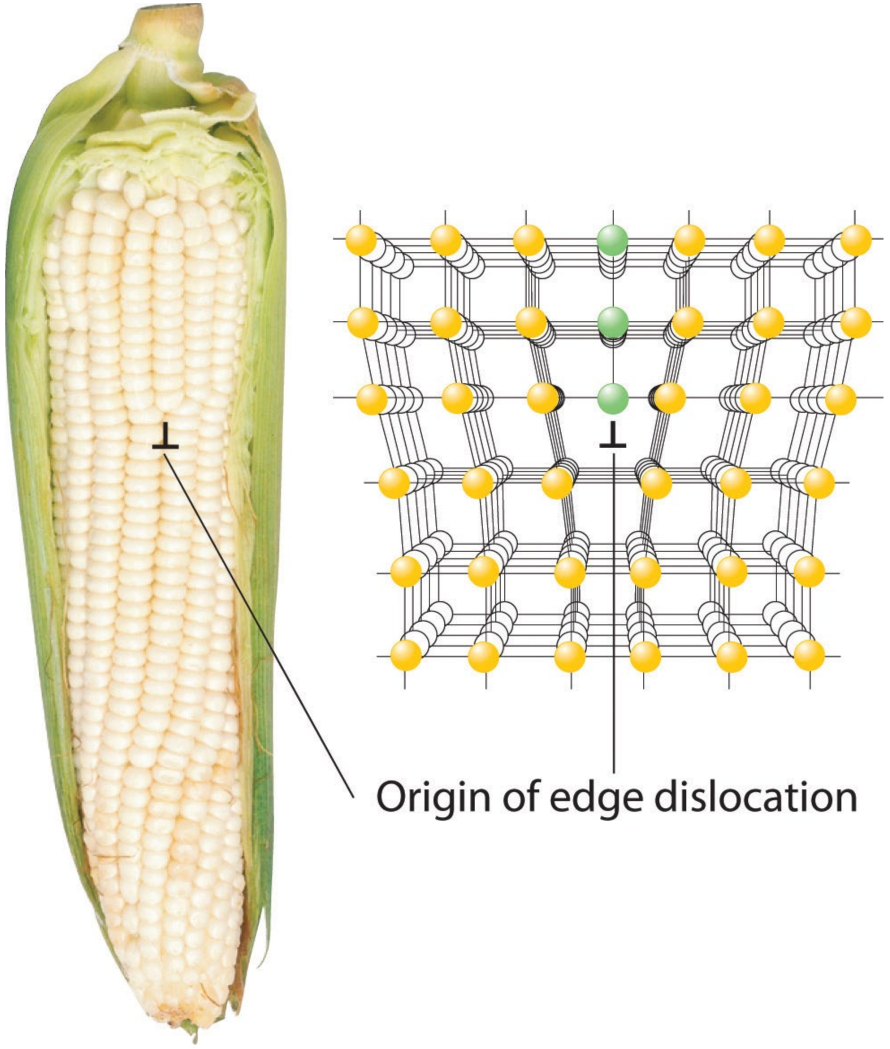
- Edge dislocation → ***b*** <u>perpendicular</u> to dislocation line
- Dislocations possess extra energy due strain imposed on lattice

Vector to complete circuit
= Burgers vector ***b***



Must take equal number of hops in (anit)parallel directions.

Edge Dislocations Abound in Nature



http://web.mit.edu/3.091/www/Fall07/lectures/lecture%2019.pdf

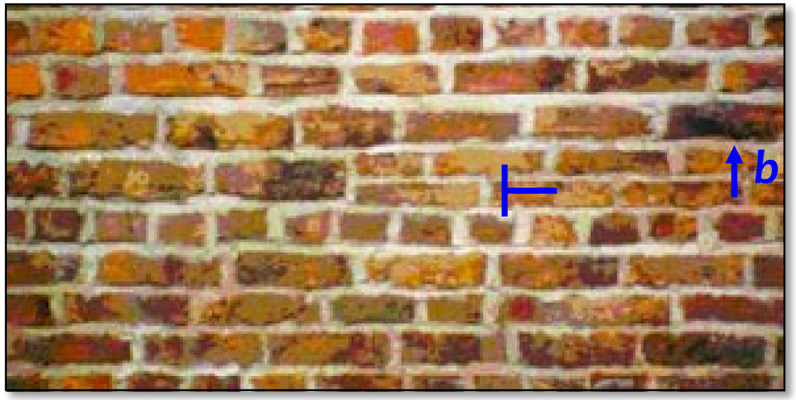
Screw Dislocation

- Linear Defects (dislocations)
  - 1D defects around which atoms are misaligned.

Edge dislocation

•Extra half-plane of atoms inserted in a crystal structure

•$\boldsymbol{b}$ perpendicular (⊥) to dislocation *line*



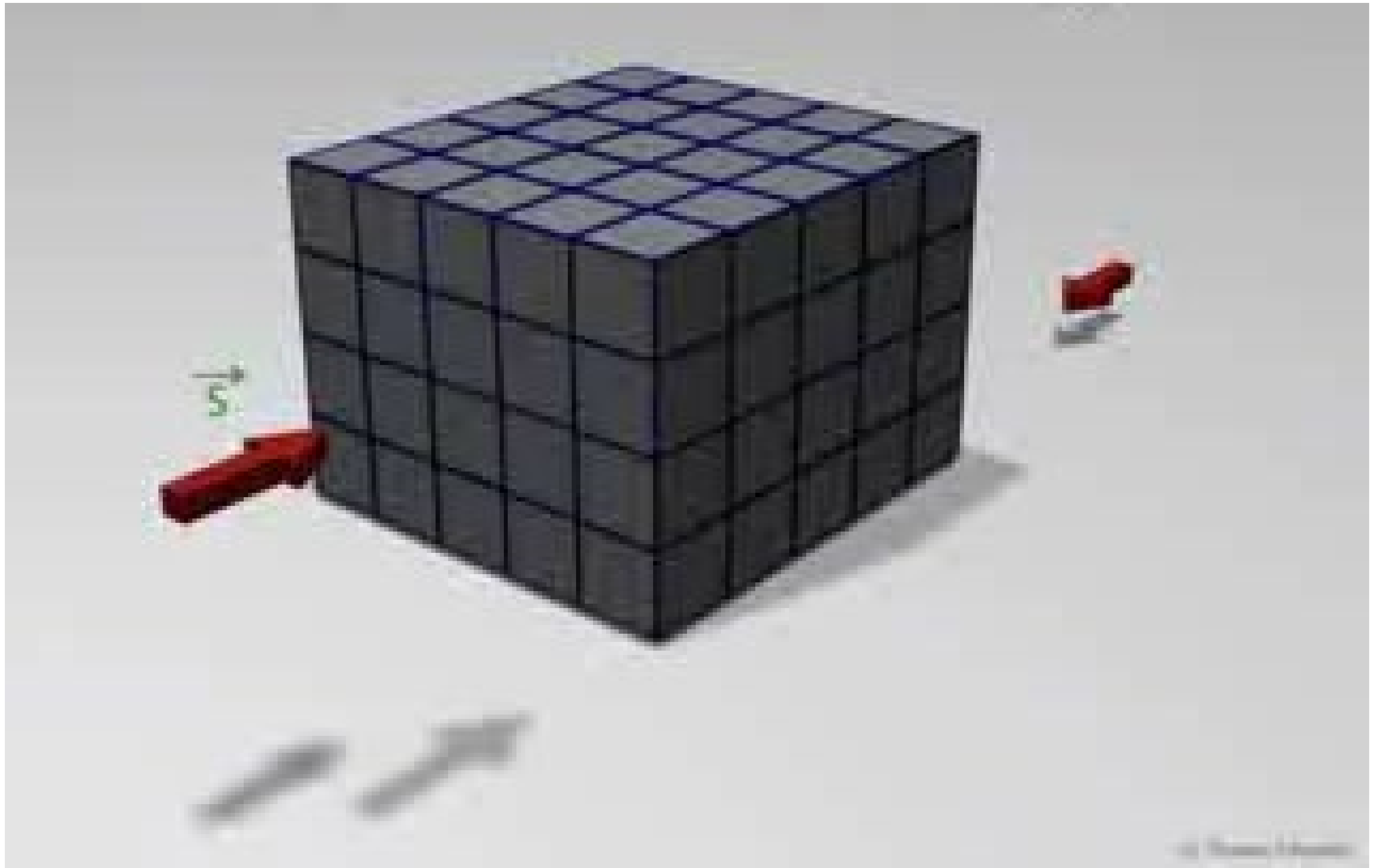
Screw dislocation

•Spiral planar ramp resulting from shear deformation

•$\boldsymbol{b}$ parallel (||) to dislocation *line*

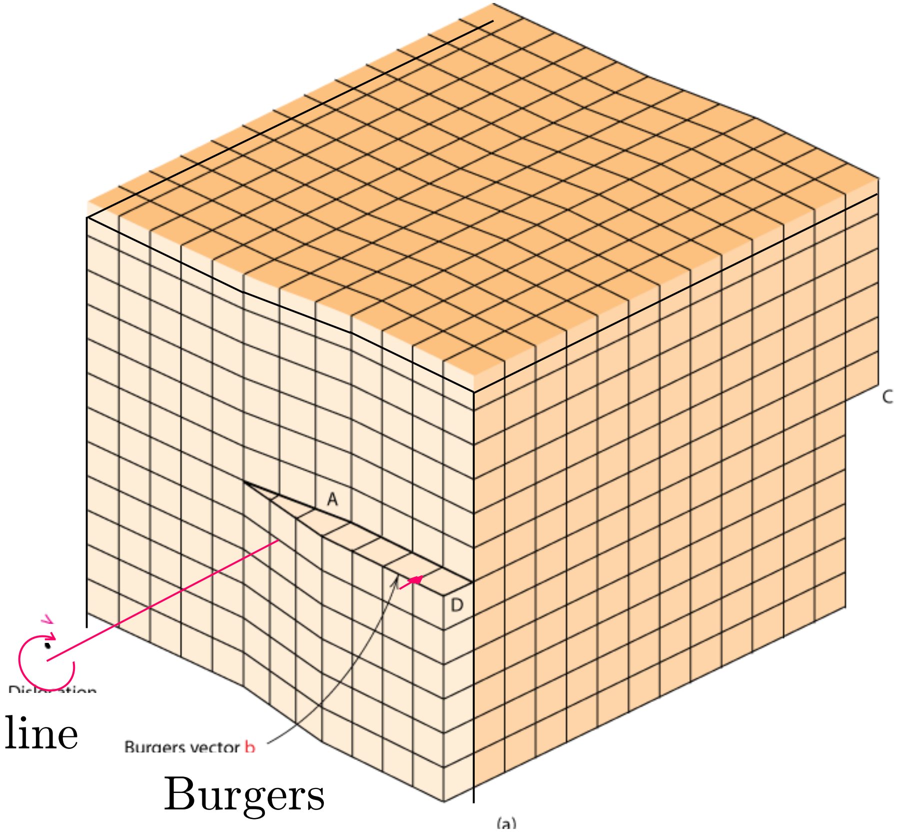
Screw Dislocation

- Screw dislocations propagate steps along the end of the crystal



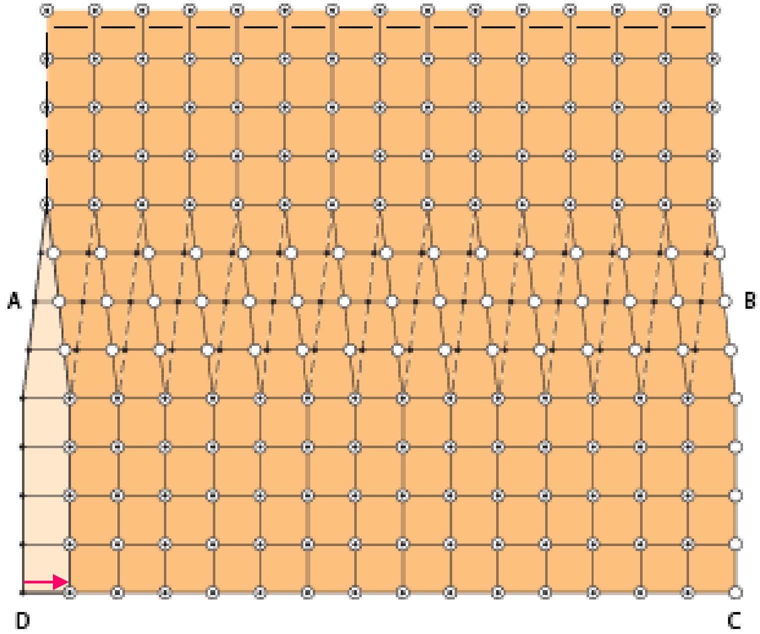
Screw Dislocation

- Screw dislocation is in a state of total shear (no tension or compression)
- Dislocations possess *strain energy*
- → Critical for mechanical deformation and plasticity



Dislocation line

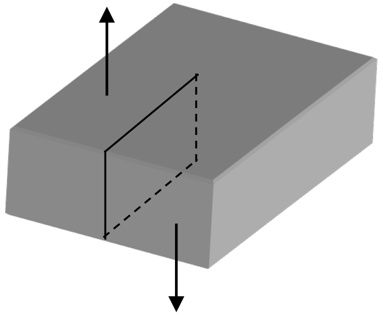
Burgers vector $\boldsymbol{b}$

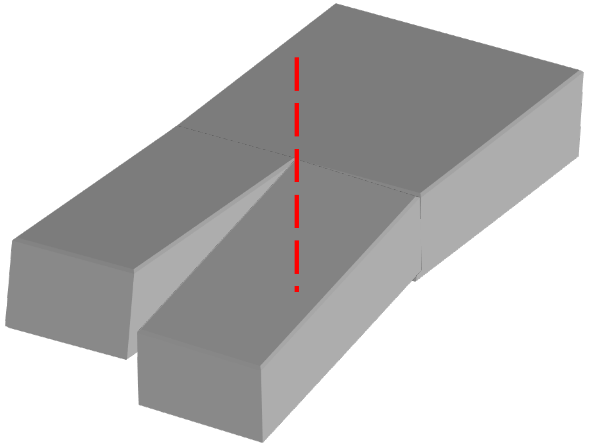


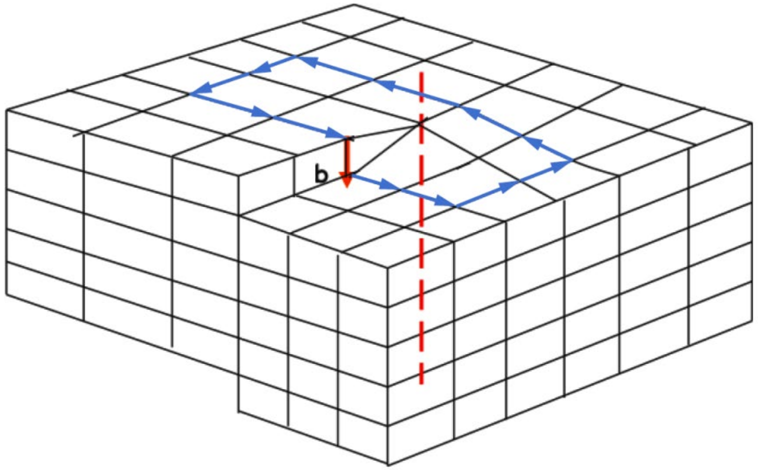
Burgers vector $\boldsymbol{b}$

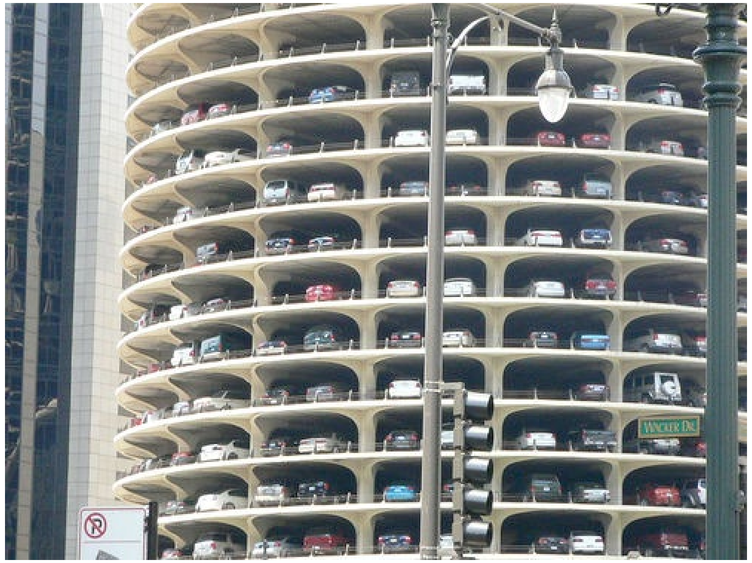
Defining the Burgers vector for a screw dislocation

Burgers vector is *parallel* to dislocation line





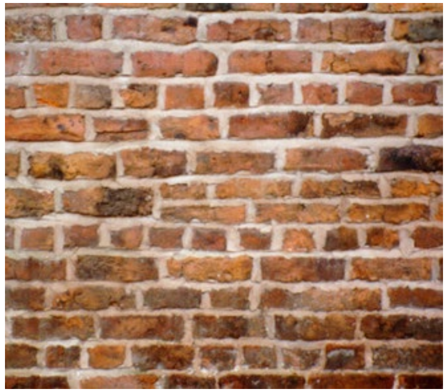


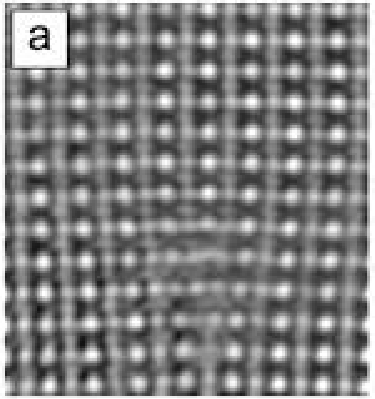


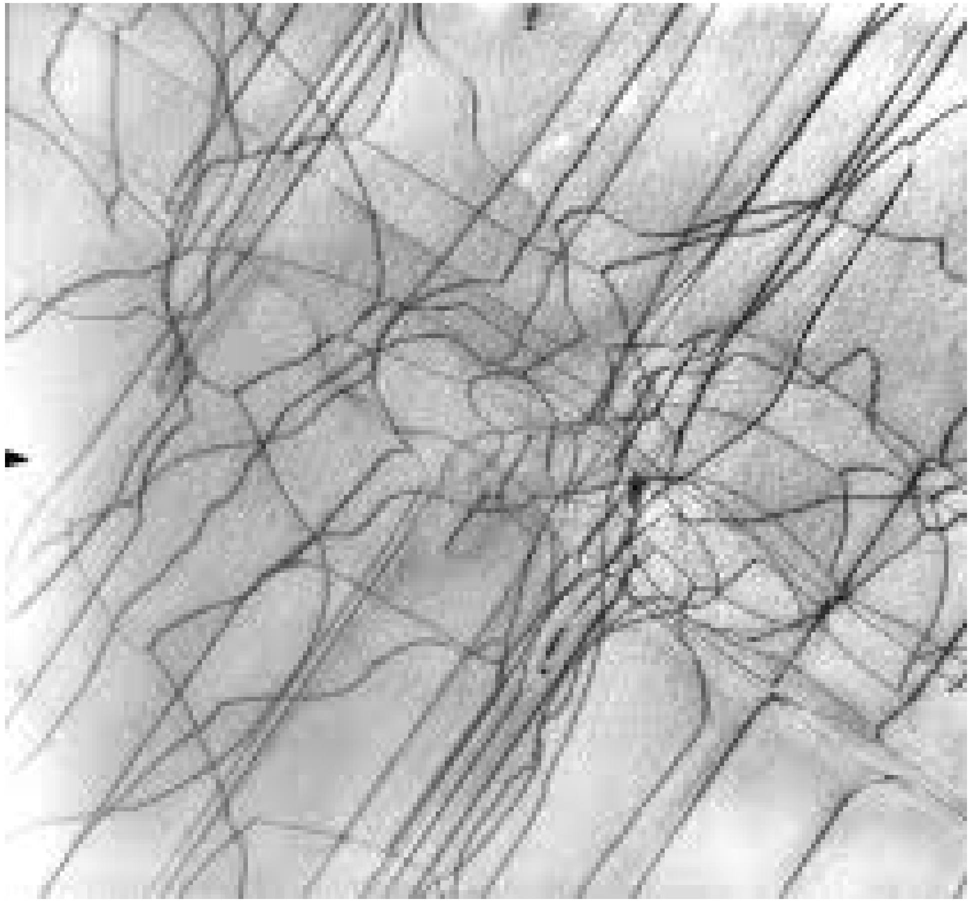
Marina City
(Corncob Building)

Dislocations and Plasticity

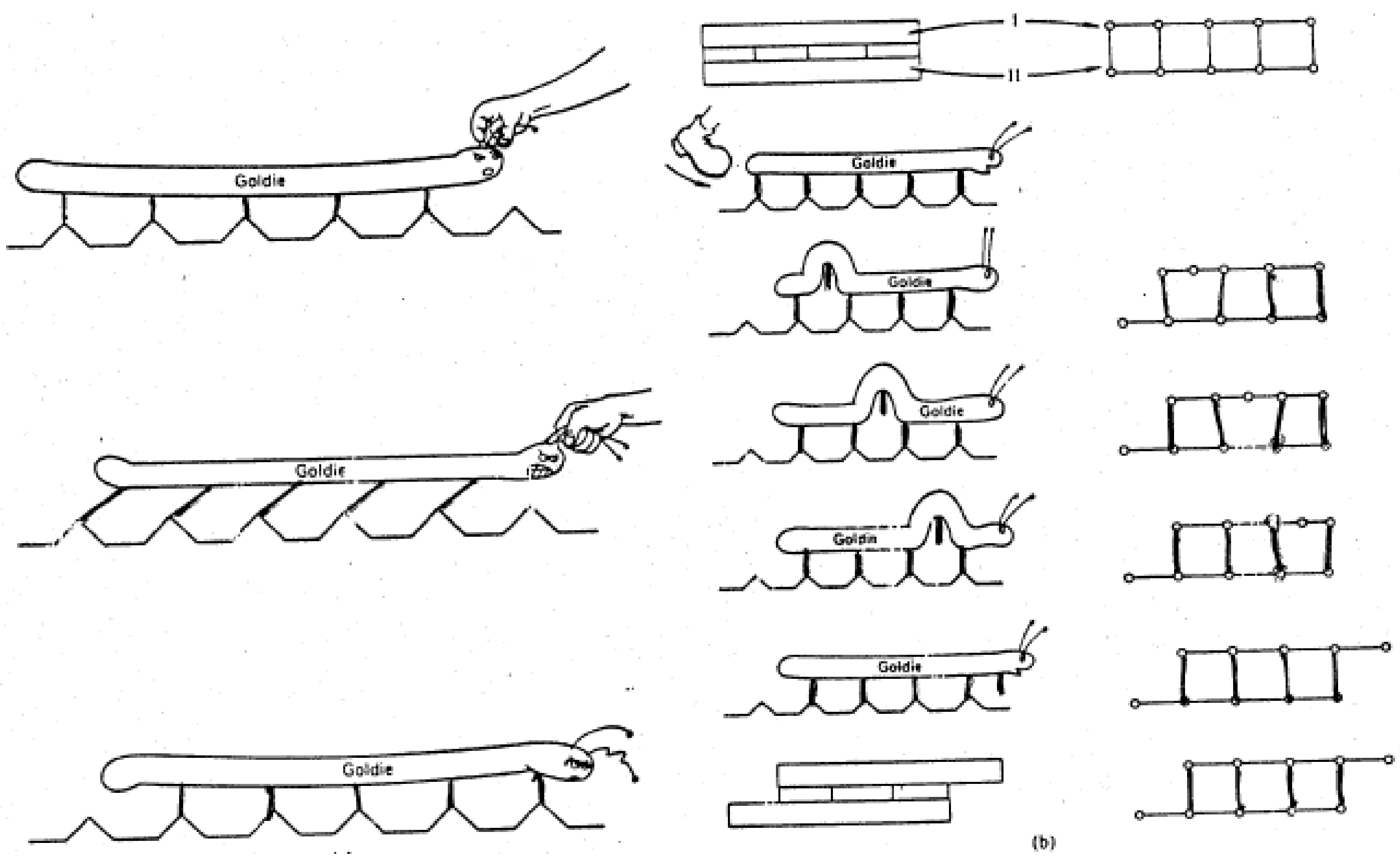
- **Dislocation Motion and Behavior**
  - Edge dislocation
  - Screw dislocation
  - The Burgers vector
  - **Dislocation motion and slip systems (qualitative)**
- Plastic Deformation in Single Crystals



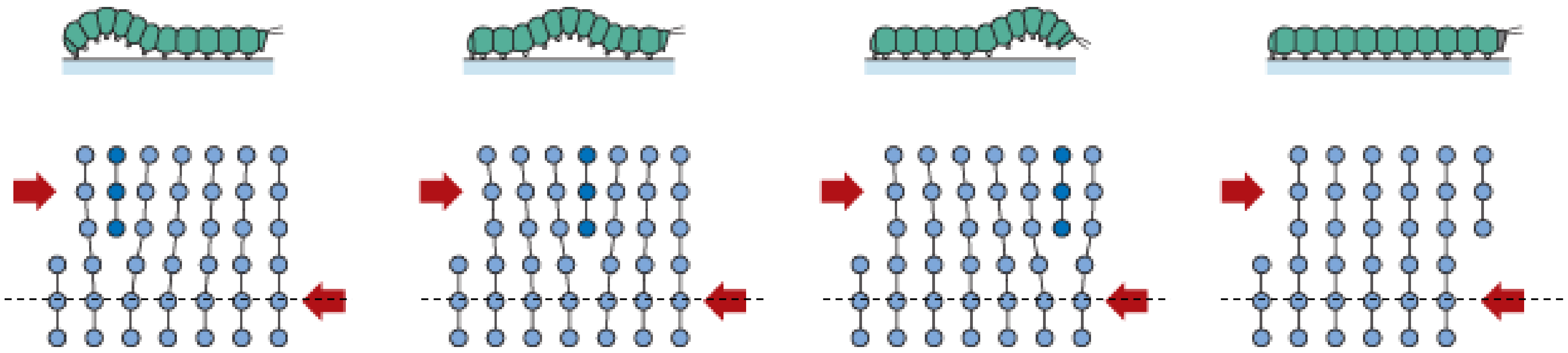




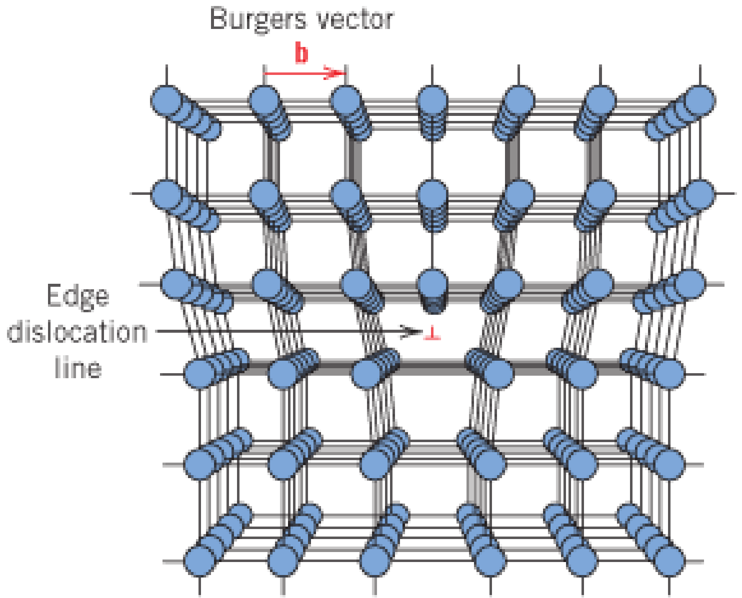
Dislocation Motion → Mechanism for Plastic Deformation



Motion of an Edge Dislocation

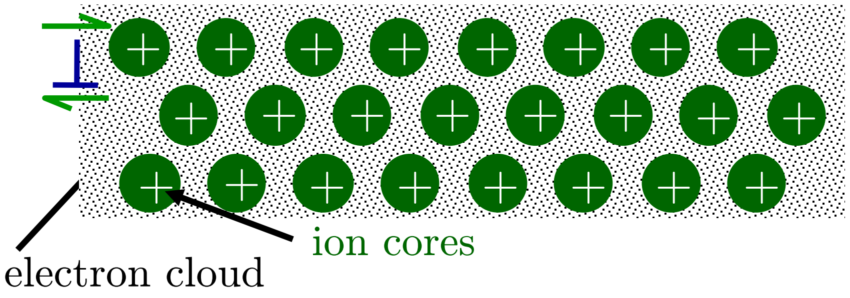


- Dislocation motion requires the successive *shifting* of a half-plane of atoms.
- Bonds formed across the slipping planes are broken and remade in succession.
- After the dislocation moves through the crystal, a step is left on the surface equal to the length of the Burgers vector.
- When a great number of dislocations have moved, we observe macroscopic permanent deformation.

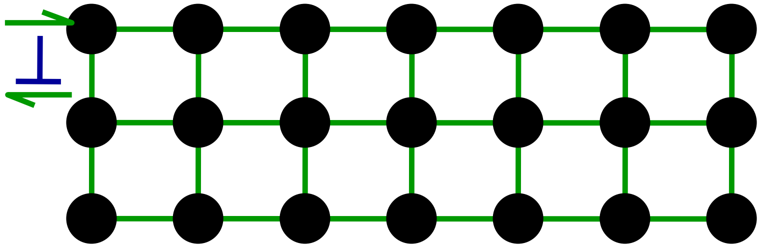


Bonding and Dislocation Motion

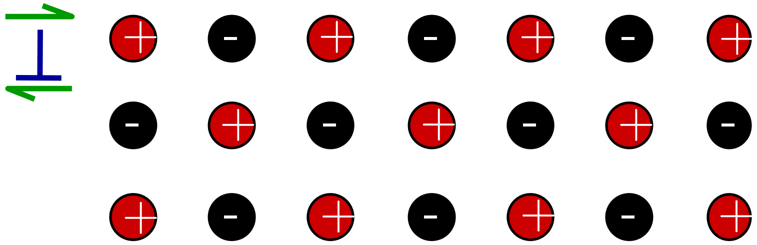
- Metals (Al, Cu):
  - Dislocation motion “easy”
  - Non-directional bonding
  - Close-packed directions for slip



- Covalent Ceramics (Si, C):
  - Motion difficult
  - Directional (angular) bonding



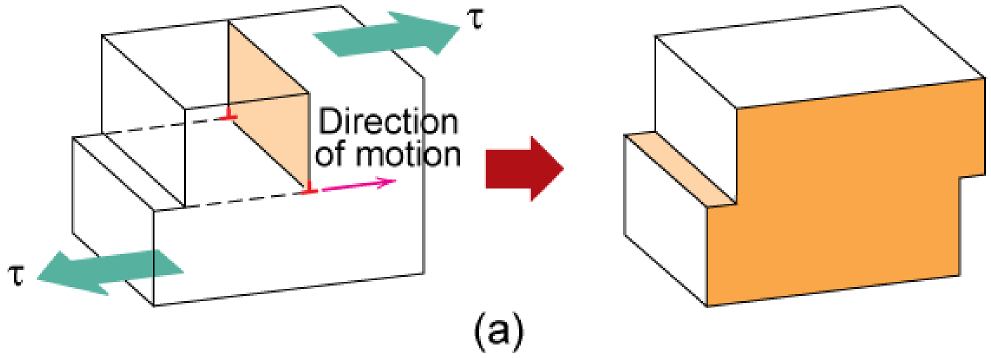
- Ionic Ceramics (NaCl):
  - Motion difficult
  - Need to avoid nearest neighbors of same charge



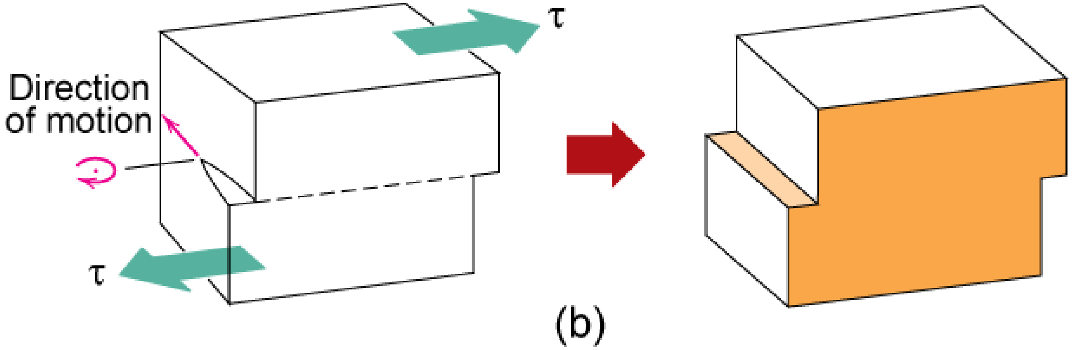
Dislocation Motion: Edge and Screw

- A dislocation moves in a slip plane in a slip direction *perpendicular* to the dislocation line.
- The Burger's vector is always *parallel* to the *slip direction* (atomic motion).
- Edge: The motion of the dislocation line is *parallel* to the Burger's vector.
- Screw: The motion of the dislocation line is *perpendicular* to the Burger's vector

Edge dislocation motion



Screw dislocation motion



Understand what each means: dislocation line, dislocation motion direction, slip direction, Burger's vector.

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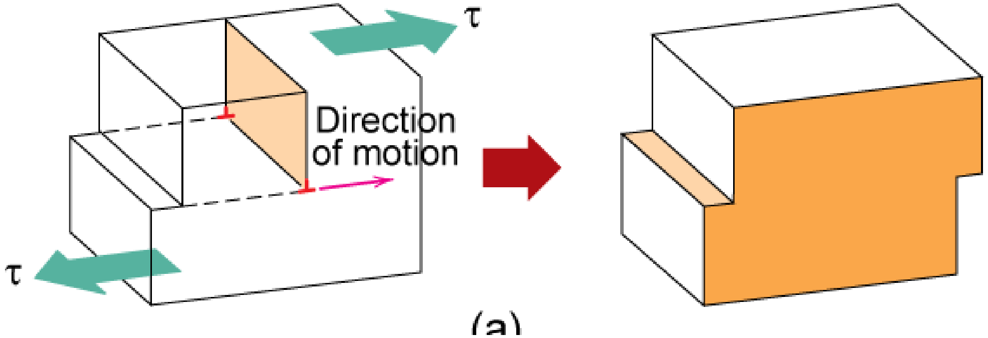
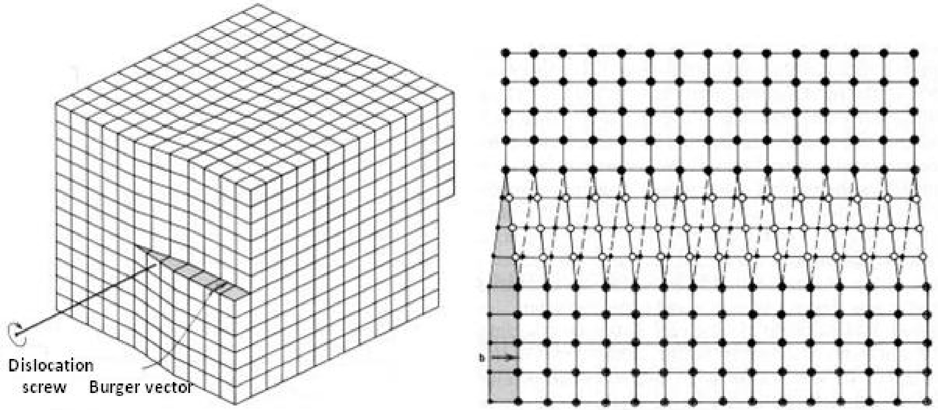
Edge dislocation motion



Screw dislocation motion



Understand what each means: dislocation line, dislocation motion direction, slip direction, Burger's vector.

Concept Check

Fig. 1 shows a plane passing through a screw dislocation. Match the three arrows to what the arrow represents.

1. Dislocation core
2. Burger's vector
3. Dislocation motion

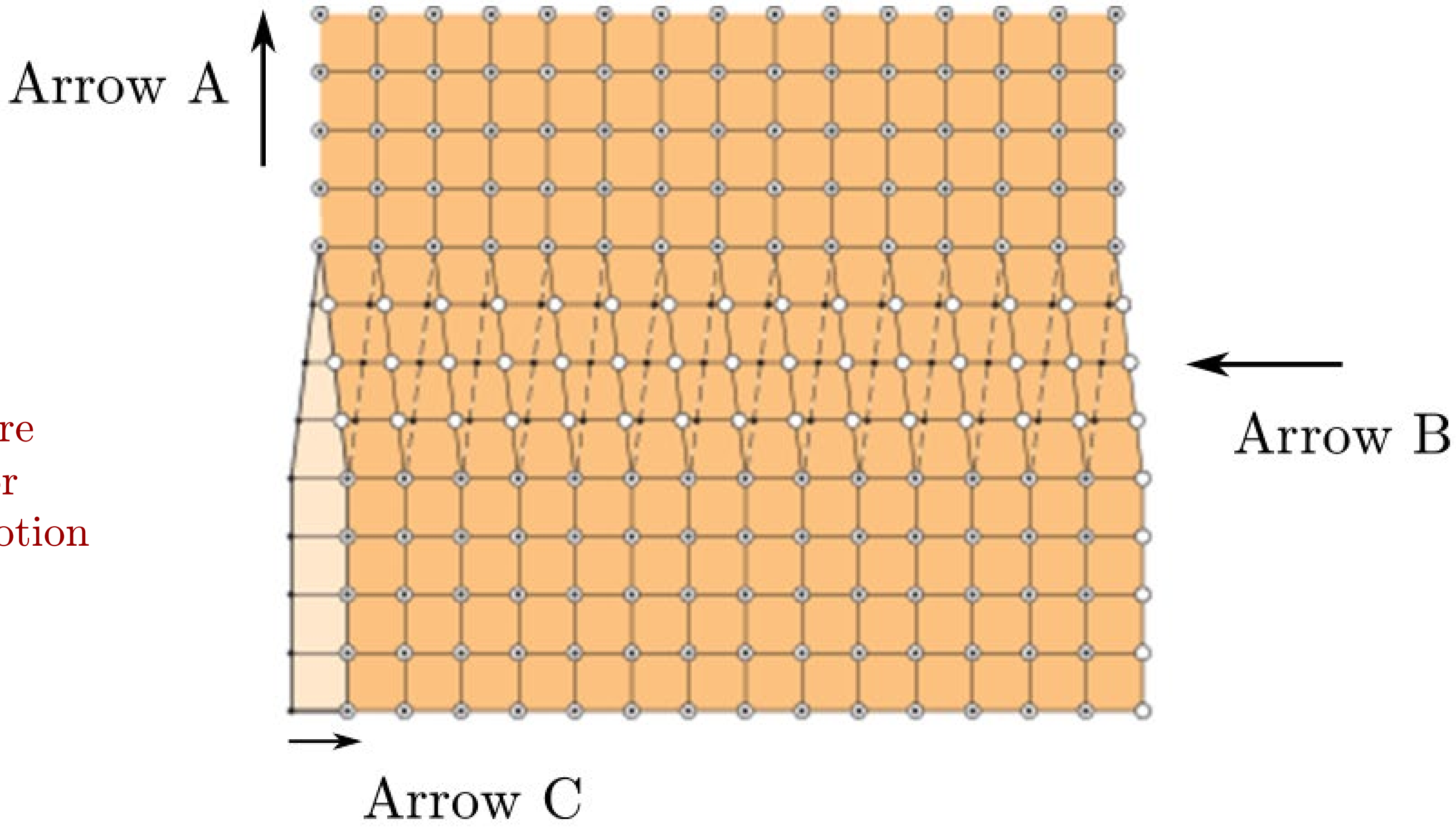


FIGURE 1: A 2D projection of two atomic planes passing through a dislocation.

Concept Check – Solution

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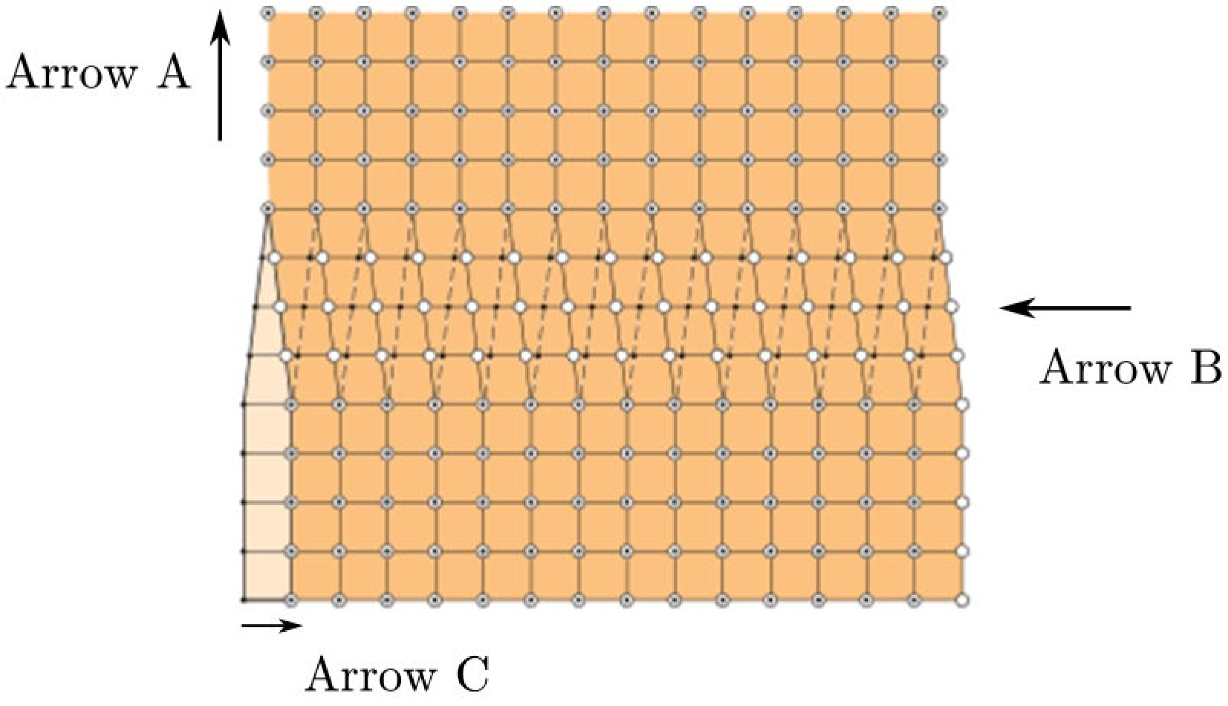
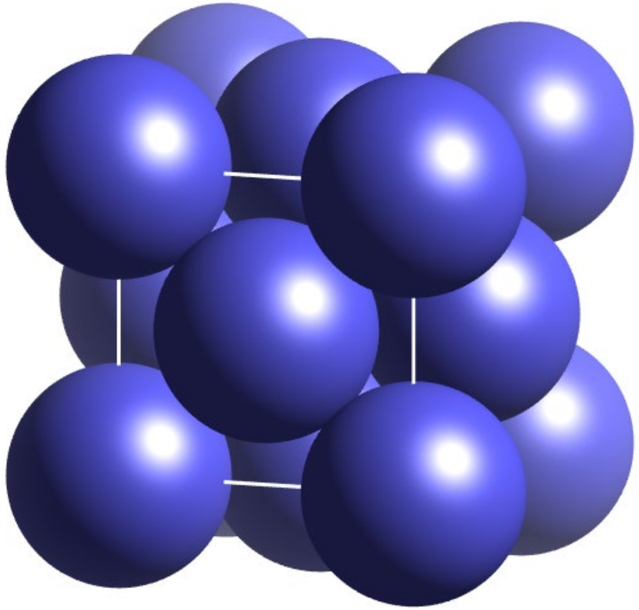


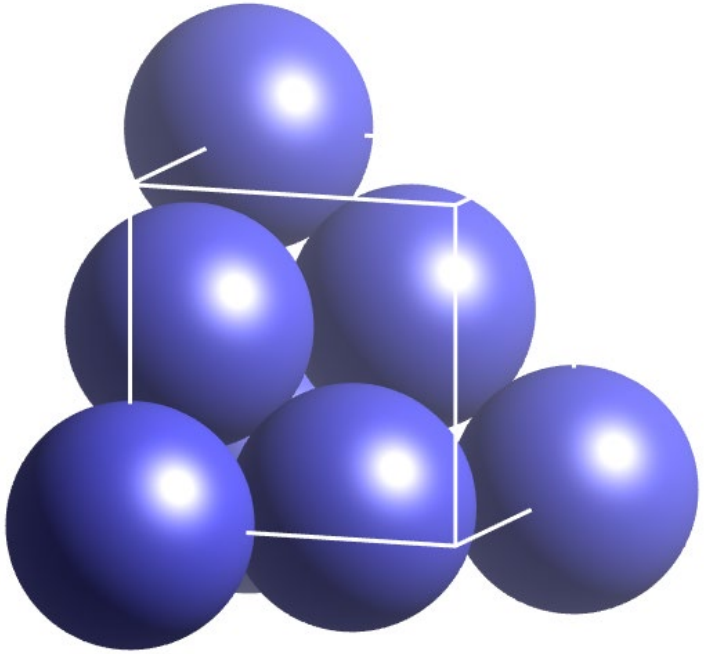
FIGURE 1: A 2D projection of two atomic planes passing through a dislocation.

Solution:

- Arrow A is the direction of dislocation motion.
- Arrow B is the dislocation core (also the direction in which atoms slip)
- Arrow C is the Burger's vector (also the direction in which the atoms slip)

Which Direction Will Slip Occur?





- Dislocation motion is not equivalent in all directions and planes
- Slip *plane* - plane on which easiest slippage occurs
    - *Highest planar densities*
- Slip directions – direction in which atoms move
    - *Highest linear densities, shortest jump distance*

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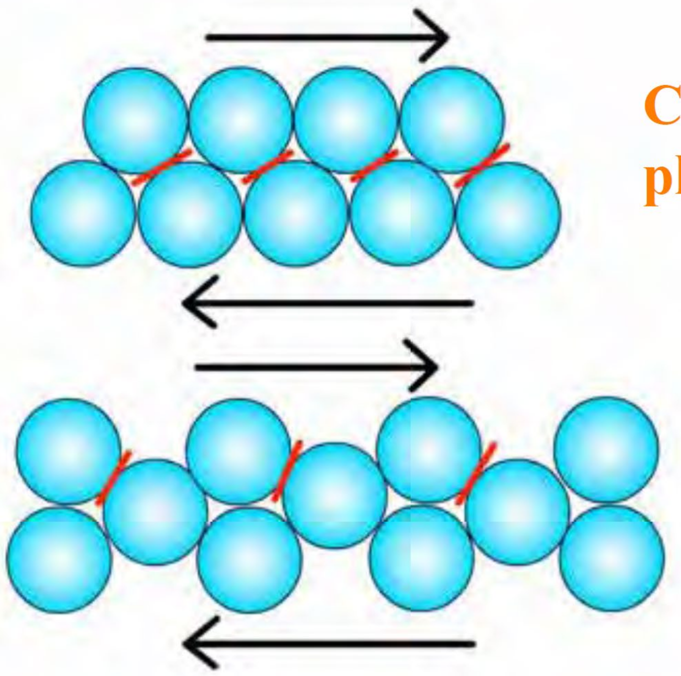

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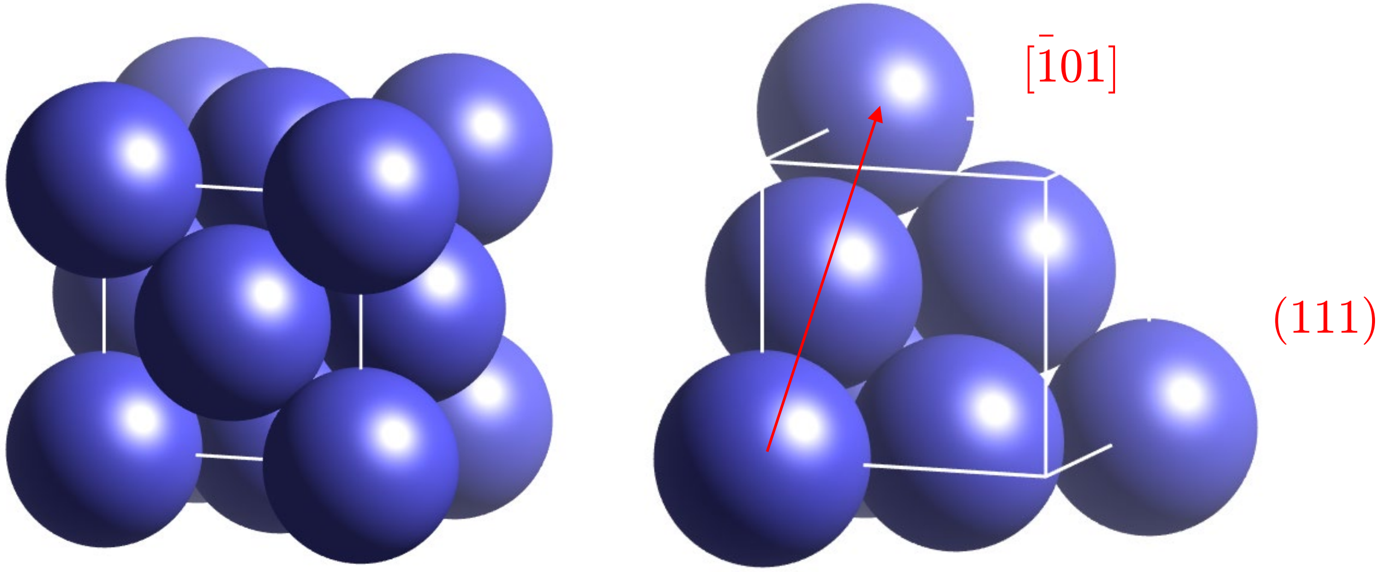


- FCC Crystals
  - FCC slip occurs on {111} planes (close-packed) and along ⟨110⟩ directions (close-packed).
  - *12* total slip systems (4 unique (111) planes, 3 ⟨110⟩ per plane)
- BCC Crystals
  - BCC slip occurs on a number of planes (similar packing densities) along ⟨111⟩ directions

Slip Systems

.1 **Slip Systems for Face-Centered Cubic, Body-Centered Cubic, and Hexagonal Close-Packed Metals**

Metals	*Slip Plane*	*Slip Direction*	*Number of Slip Systems*
	Face-Centered Cubic		
Cu, Al, Ni, Ag, Au	$\{111\}$	$\langle 1\bar{1}0 \rangle$	12
	Body-Centered Cubic		
α-Fe, W, Mo	$\{110\}$	$\langle \bar{1}11 \rangle$	12
α-Fe, W	$\{211\}$	$\langle \bar{1}11 \rangle$	12
α-Fe, K	$\{321\}$	$\langle \bar{1}11 \rangle$	24
	Hexagonal Close-Packed		
Cd, Zn, Mg, Ti, Be	$\{0001\}$	$\langle 11\bar{2}0 \rangle$	3

- Slip systems → *which direction and plane* upon which slip will prefer to occur in a crystal.
- Slip systems → *little information* about how much force is required to initiate slip.
  - For that, you need Peierls-Nabarro* theory.

$$\text{Slip plane} + \text{slip direction} = \text{slip system (representation: } \{hkl\}\langle uvw \rangle)$$

- BCC { 110 }, { 211 }, and { 321 } planes have very similar packing densities/surface energies.

*Assesses how strain due to a dislocation is embodied in different crystal structures.

Concept Check

What is the slip system for the SC crystal below?

A. $\{100\}\langle 100\rangle$

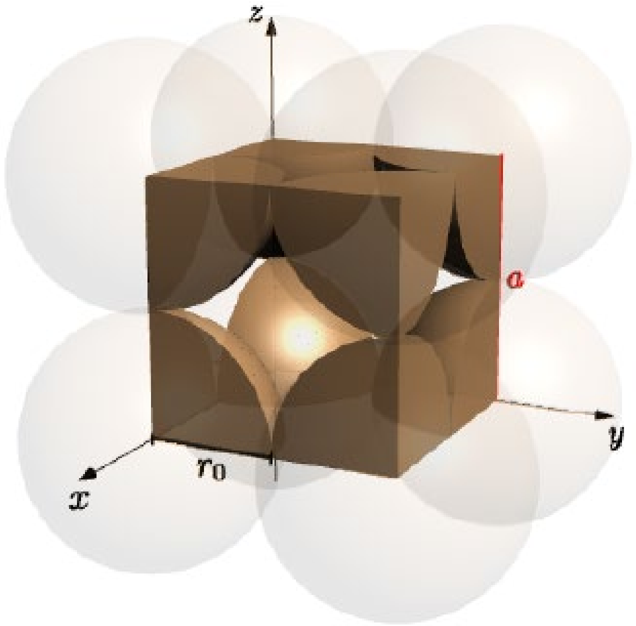
B. $\{100\}\langle 110\rangle$

C. $\{100\}\langle 111\rangle$

D. $\{110\}\langle 100\rangle$

E. $\{110\}\langle 110\rangle$

F. $\{110\}\langle 111\rangle$



Concept Check – Solution

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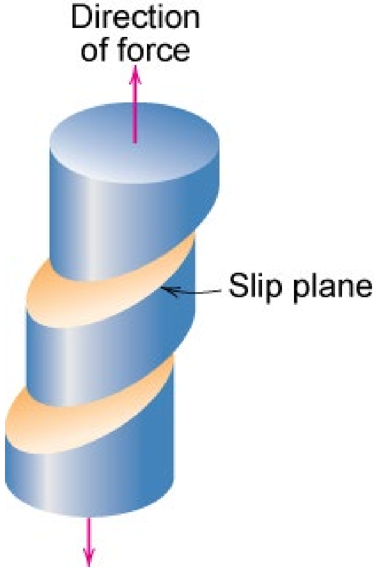
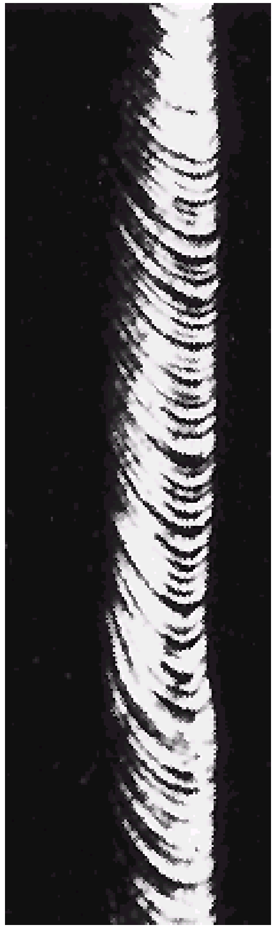


Solution:

It is always easiest to first find the slip direction. This will be the highest linear density atoms — the close-packed directions. In SC, this is the $\langle 100\rangle$ family.

Then, we think about the closest-packed plane. This isn't terribly easy to see, but for (100) there is $1\,\mathrm{atom}/\mathrm{a}^2$, for the (110) there is $1\,\mathrm{atom}/\sqrt{2}\mathrm{a}^2$. The (100) is more dense. Low-index planes (e.g., (100), (110), (111)) are typically the highest density, so check those first.



Slip in a Zn (HCP)
Single crystal

Summary to Here

- Stress-strain curves can be analyzed to find
  - Young's modulus
  - Yield strength
  - Ultimate tensile strength
  - Ductility
  - Resilience
  - Toughness

- The physical mechanism behind plasticity is the permanent motion of atoms. This is embodied through dislocation (e.g., edge and screw) motion.

- Edge and screw dislocations can be quantified using Burger's circuits to acquire a Burger's vector, which has a direction and magnitude.

- Slip will occur along preferred planes in crystals – the lowest energy barriers are along close-packed direction within close-packed planes.

Outcomes

- Describe simple mechanisms behind plasticity (dislocation motion, slip systems).
- Analyze stress-strain curves to derive values of interest with respect to mechanical properties. Use the data to evaluate materials for their suitability in structural applications.
- Distinguish edge and screw dislocations with regards to:
  - Dislocation characteristics.
  - Burger's vector (no 3D derivation of Burger's vectors).
  - Slip direction.
  - Dislocation motion.
- Differentiate slip systems in various structures