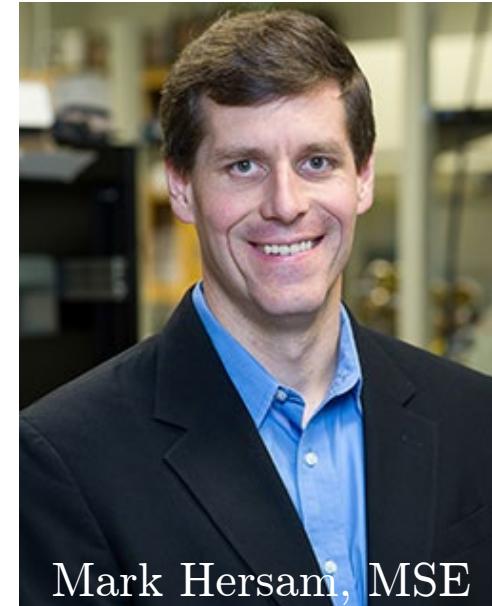


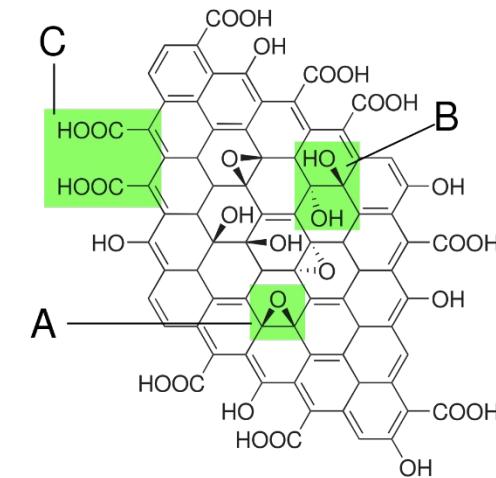
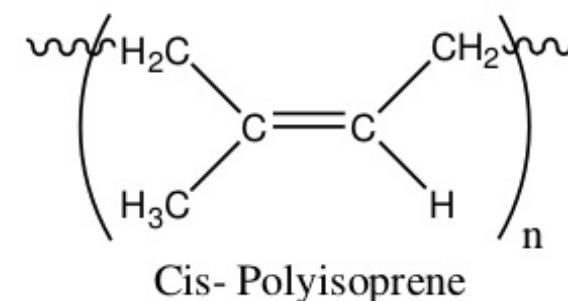
UV-resistant elastic for N95

Can we reuse N95s?

- N95s are *not* approved for routine decontamination by the CDC.
- Time – 5 days between uses
- Vaporous hydrogen peroxide treatments
 - Reduced filtration efficacy after 3 cycles (Bergman)
 - Degradation of elastomer straps after 20 cycle (Battelle)
- Moist heat
 - 99.88% reduction in CoV loads
 - Minimal degradation in filtration and fit
 - High uncertainty with regards to disinfection efficacy
- Ultraviolet germicidal irradiation
 - No effect on filtration at inactivation doses
 - CoV inactivation of greater than 99.9%
 - Damage (“aging”) of polyisoprene straps
- Material Vignette idea: what happens to polyisoprene during UV exposure that leads to *mechanical* degradation (embrittlement/softening)
- Idea – new type of elastic composite using hydrated graphene oxide.



Mark Hersam, MSE



Strengthening + Electronic Properties I

-Electrical Conduction

Dr. Jonathan Emery

Cook 3035 — jonathan.emery@northwestern.edu

ANNOUNCEMENTS — May 21st, 2020

Lecture Topic

- Strengthening Mechanisms
- Recovery, Recrystallization,
- Electrical Conduction
- Band Structure

Logistics

- Wednesday: P-set D8
- Thursday: Quiz D8 Due

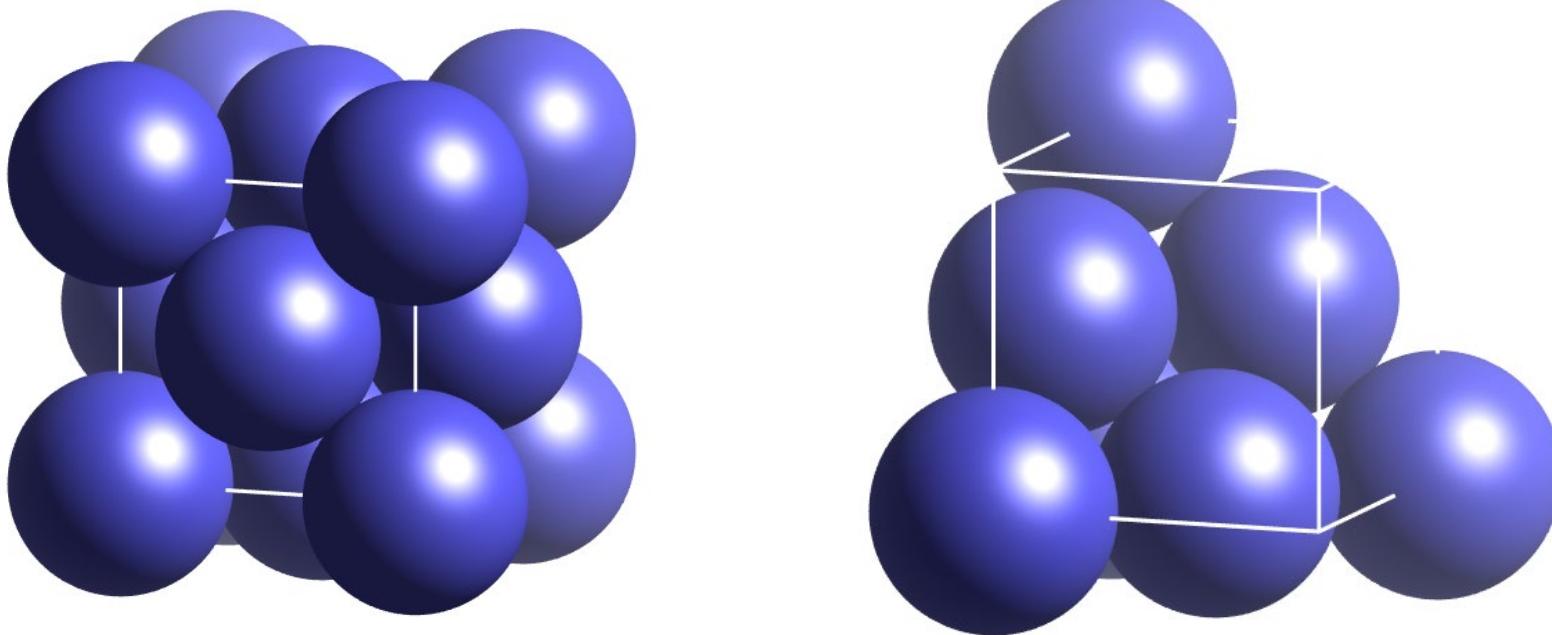
Reading

- Callister Ch. 18.1-18.9.

Outline

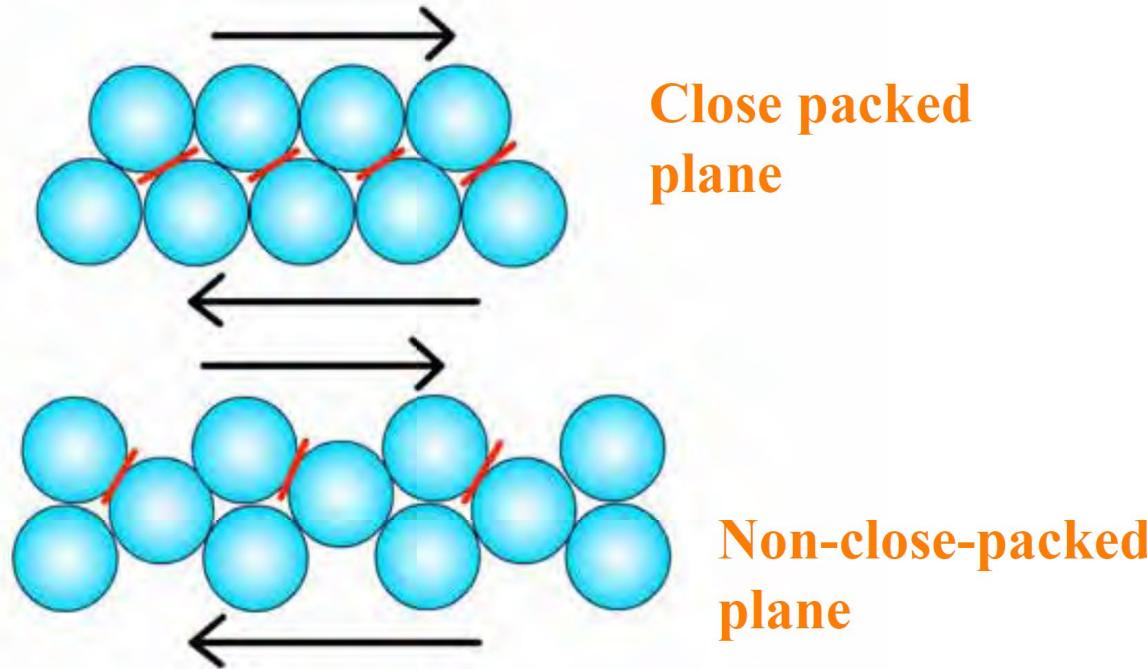
- Slip systems in common crystals
- Strengthening Mechanisms [Video Lecture]
- Heat treatments – Recovery, Recrystallization, and Grain Growth
- Electrical Conduction
 - Materials properties of charge transport (conductivity and resistivity) [Video Lecture]
 - Charge carrier mobility
 - Sources of resistivity (Matthiessen's Rule)
- Electronic Structure
 - Review electronic states in isolated atoms
 - What happens when we push atoms together?
→ Electronic band structure [Video Lecture]
 - Difference between electronic structure of metals, insulators, and semiconductors.

Which Direction Will Slip Occur?



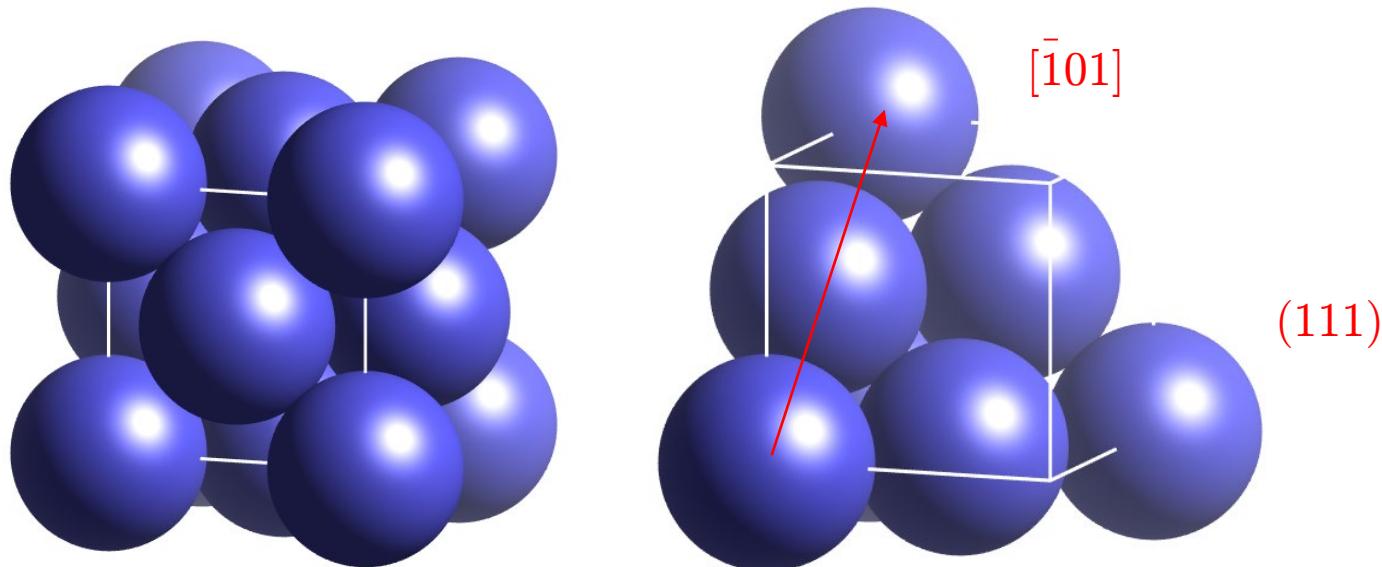
- Dislocation motion is not equivalent in all directions and planes
- **Slip plane** - plane on which easiest slippage occurs
 - *Highest planar densities*
- **Slip directions** – direction in which atoms move
 - *Highest linear densities, shortest jump distance*

Which Direction Will Slip Occur?



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

Which Direction Will Slip Occur?



- FCC Crystals
 - FCC slip occurs on $\{111\}$ planes (close-packed) and along $\langle 110 \rangle$ directions (close-packed).
 - 12 total slip systems (4 unique (111) planes, 3 $\langle 110 \rangle$ per plane)
- BCC Crystals
 - BCC slip occurs on a number of planes (similar packing densities) along $\langle 111 \rangle$ 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 }	⟨ 110 ⟩	12
Body-Centered Cubic			
α-Fe, W, Mo	{ 110 }	⟨ 111 ⟩	12
α-Fe, W	{ 211 }	⟨ 111 ⟩	12
α-Fe, K	{ 321 }	⟨ 111 ⟩	24
Hexagonal Close-Packed			
Cd, Zn, Mg, Ti, Be	{ 0001 }	⟨ 11̄20 ⟩	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.

Slip plane + slip direction = slip system (representation: {hkl}⟨uvw⟩)

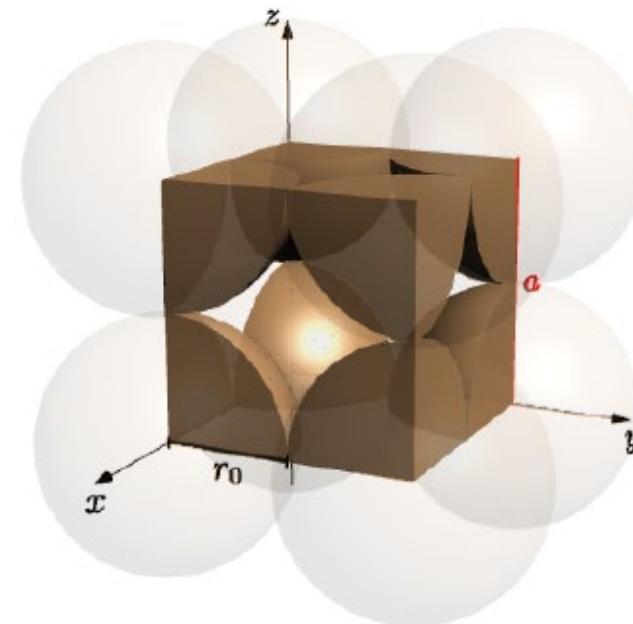
- BCC { 110 }, { 211 }, and { 321 } planes have very similar packing densities/surface energies.

*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

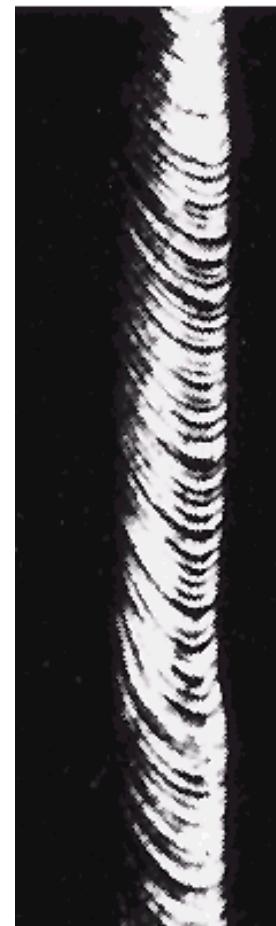
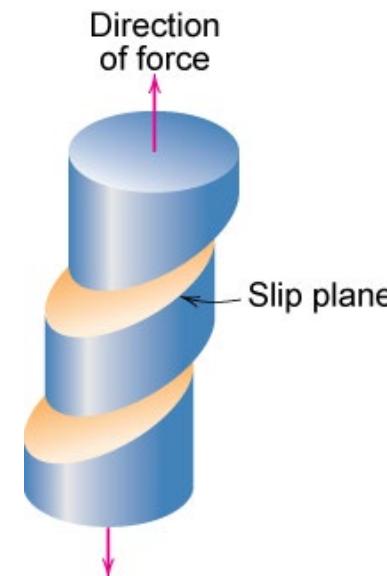
1. What is the slip system for the SC crystal below?

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

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.

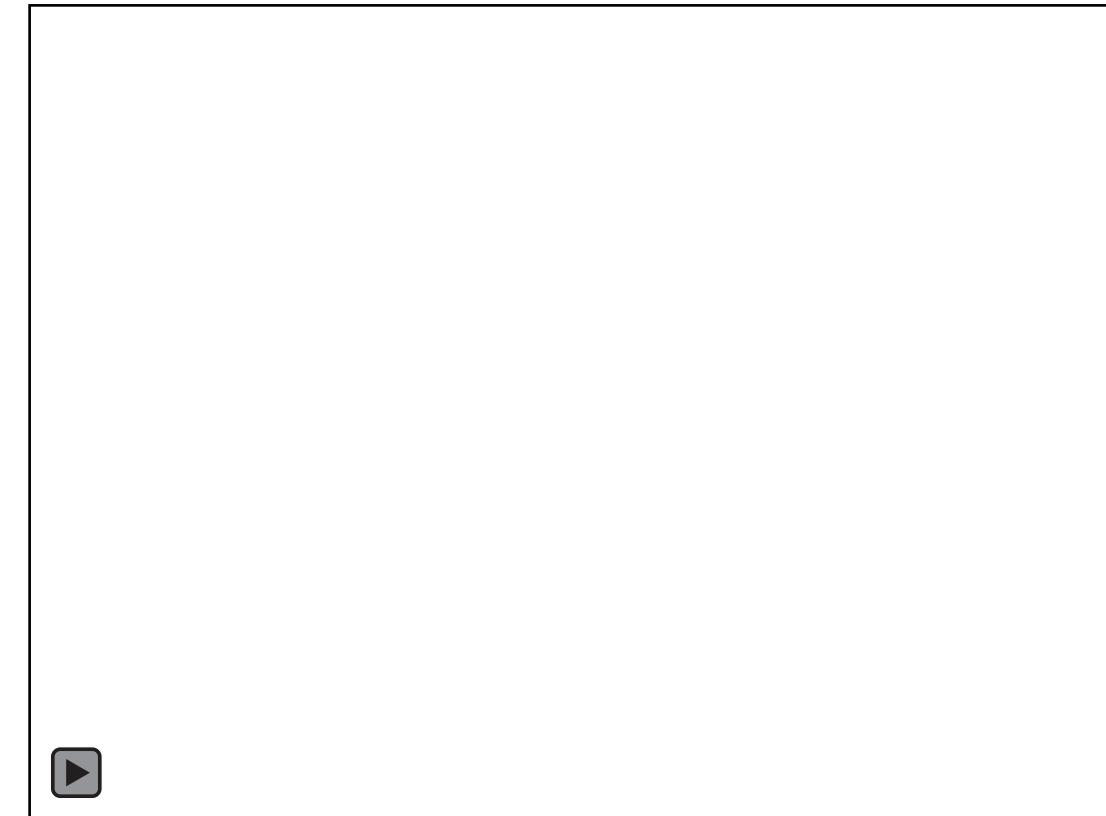
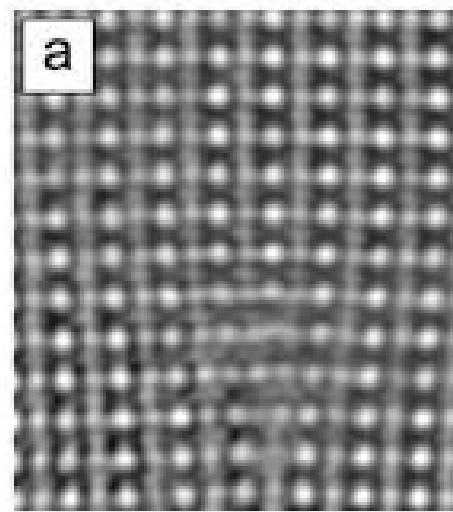
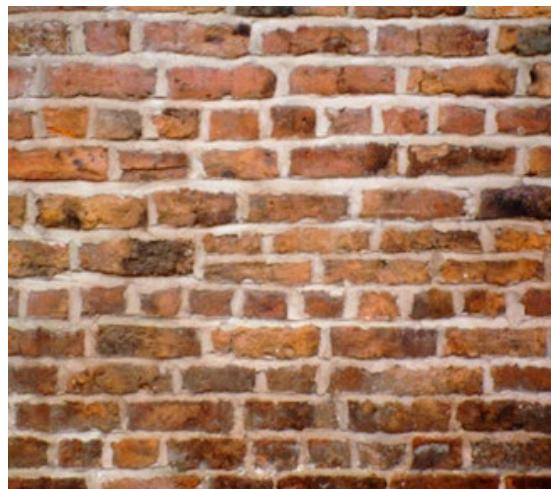
Then, we think about the closest-packed plane. This isn't terribly easy to see, but for (100) there is $1 \text{ atom}/a^2$, for the (110) there is $1 \text{ atom}/\sqrt{2}a^2$. The (100) is more dense. Low-index planes (e.g., (100) , (110) , (111)) are typically the highest density, so check those first.



Slip in a Zn (HCP)
Single crystal

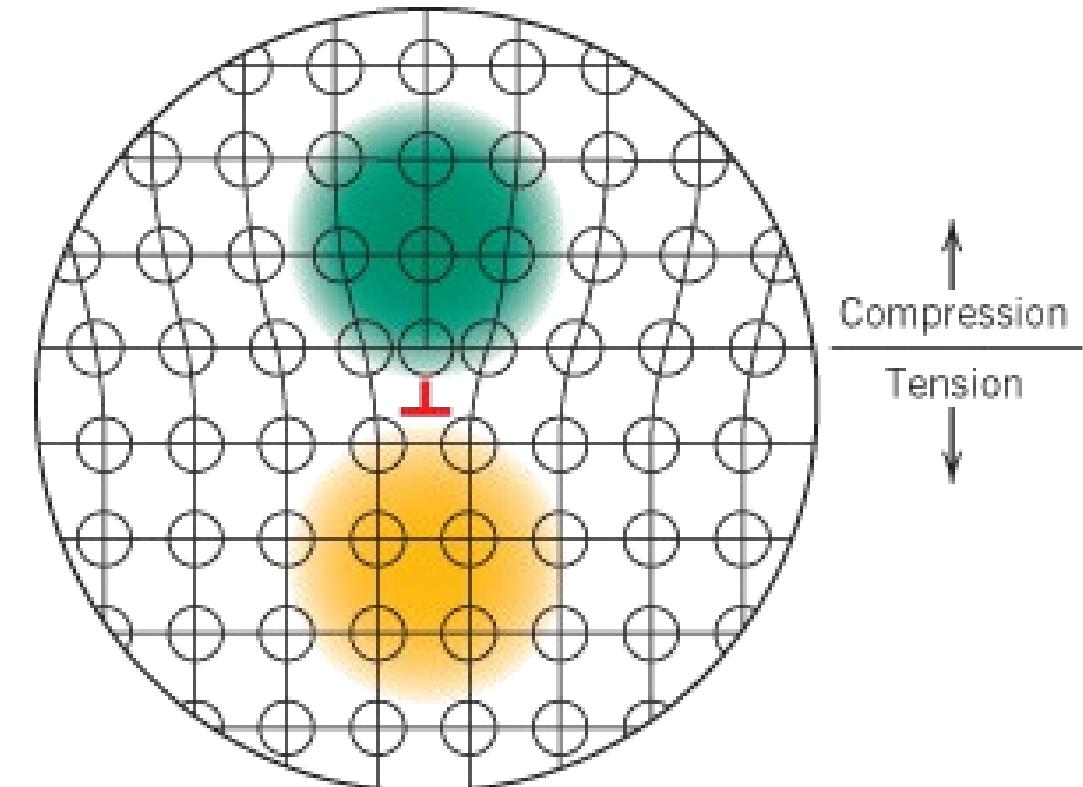
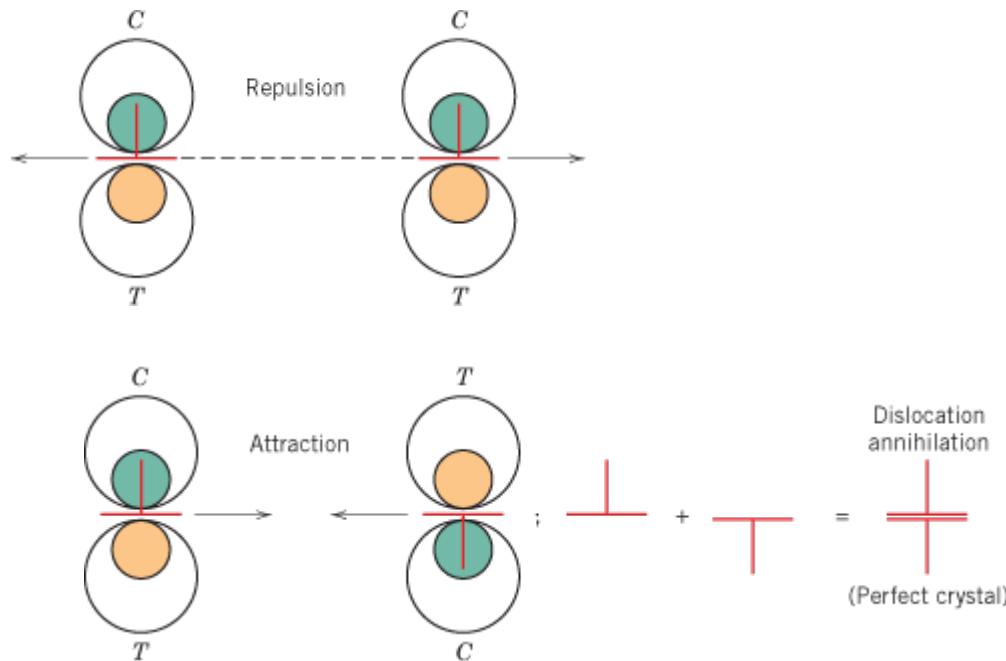
Dislocations and Plasticity [VL]

- Strengthening Mechanisms
 - Grain size effects
 - Solid-solution strengthening
 - Strain hardening
 - Precipitate hardening
- Processing
 - Recovery
 - Recrystallization
 - Grain growth



Characteristics of Edge Dislocations [VL]

- Compressive region
- Tensile region
- Lattice strain → energy
- Dislocation-dislocation interaction → mechanical properties
- Interaction is, *on average*, repulsive*.



*Calculating the global interactions of discrete dislocations to explain work-hardening is still an [active area](#) of research for computational metallurgists.

Strengthening Mechanisms [VL]

Goal:

Increase σ_y , TS (tensile strength)

Approach:

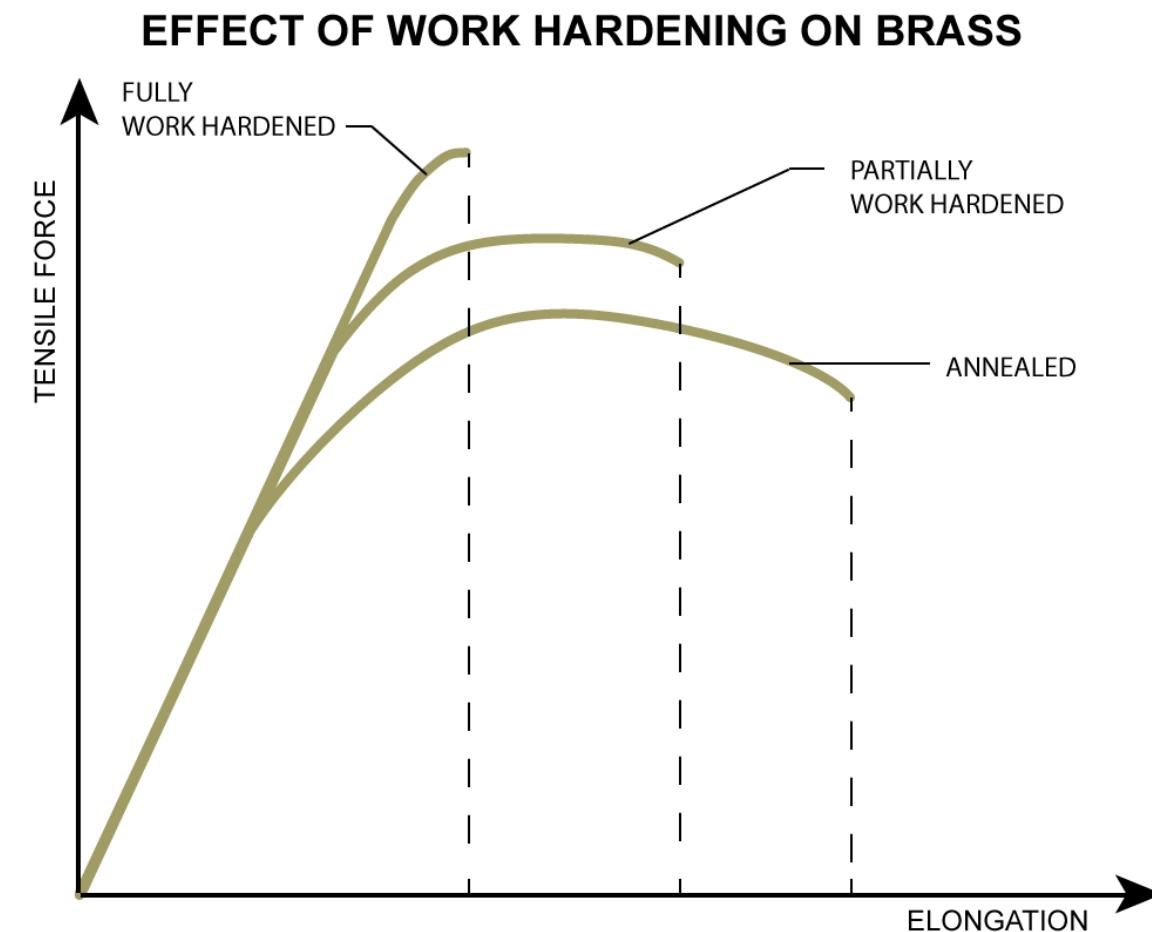
Inhibit motion of dislocations/sliding

Tradeoff:

Stronger usually → less ductile (more brittle)

No/little influence on elastic modulus

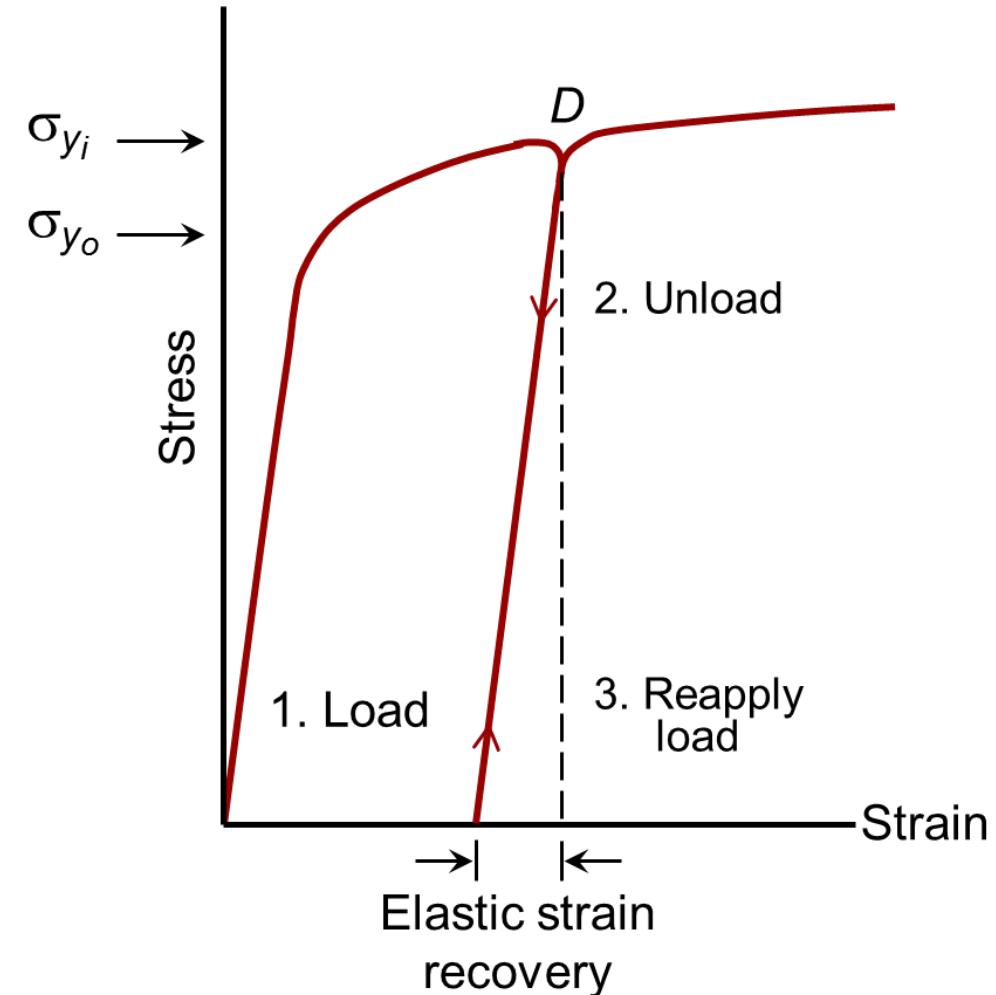
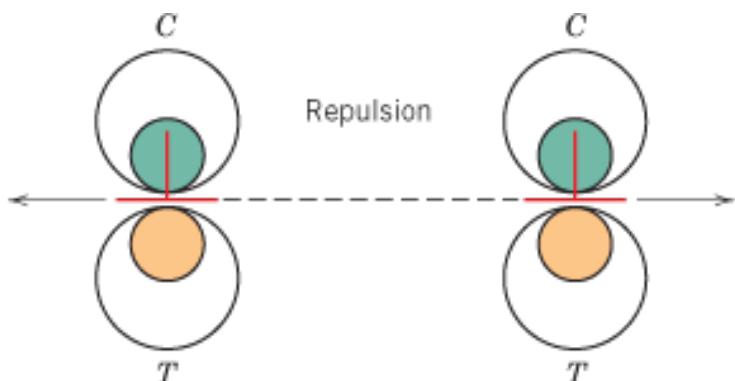
(nature of bond does not change)



Four Strategies for Strengthening [VL]

1.) Strain Hardening (Cold Working)

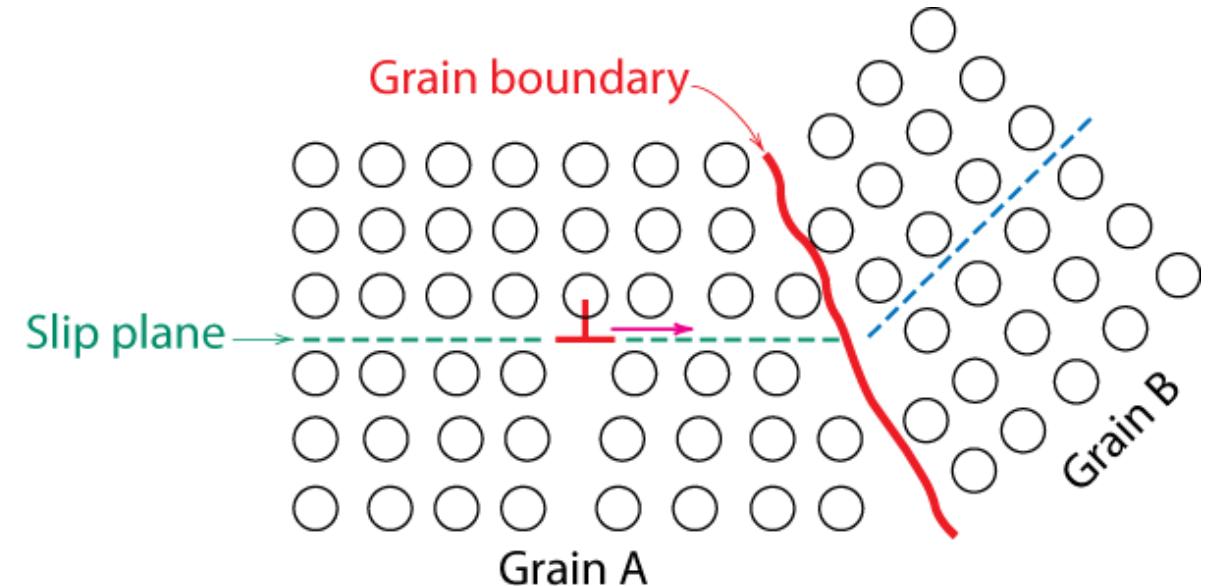
- Deform metal into the plastic regime.
- Unload sample → maintain plastic deformation *and* dislocations
- Achieve increase in σ_y due to repulsive interactive nature of large quantities dislocation.



Four Strategies for Strengthening [VL]

2.) Grain Size Reduction

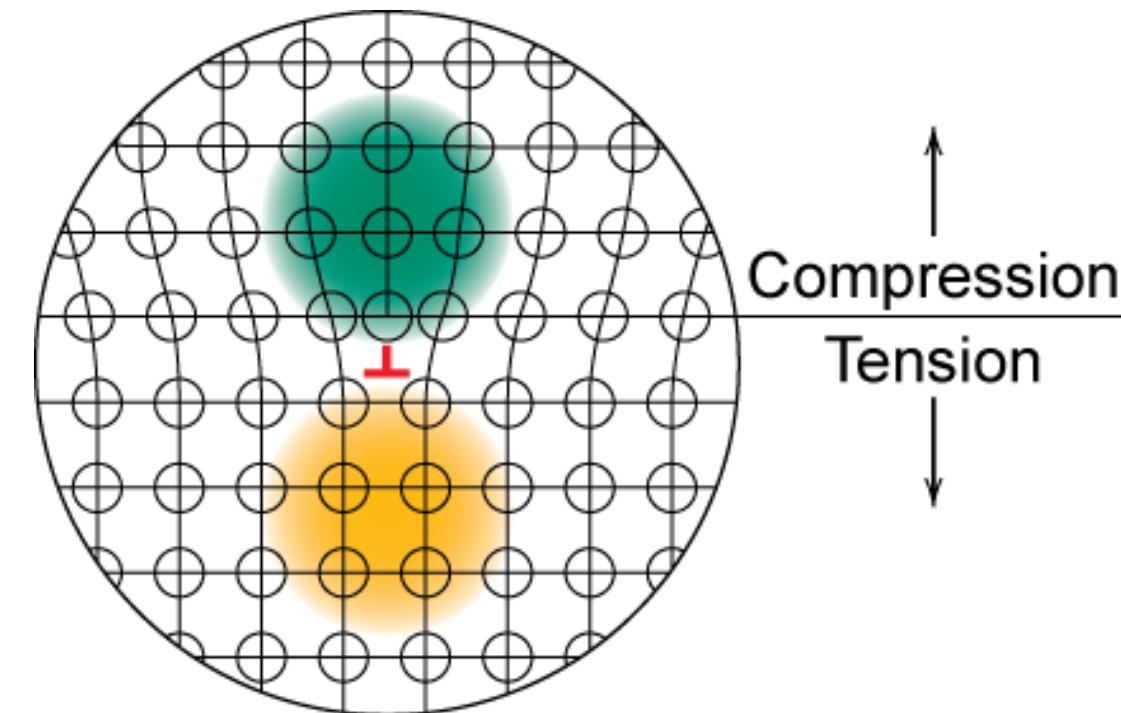
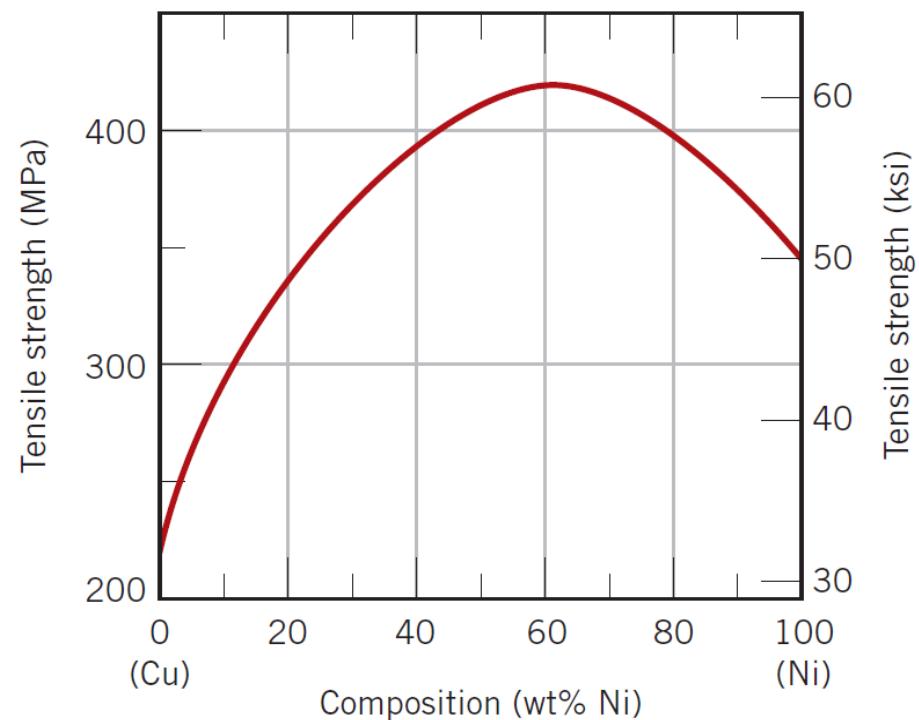
- Dislocation motion has to change direction at grain boundaries
- Grain boundaries create discontinuity for slip planes → form barriers to slip
- Smaller grain size: more barriers to slip



Four Strategies for Strengthening [VL]

3.) Solid-solution Strengthening

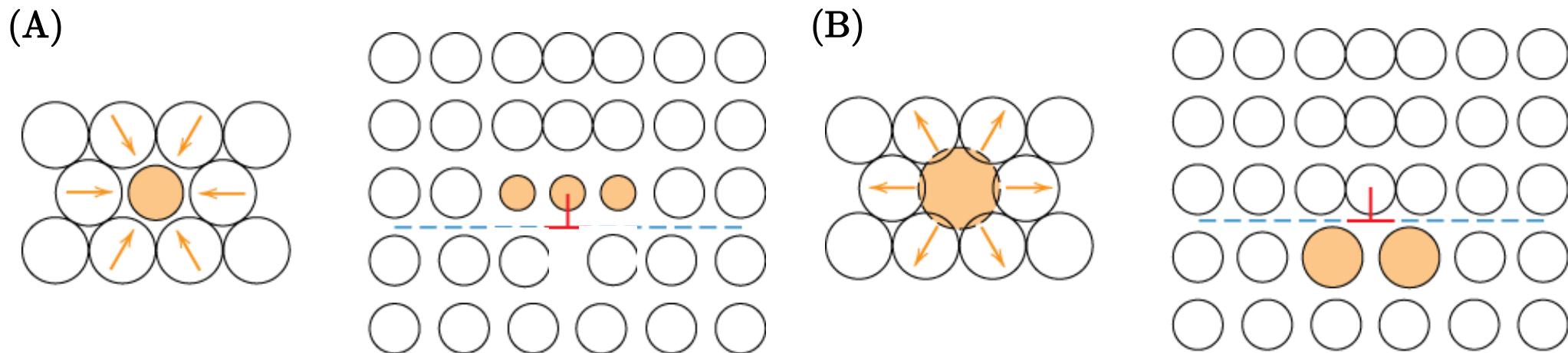
- Strengthen metals by introducing impurities
- High purity metals are typically softer than their alloys



Four Strategies for Strengthening [VL]

3.) Solid-solution Strengthening

- Lower energy for the dislocation to stay put



(A.) Small substitutional impurities – add tension

- Act to reduce *compressive* lattice strain
- Segregate *above* slip plane to *cancel compressive strain* of edge dislocation

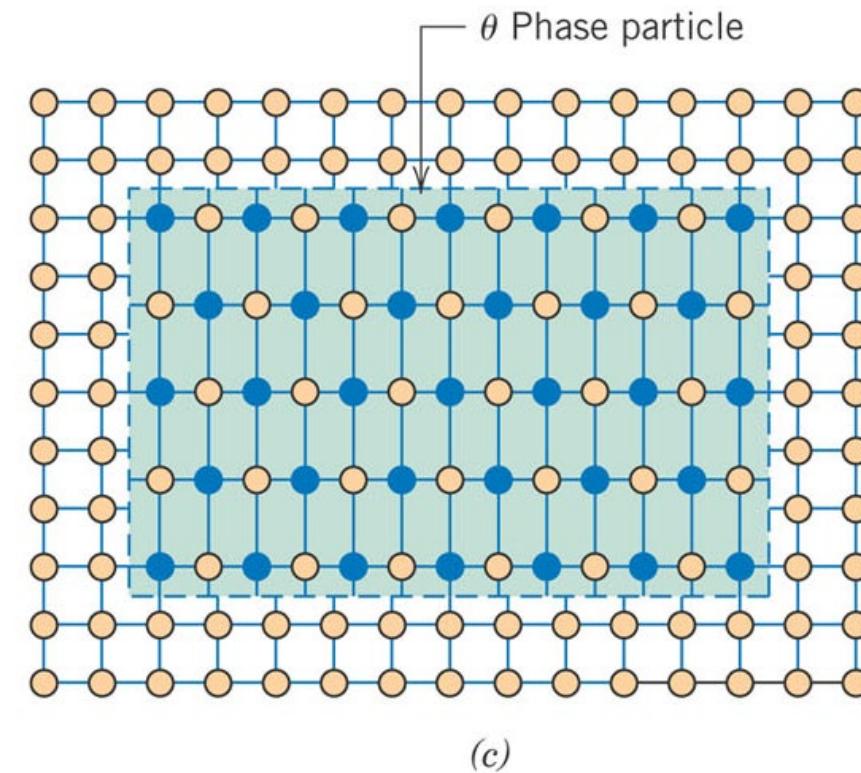
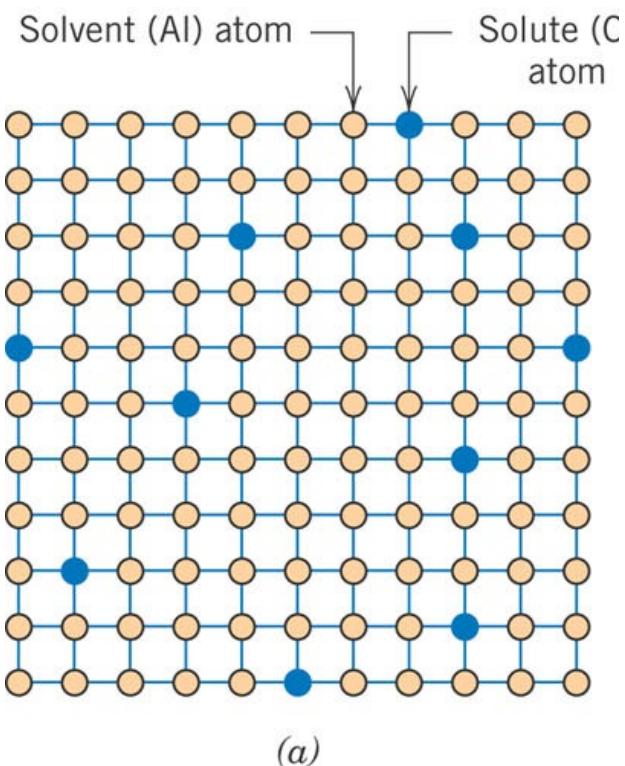
(B.) Large substitutional impurities – add compression

- Acts to reduce *tensile* lattice strain
- Segregate *below* slip plane to *cancel tensile strain* of edge dislocation

Four Strategies for Strengthening [VL]

4.) Precipitate Hardening

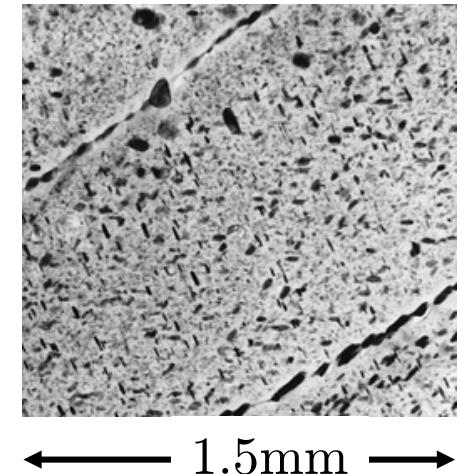
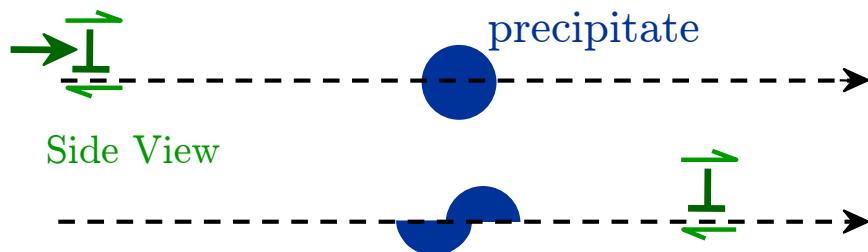
- Inserting precipitates (small volumes) of other phases (strong ones)
 - Intermetallics (ionic character)
 - Covalent precipitates
 - Ionic precipitates



Four Strategies for Strengthening [VL]

4.) Precipitate Hardening

- Strong precipitates (ceramics, e.g. SiC in Fe or Al) act as dislocation motion blockades.



6000-series aluminum alloy: Al-Cu (Duralumin)

~20% lighter

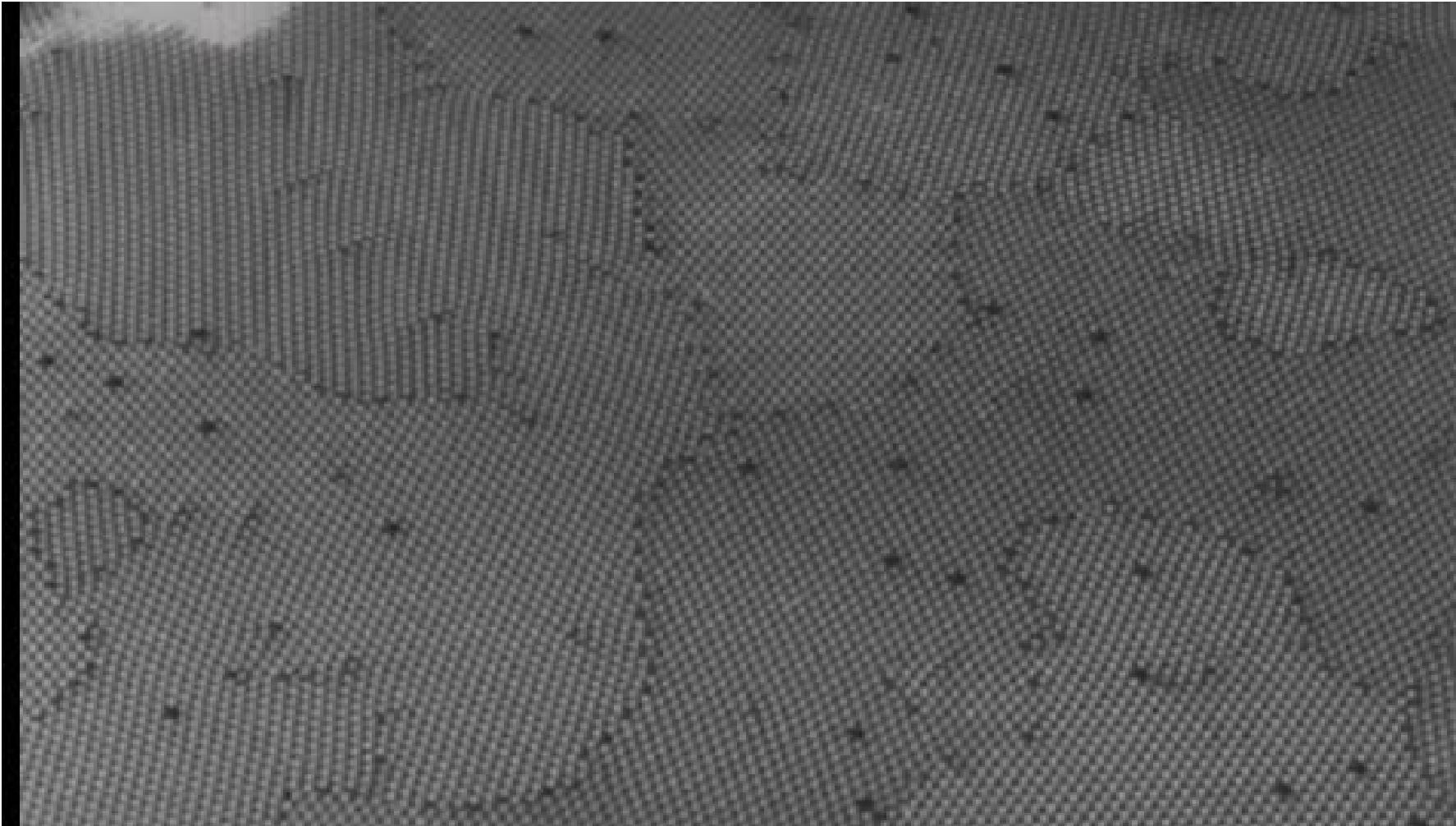
~20% improved fuel efficiency

Approaches strength of steel
(More expensive)

Al_3Sc precipitates

Bubble Raft Dislocation Analog [VL]

11:40 Impurity Atoms



Concept Check

Select one or more answers for this question: Grain size reduction, formation of solid-solutions, precipitate hardening, and strain hardening can all lead to *strengthening* of metals.

Which mechanical property(ies) is(are) often sacrificed to achieve larger strengths?

- A. Stiffness (elastic modulus)
- B. Resilience
- C. Ductility
- D. Toughness

Concept Check – Solution

Select one or more answers for this question: Grain size reduction, formation of solid-solutions, precipitate hardening, and strain hardening can all lead to *strengthening* of metals.

Which mechanical property(ies) is(are) often sacrificed to achieve larger strengths?

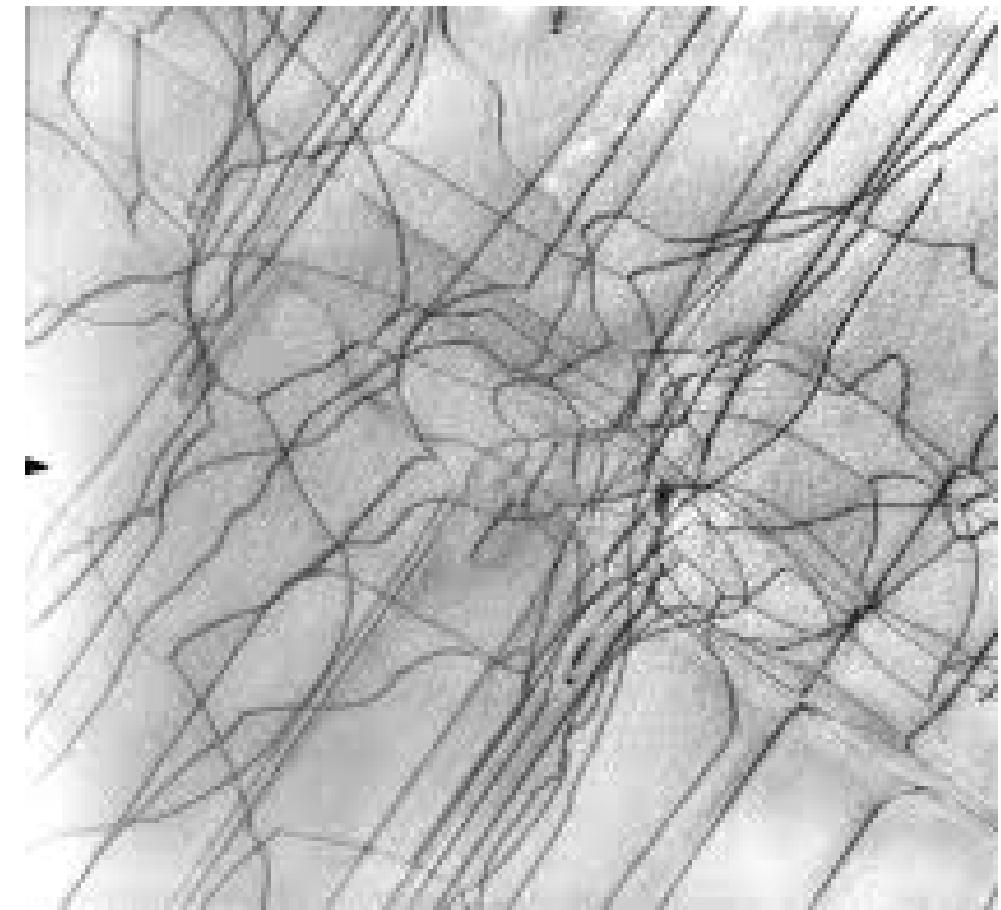
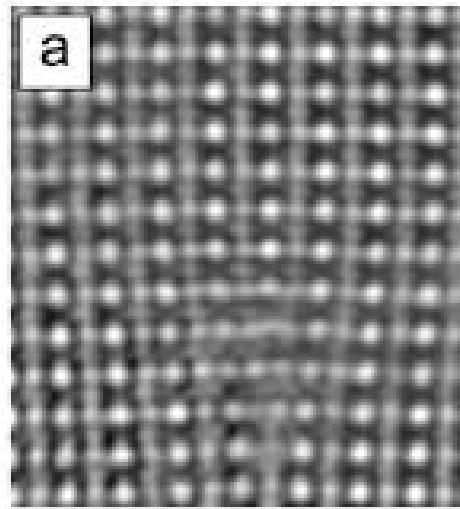
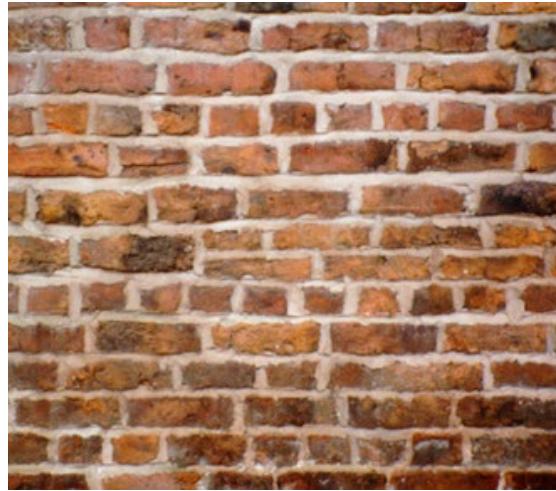
- A. Stiffness (elastic modulus)
- B. Resilience
- C. Ductility**
- D. Toughness

Solution: Just ductility. Build-up of dislocations when we impede them lead to the formation of cracks (more on this later) and then fracture.

- ◊ Stiffness is not affected (bond strength does not change).
- ◊ Toughness may go up or down, depending on the degree of strengthening (you can embrittle a material greatly through strengthening).
- ◊ Resilience is likely to rise as the strength rises (it isn't sacrificed) but the elastic modulus is constant.

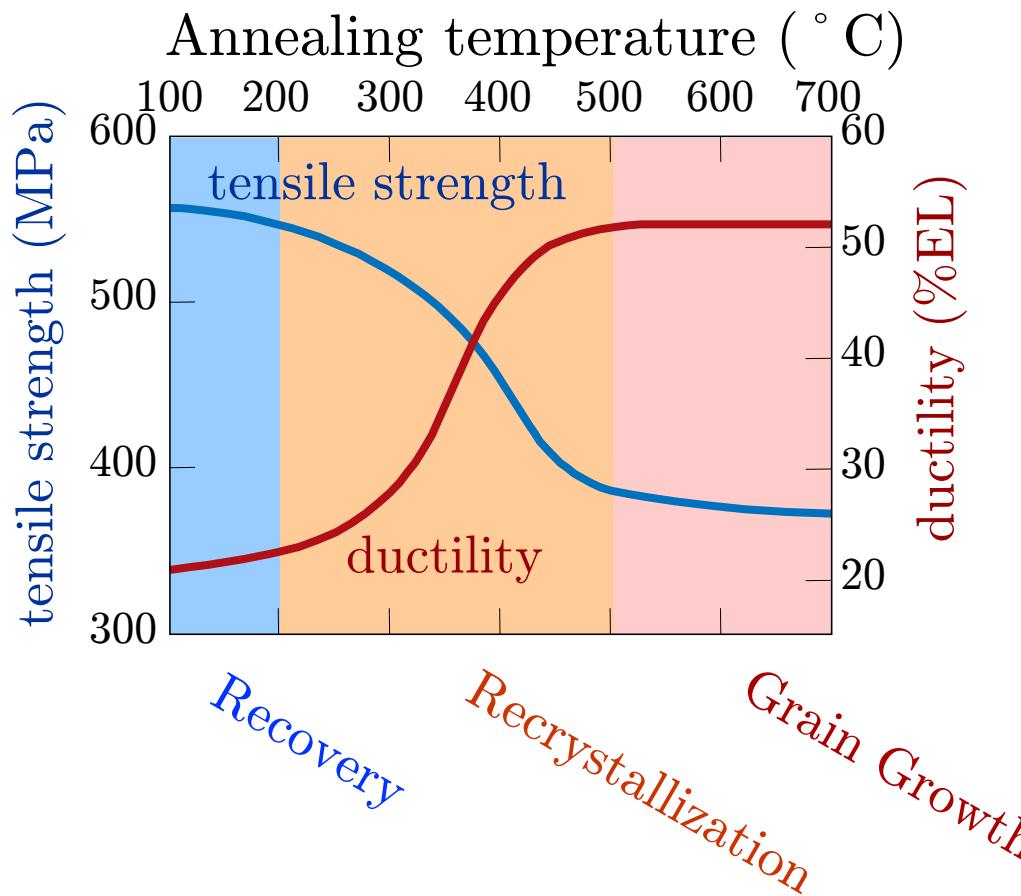
Dislocations and Plasticity

- Strengthening Mechanisms
 - Grain size effects
 - Solid-solution strengthening
 - Strain hardening
 - Precipitate hardening
- Processing
 - Recovery
 - Recrystallization
 - **Grain growth**
- Biomaterials



Heat Treatments - Annealing

- Much of the structural/mechanical changes caused by plastic deformation can be reversed via *annealing*, or heat treatment.



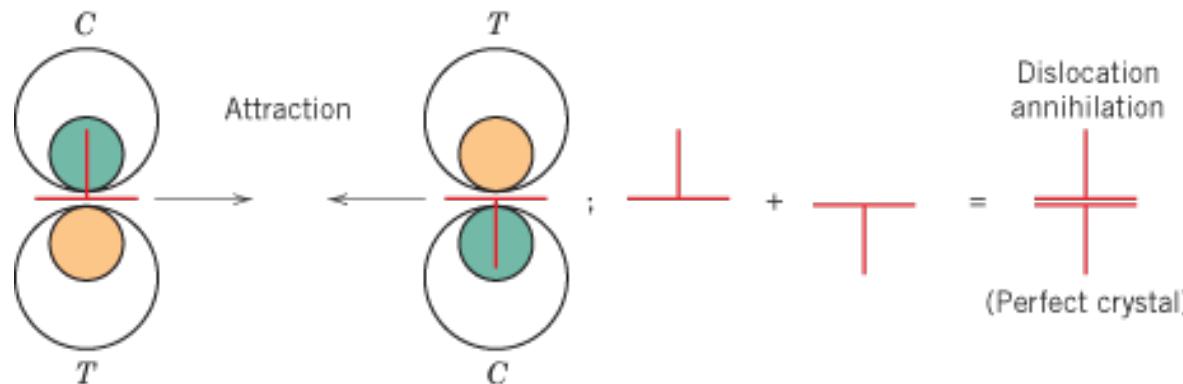
- Three annealing stages:
 - Recovery
 - Recrystallization
 - Grain Growth

Heat Treatments – Three Microstructural Stages

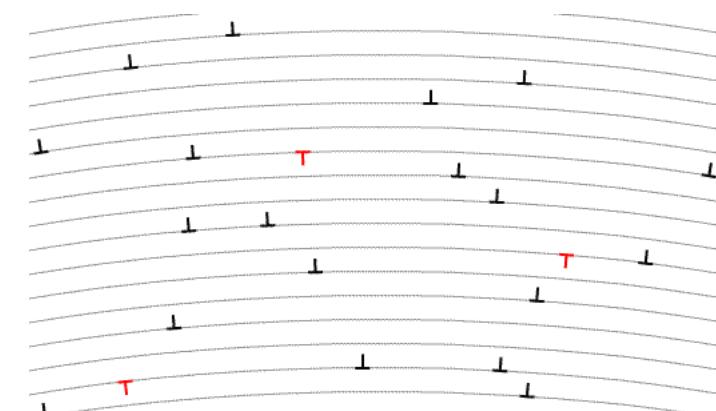
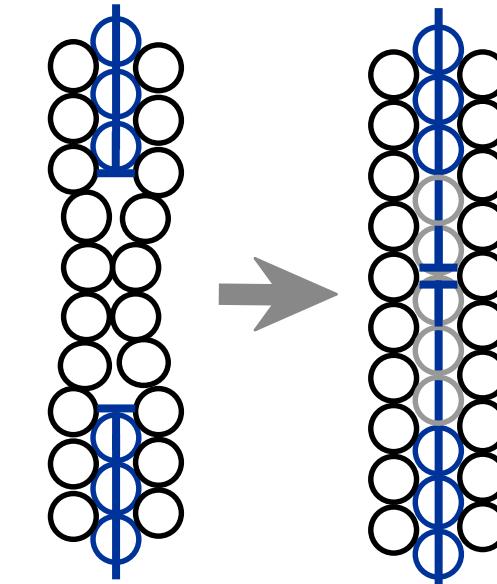
1.) Recovery:

- Reduction of *dislocation density* by annihilation.
- Rearrangement of dislocations in low-energy configurations.

Dislocation annihilation → perfect crystal.



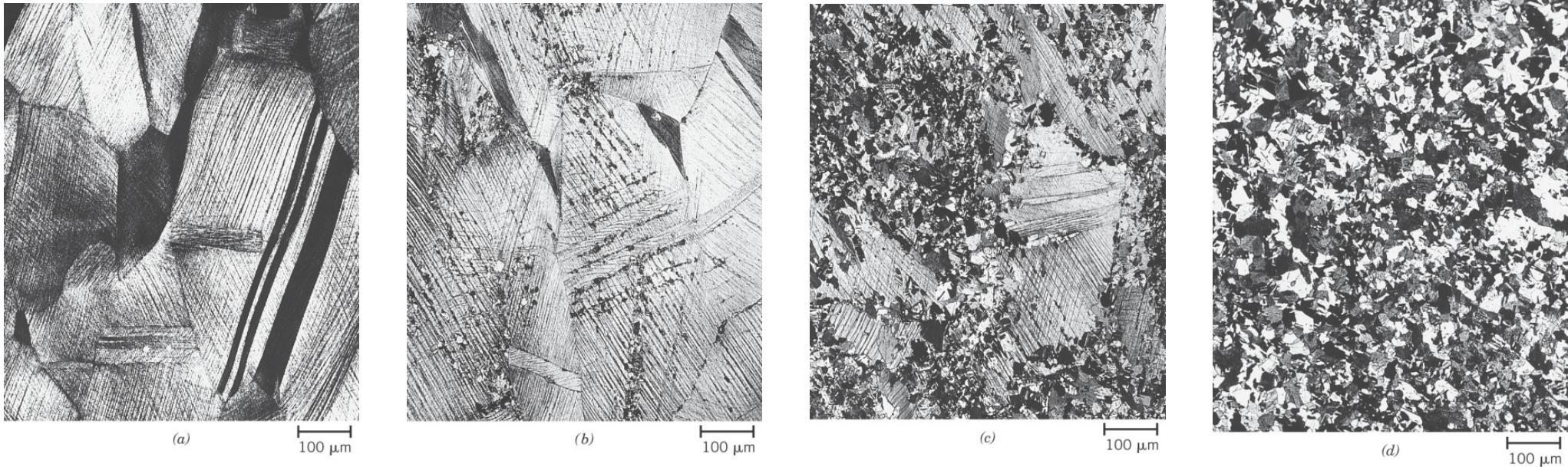
- Temperature increases → atomic diffusion increases
- Dislocations combine/align to reduce overall strain energy in the lattice



Heat Treatments - Annealing

2.) Recrystallization:

- After recovery, strain still exists in crystals.
- Small, unstrained grains nucleate inside large, strained grains.
- These grains consume the strained grains.
- Strained grains are completely consumed – driving force is reduction in strain energy.

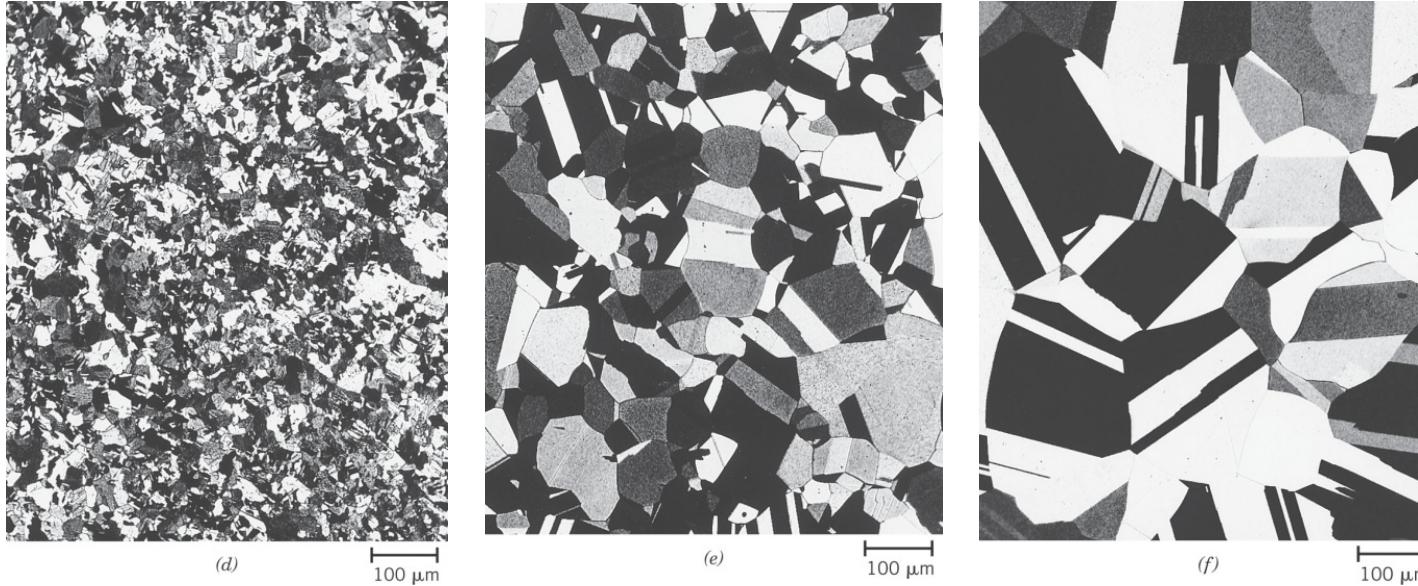


Recrystallization

Heat Treatments - Annealing

3.) Grain Growth:

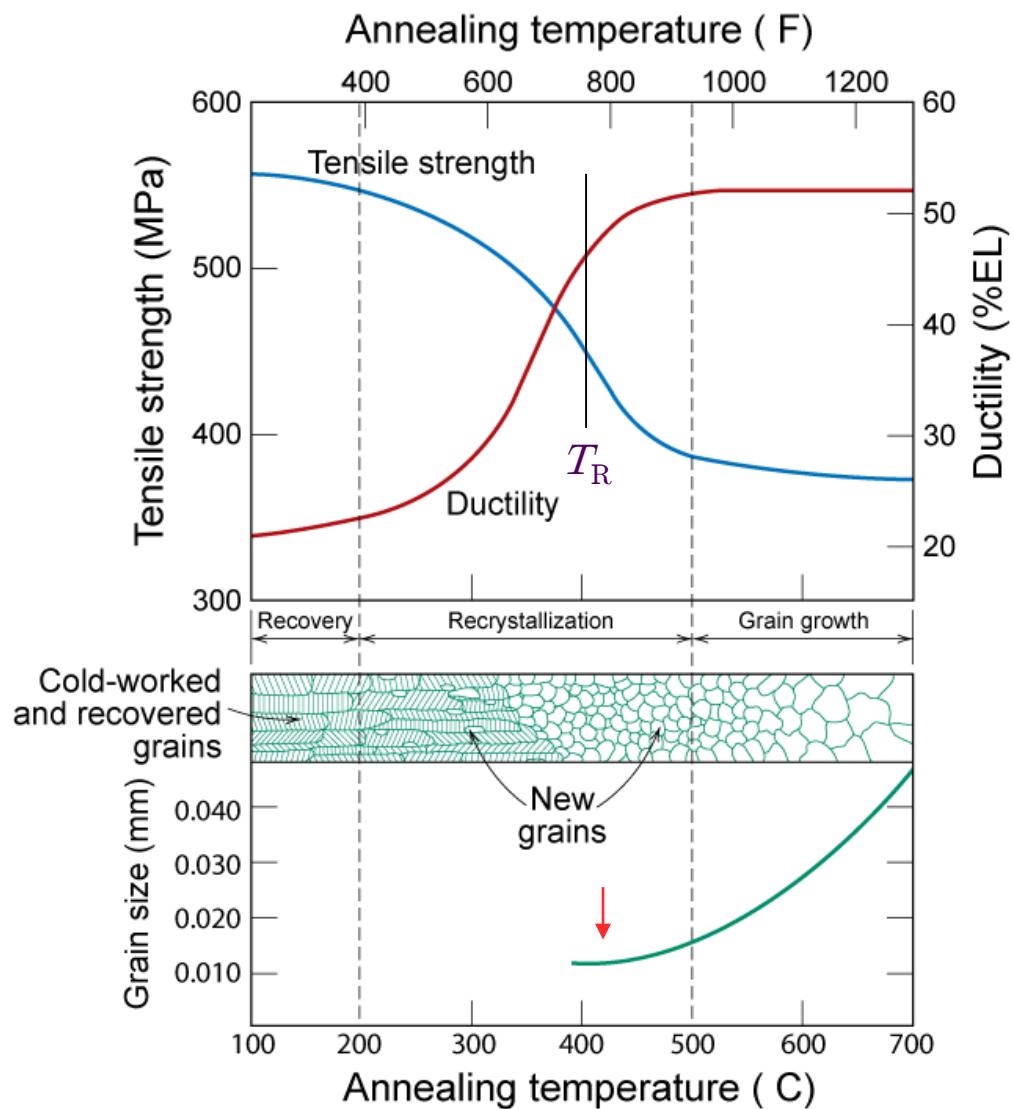
- Small grains shrink (disappear)
- Large grains grow to reduce grain boundary energy



Grain Growth

- Large grains, few dislocations → lower strength
- Large grains, few dislocations → improved ductility

Annealing after Strain Hardening



T_R = “recrystallization temperature”

→ Temperature at which recrystallization just reaches completion in 1 h.

$$0.3T_m < T_R < 0.6T_m$$

Note – all processes are thermally activated (Arrhenius type behavior)

- Near the “recrystallization temperature”, all processes will proceed: recovery, recrystallization, grain growth over long times.
- Activation energies for recovery are lower than recrystallization (etc.)

Concept Check

Lead is a metal with an interesting combination of properties: it is heavy, ductile, an inert, and it is relatively easily extracted from galena and therefore inexpensive. It also has a low melting temperature ($T_M = 600\text{ K}$).

Let's say you've been living under a rock for 80 years, and you decide to install lead pipe in your house. Which of the following techniques could you use to go about strengthening the lead pipe prior to installation?

- A. Annealing the lead to increase grain size.
- B. Work-hardening the lead pipe.
- C. Alloying the lead with antimony to create a solid solution.
- D. Alloying the lead with copper to acquire a Cu-phase precipitate.

Concept Check – Solution

Lead is a metal with an interesting combination of properties: it is heavy, ductile, an inert, and it is relatively easily extracted from galena and therefore inexpensive. It also has a low melting temperature ($T_M = 600\text{ K}$).

Let's say you've been living under a rock for 80 years, and you decide to install lead pipe in your house. Which of the following techniques could you use to go about strengthening the lead pipe prior to installation?

- A. Annealing the lead to increase grain size.
- B. Work-hardening the lead pipe.
- C. Alloying the lead with antimony to create a solid solution.**
- D. Alloying the lead with copper to acquire a Cu-phase precipitate.**

Solution:

Alloying to create solid solutions or precipitates will certainly strengthen the material (and this is what is done). Increasing grain size will have the opposite effect — eliminating barriers for dislocation motion. Cold working won't do anything for lead! It is at its recrystallization temperature at room temperature and “anneals” in ambient.

Outline

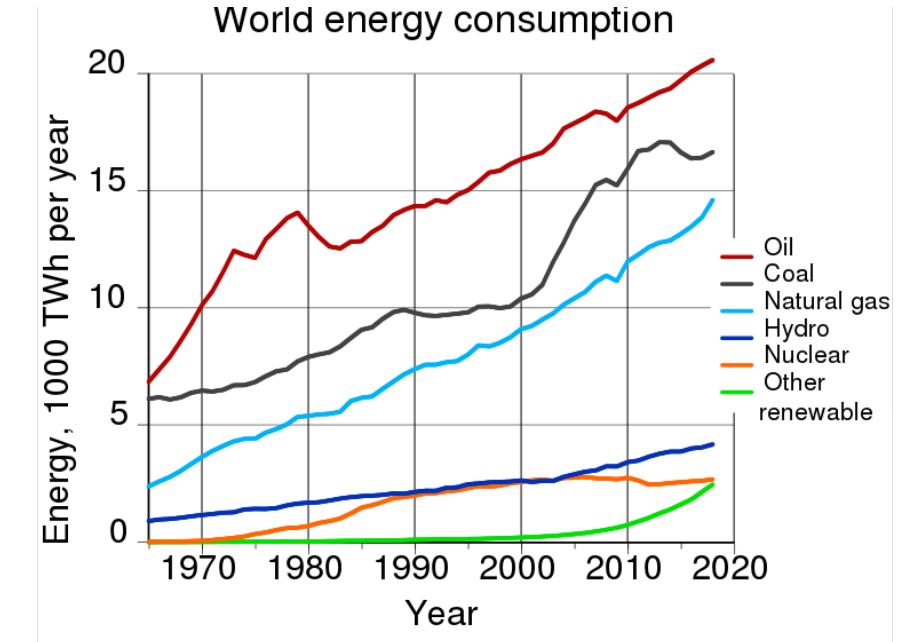
- Electrical Conduction
 - Materials properties of charge transport (conductivity and resistivity) [Video Lecture]
 - Charge carrier mobility
 - Sources of resistivity (Matthiessen's Rule)
- Electronic Structure
 - Review electronic states in isolated atoms
 - What happens when we push atoms together?
→ Electronic band structure [Video Lecture]
 - Difference between electronic structure of metals, insulators, and semiconductors.

Electronic Properties I: Objectives

- How are electrical conductance and resistance characterized?
 - Classical perspective
- For metals, how is conductivity affected by imperfections, temperature, and deformation?
- What are the physical phenomena that distinguish conductors, semiconductors and insulators?
 - Quantum-mechanical approach
 - Remember *electronic* structure from Ch. 2

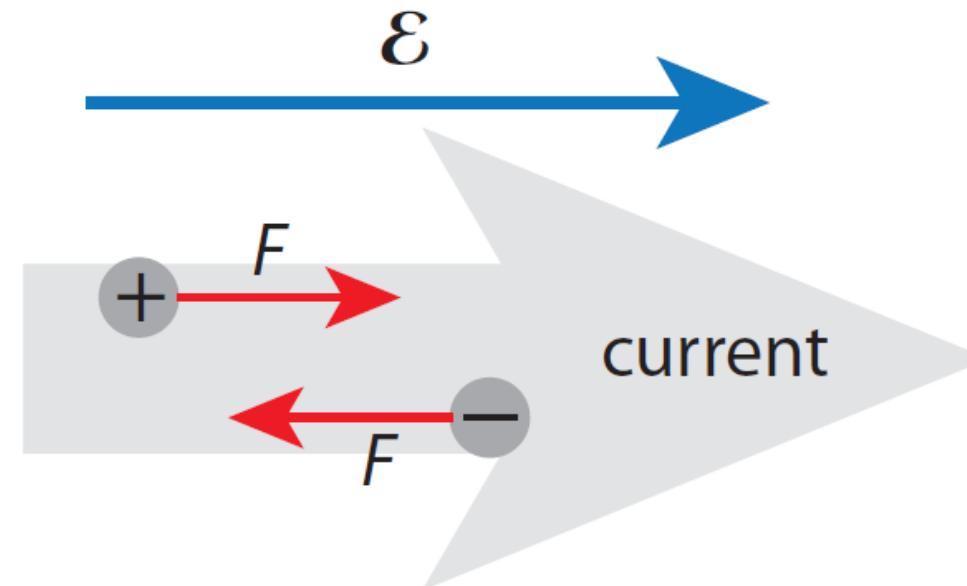
Electronic Properties and the Information Age

- Critical in transport and storing of electricity and power
- Used to operate machines, appliances, and devices
- Central to storing and processes digital information
- Central to Renewable Energy Age?



Electrical Conduction: Classical Description [VL]

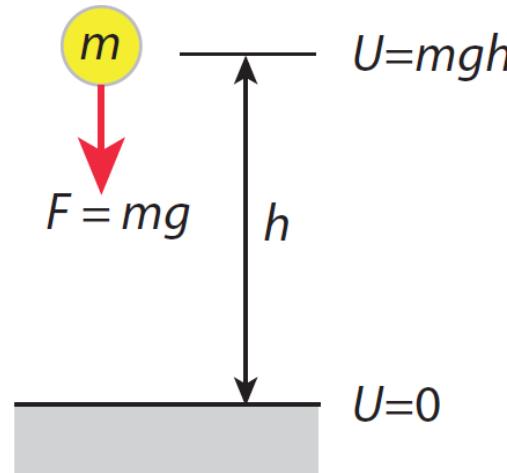
- Charged particles experience a force, F , when an electric field, \mathcal{E} , is present.
- The motion of the charged particles brought about by this force is the current, I .
- Force accelerates *positive* charge in direction of the \mathcal{E} -field.*



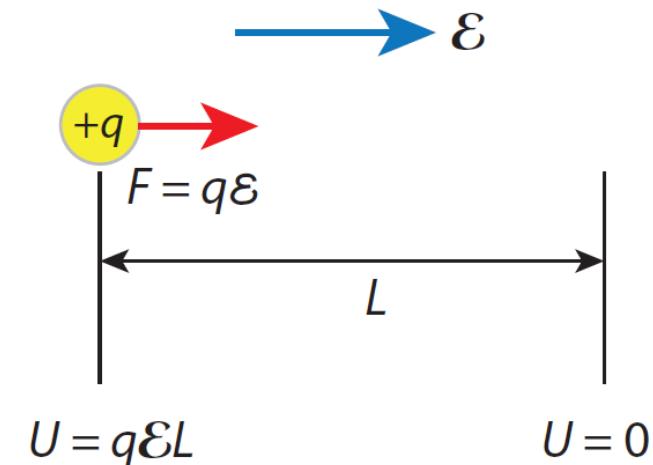
Electric Potential (V) [VL]

- Defined as the potential energy per unit charge
 - Analogous to gravitational potential energy
 - Energy of an electrically charged particle at rest in an electric field

$$V = \frac{U}{q} = \mathcal{E}L$$



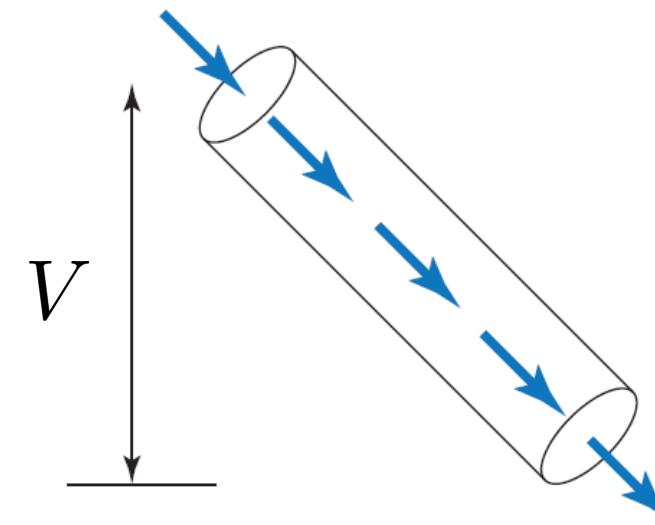
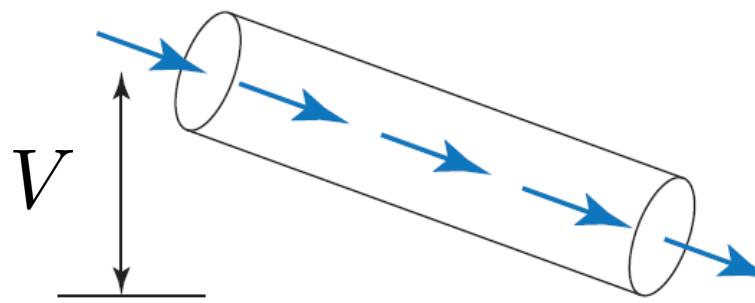
Potential energy due to a gravitational field



Potential energy due to an electric field

Electrical Conduction [VL]

- The flow of current through a potential difference is analogous to the flow of water downhill
- Increasing the difference in potential between the two ends of a wire causes charges to flow faster, and thereby increases the current



$$I \propto V$$

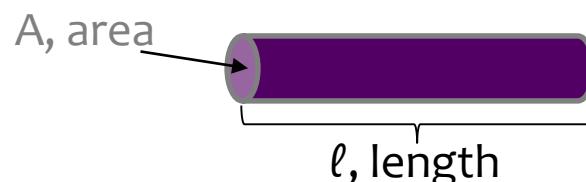
Ease of Electrical Conduction: Resistance [VL]

- Ohm's Law expresses this linear relationships between the current and applied potential

$$V = IR$$

Electric potential difference (volts, V*) Current (amps, A) Resistance (Ohms, Ω)

- Resistivity, ρ ($\Omega \cdot \text{m}$)
 - A *material property* that is *independent* of sample size and geometry



Area of current flow

Current flow path length

- Conductivity, σ [$(\Omega \cdot \text{m})^{-1}$ or S/m]
 - A *material property* that is independent of sample size and geometry

$$\rho = \frac{RA}{l}$$
$$\sigma = \frac{1}{\rho}$$

*Sometimes you see a ΔV here.

An Alternate Expression of Ohm's law

- It can also be expressed as an electron *flux*

$$J = \sigma \epsilon$$

$J \equiv$ Current Density

$\epsilon \equiv$ Electric field potential $\equiv V/\ell$

$$J = \sigma \frac{V}{\ell}$$

The diagram shows the equation $J = \sigma \frac{V}{\ell}$ with three arrows pointing to its components: "Electron flux" points to J , "conductivity" points to σ , and "voltage gradient" points to $\frac{V}{\ell}$.

→ Similar to mass flux for steady-state diffusion

Electrical Conduction: Summery Table [VL]

Value	Symbol	Unit	Material Property?	Relationship
Conductance	G	Ω^{-1} or S	No	$G = 1/R$
Conductivity	σ	$\Omega^{-1}\text{-m}^{-1}$ or $\text{S}\text{-m}^{-1}$	Yes	$\sigma = G\ell/A$
Resistance	R	Ω	No	$R = 1/G$
Resistivity	ρ	$\Omega\text{-m}$	Yes	$\rho = RA/\ell$

- Conductivity and resistivity *only* depend on the material the wire is made of (neglecting a few things we'll talk about later) and are therefore materials properties

Concept Check

Select all that apply: Which of the following quantities are *independent* of circuit geometry?

- A. Resistance
- B. Conductivity
- C. Conductance
- D. Resistivity

Concept Check – Solution

Select all that apply: Which of the following quantities are *independent* of circuit geometry?

- A. Resistance
- B. Conductivity**
- C. Conductance
- D. Resistivity**

Solution:

Both resistance and conductance are measured values dependent on circuit geometry (length and width of wire). Resistivity and conductivity are intrinsic materials properties that depend only on the material itself.

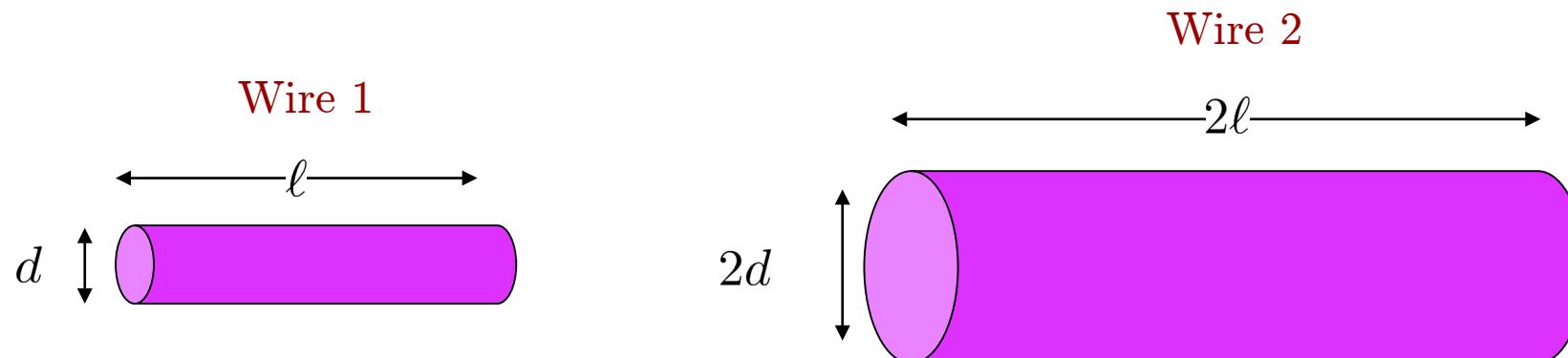
Value	Symbol	Unit	Material Property?	Relationship
Conductance	G	Ω^{-1} or S	No	$G = 1/R$
Conductivity	σ	$\Omega^{-1}\text{-m}^{-1}$ or S-m $^{-1}$	Yes	$\sigma = G\ell/A$
Resistance	R	Ω	No	$R = 1/G$
Resistivity	ρ	$\Omega\text{-m}$	Yes	$\rho = RA/\ell$

Concept Check

The wires shown below are made of the same material. Write an expression relating the resistances of the two wires. What is the relationship between the *resistance* of the two wires?

- A. $R_1 = R_2$
- B. $4R_1 = R_2$
- C. $2R_1 = R_2$
- D. $R_1 = 2R_2$
- E. $R_1 = 4R_2$
- F. Can't say, need resistivity.

Value	Symbol	Unit	Material Property?	Relationship
Conductance	G	Ω^{-1} or S	No	$G = 1/R$
Conductivity	σ	$\Omega^{-1}\text{-m}^{-1}$ or S-m $^{-1}$	Yes	$\sigma = G\ell/A$
Resistance	R	Ω	No	$R = 1/G$
Resistivity	ρ	$\Omega\text{-m}$	Yes	$\rho = RA/\ell$



Concept Check – Solution

- Analogous to flow of water in a pipe
- Resistance depends on sample geometry and size

$$R = \frac{\rho\ell}{A}$$

$$R \propto \frac{1}{A}$$

$$R \propto \frac{1}{d^2}$$

$$R \propto \ell$$

$$\frac{R_1}{R_2} = \frac{\frac{\rho_1 \ell_1}{A_1}}{\frac{\rho_2 \ell_2}{A_2}}$$

$$\frac{R_1}{R_2} = \cancel{\frac{\rho_1}{\rho_2}} \frac{\ell_1}{\ell_2} \frac{A_2}{A_1}$$

$$\frac{R_1}{R_2} = \cancel{\frac{\pi(\frac{2d}{2})^2}{\pi(\frac{d}{2})^2}} \frac{\cancel{\ell_1}}{\cancel{2\ell_1}}$$

$$\frac{R_1}{R_2} = \frac{4}{2} = 2$$

Conductivity: A Comparison

- Room temperature values ($\Omega\text{-m}$)⁻¹

METALS

Silver	6.8×10^7
Copper	6.0×10^7
Iron	1.0×10^7

conductors

CERAMICS

Soda-lime glass	$10^{-10} - 10^{-11}$
Concrete	10^{-9}
Aluminum oxide	$\sim 10^{-13}$

SEMICONDUCTORS

Silicon	4×10^{-4}
Germanium	2×10^0
GaAs	1×10^{-6}

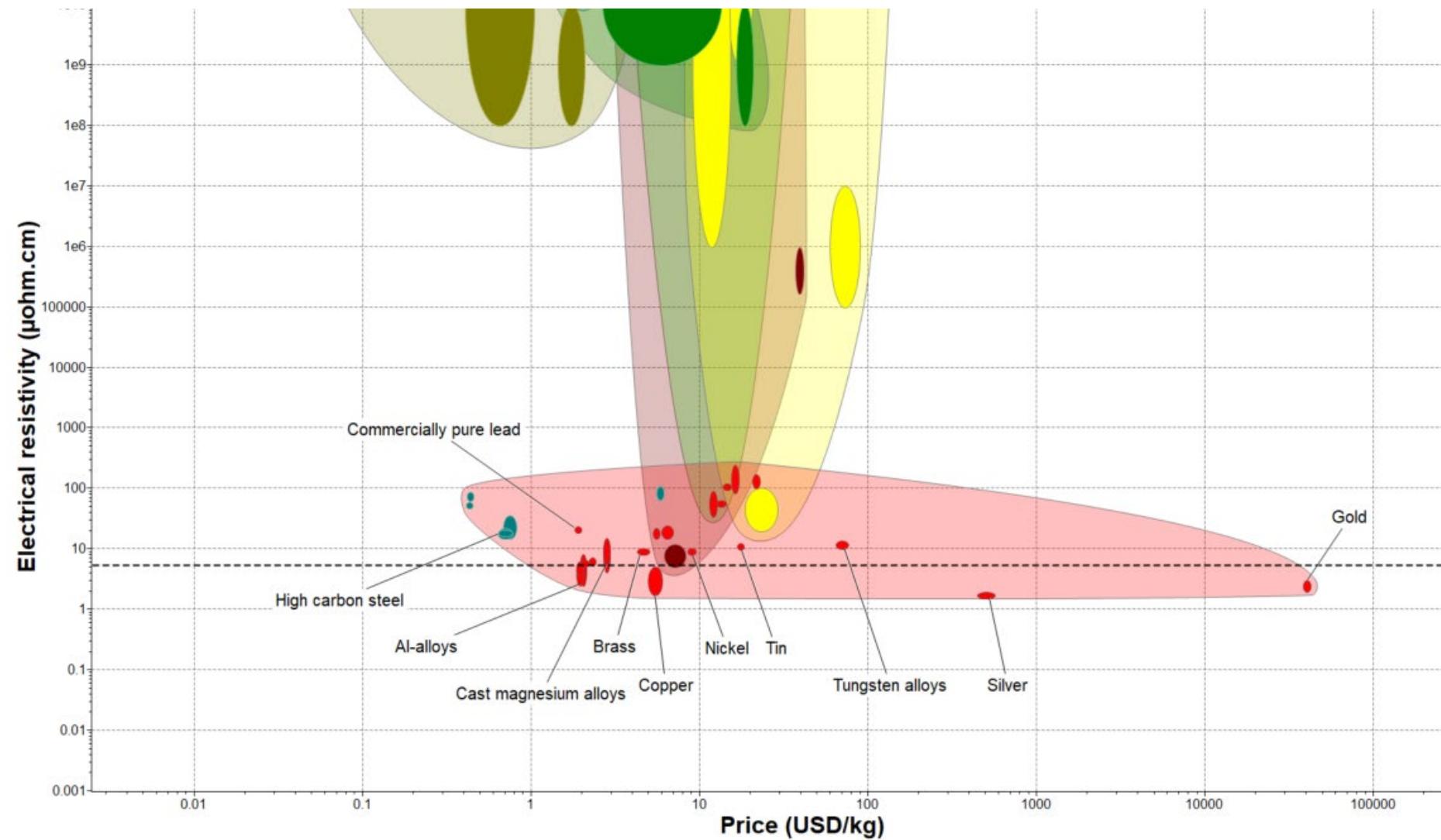
Semiconductors*

POLYMERS

Polystyrene	$\sim 10^{-14}$
Polyethylene	$10^{-15} - 10^{-17}$

insulators

Conductivity: A Comparison

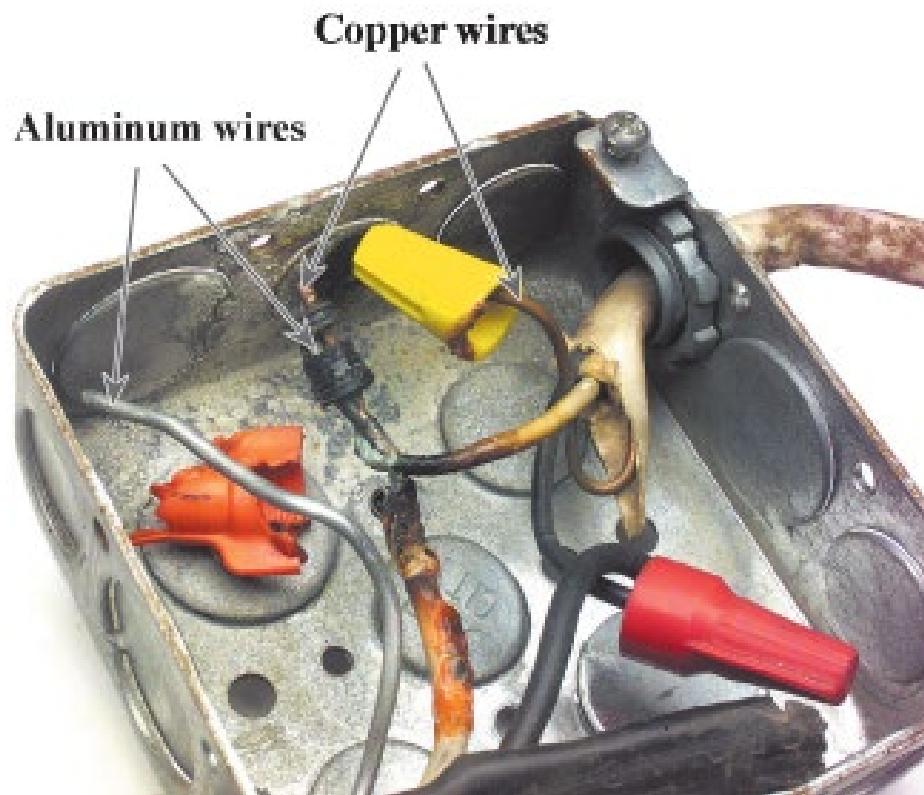


Ni

Case Study: Cu vs Al

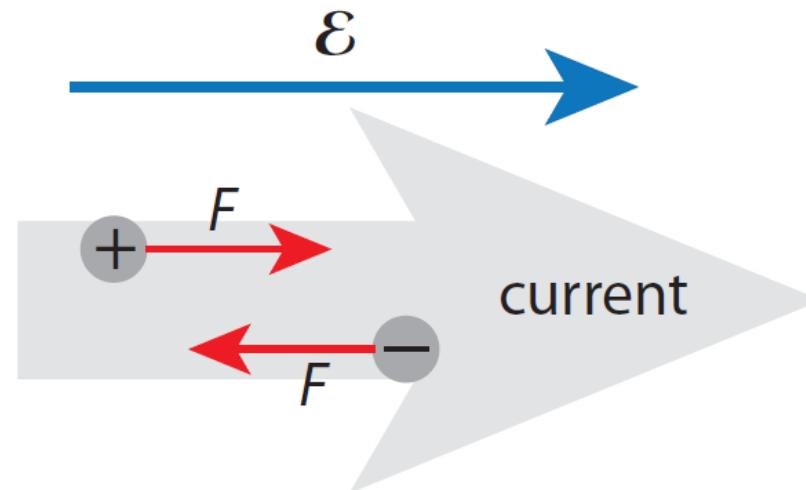
- Rise in price in Cu in 1970s → use aluminum!

Alloy	Composition	Electrical Conductivity	Coefficient of Thermal Expansion
Al-1350	99.50 Al, 0.1 Si, 0.05 Cu...	$3.57 \times 10^7 \text{ } (\Omega\text{-m})^{-1}$	$23.8 \times 10^{-6} \text{ } ^\circ\text{C}^{-1}$
Cu-C1100	99.90 Cu, 0.04 O, ...	$5.88 \times 10^7 \text{ } (\Omega\text{-m})^{-1}$	$17.0 \times 10^{-6} \text{ } ^\circ\text{C}^{-1}$



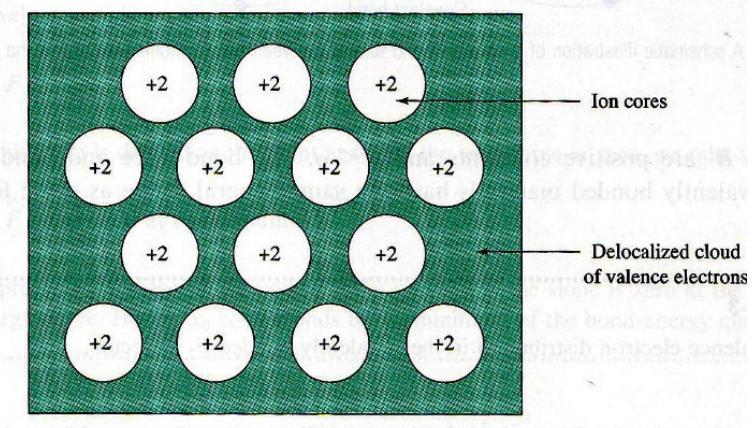
Conduction in Metals, Electron Mobility

- An electric field acts on free electrons to accelerate them in a direction opposite the applied field due to their negative charge

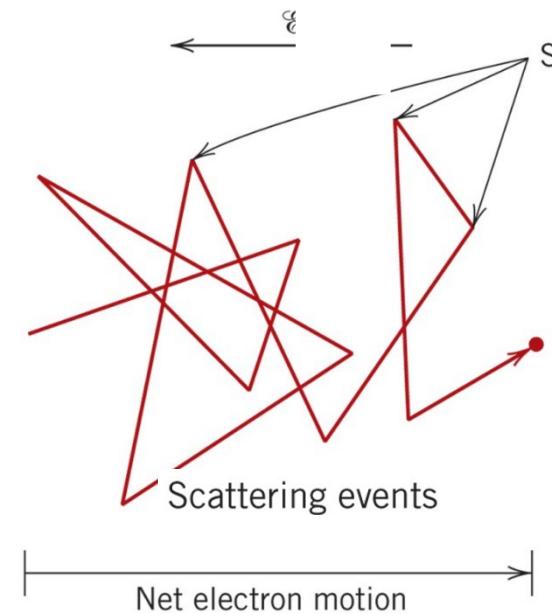


Conduction in Metals, Electron Mobility

- *E*-fields will accelerate “free” electrons in the Fermi Sea.
- According to quantum mechanics*, electrons do not interact with the rest of the atoms in a perfect lattice.
- But → current reaches a constant value due to “frictional forces”
 - These result from scattering of electrons by imperfections such as:
 - 0D defects impurity atoms, vacancies, interstitials,
 - 1D defects – dislocations
 - 2D defects – grain boundaries
 - Thermal vibrations of the atoms and lattice
 - Scattering leads to electron “deflections”*

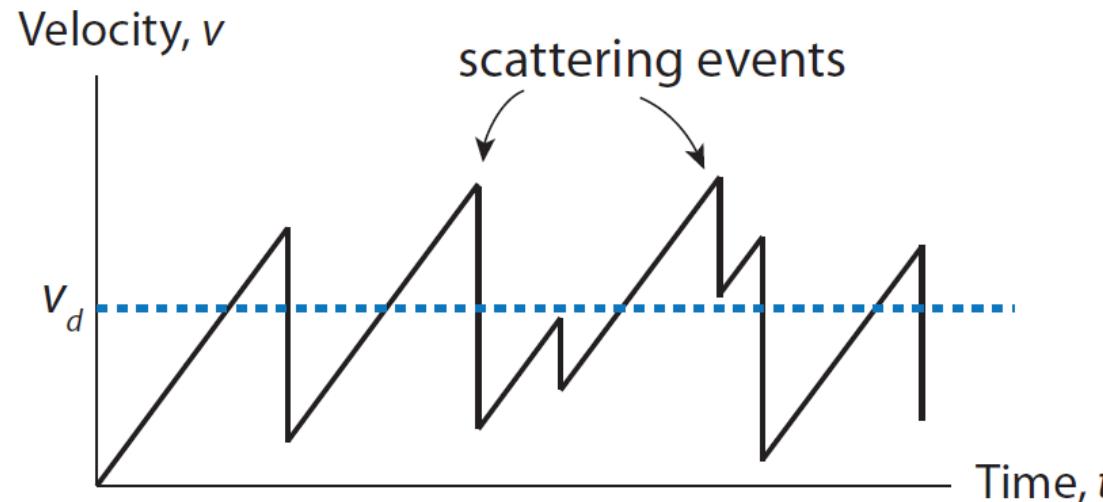


Many Mg atoms combine to form a solid metal



Electron Mobility

- Drift velocity represents the average electron velocity in the direction (opposite) of applied force (electrical field)



$$v_d = \mu_e \mathcal{E} \text{ where } \mu_e \text{ is the electron mobility } \text{m}^2/(\text{V}\cdot\text{s})$$

- Mobility indicates the *frequency of scattering*.
- Mobility decreases with an *increasing* frequency of scattering events.

$$\mu_e \propto \frac{1}{f_s}$$

Conduction in Metals: Electron Mobility

- The conductivity of metals is given by

$$\sigma = n|e|\mu_e$$

where

- n = concentration of free electrons ($/m^3$)
- $|e|$ = magnitude of electron charge ($1.6 \times 10^{-19} C$)
- μ_e = electron mobility ($[m^2 V^{-1}s^{-1}]$)

$$\sigma [(\Omega\text{-m})^{-1}] = n [m^{-3}] |e| [C] \mu_e [m^2/(V\text{-s})]$$

Conduction in Metals: Example

- Ag has a room temperature electrical conductivity of 6.3×10^7 ($\Omega\text{-m}$) $^{-1}$. There are 5.85×10^{22} Ag atoms per cm^3 each with one conduction electron. The mass of an electron is 9.1×10^{-31} kg.
 - What is the electron mobility?
 - What is the average time between scattering events?

$$\sigma = n|e|\mu_e$$

$$\mu_e = \frac{\sigma}{n|e|} = 0.0067 \text{m}^2/(\text{V}\text{-}\text{s})$$

Conduction in Metals: Example

- What is the average time between scattering events?

We know that $F=ma$, where m is the mass and a is the acceleration and an electron are being accelerated by an electric field:

$$\begin{aligned} F &= |e|\mathcal{E} = ma \\ a &= \frac{dv}{dt} = |e|\mathcal{E}/m \\ v &= |e|\mathcal{E}t/m \end{aligned}$$

Define average drift velocity (v_d) with respect to average time (τ) between collisions:

$$v_d = |e|\mathcal{E}\tau/m$$

and the average drift velocity in terms of mobility is:

$$v_d = \mu_e \mathcal{E}$$

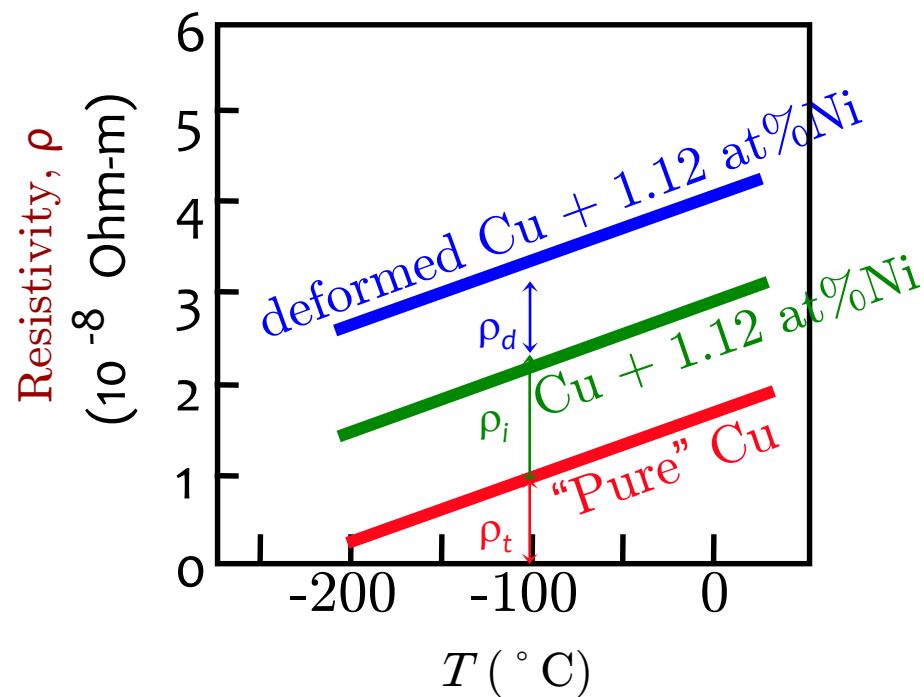
$$\tau = \frac{\mu_e m}{|e|} = \frac{0.0067 \text{ m}^2/(\text{V-s}) \times 9.1 \times 10^{-31} \text{ kg}}{1.6 \times 10^{-19} \text{ C}} = 3.83 \times 10^{-14} \text{ s}$$

Matthiessen's Rule

- Presence of imperfections (anything that flaws lattice) increases resistivity, e.g.,

- Dislocations
- Impurity atoms
- Vacancies

These act to scatter electrons, decreasing conductivity.



Resistivity increases with:

- temperature
- wt% impurity
- %cold working

$$\rho_{\text{total}}$$

$$\begin{aligned} &= \rho_{\text{deformation},d} \\ &+ \rho_{\text{impurity},i} \\ &+ \rho_{\text{thermal},t} \end{aligned}$$

Concept Check

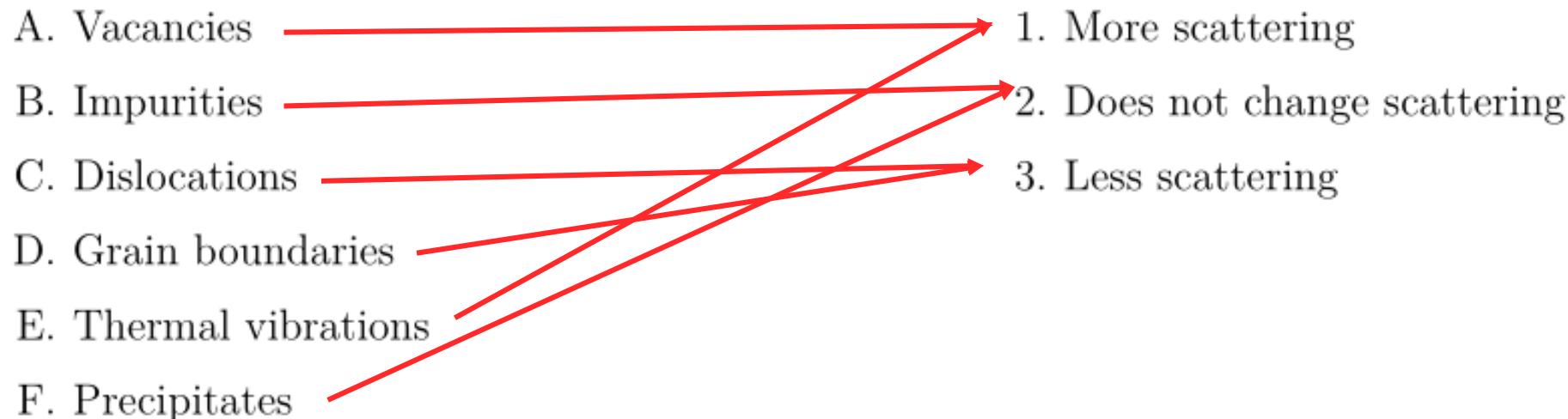
As temperature increases, defect populations will change.

In a metal, how do you expect each of the following defects to impact electron scattering (and therefore conductivity), as temperature increases?

Assume that we are working within a solid solution phase field and that we heat the material above 50% of its melting temperature. We do not go through any phase transformations.

- | | |
|-----------------------|-------------------------------|
| A. Vacancies | 1. More scattering |
| B. Impurities | 2. Does not change scattering |
| C. Dislocations | 3. Less scattering |
| D. Grain boundaries | |
| E. Thermal vibrations | |
| F. Precipitates | |

Concept Check – Solution



- ◊ As temperature increases, the number of vacancies increase according to Arrhenius behavior. This means more defects and more scattering.
- ◊ As temperature rises, impurities will stay the same (assuming we don't go through a phase transition) so scattering from impurities will not change.
- ◊ As temperature rises, dislocation may begin to annihilate (if hot enough). This would lead to less scattering.
- ◊ As temperature rises, grain boundaries may be eliminated through grain growth. This would lead to less scattering.
- ◊ At temperature rises, thermal vibrations would definitely increase, causing more scattering.
- ◊ There are no precipitates to start with (we have a solid solution) and we don't go through a phase transition, so scattering from precipitates (which is already zero...) would not change.

Outline

- **Electrical Conduction**
 - Materials properties of charge transport (conductivity and resistivity) [Video Lecture]
 - Sources of resistivity (Matthiessen's Rule)
- **Electronic Structure**
 - Review electronic states in isolated atoms
 - What happens when we push atoms together?
 - **Electronic band structure** [Video Lecture]
 - Difference between electronic structure of **metals**, **insulators**, and **semiconductors**.

Electron Energy Band Structures [VL]

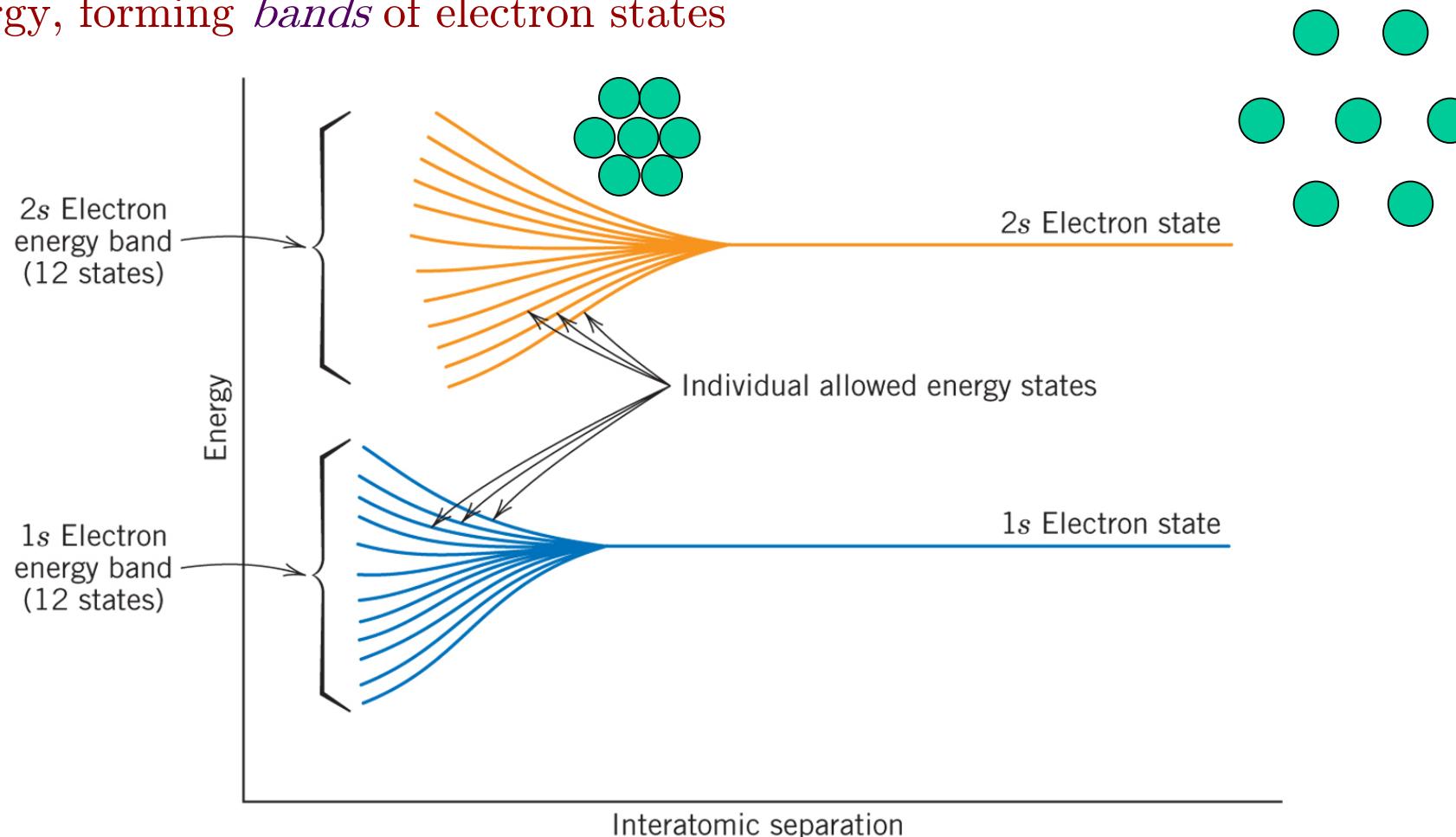
- Electrons' availability to contribute to conduction depends on:
 - The *arrangement of electron states* (quantum states) with respect to **energy**
 - The manner in which the states are occupied by electrons.
- There are shells (integers) and subshells (s, p, d, f with 1, 3, 5, 7 states)
- Electrons only fill the states with the lowest energies with two electrons of opposite spin per state.

Electron Energy Band Structures [VL]

- In a solid, atoms are in close proximity and therefore electrons interact with each other to form chemical bonds
 - Molecular orbital (MO) theory* (chemists) or band theory (physicists)
→ We'll limit our discussion to concepts.
- These theories find a *splitting* of each atomic state into a series of closely spaced electron states
- → Rather than talking about *discrete* states we will talk about bands in solids
- This splitting begins with the outermost shell
 - Valence electrons are those that interact with electrons from other atoms most.
 - Valence electrons are the most loosely bound and are most easily perturbed.

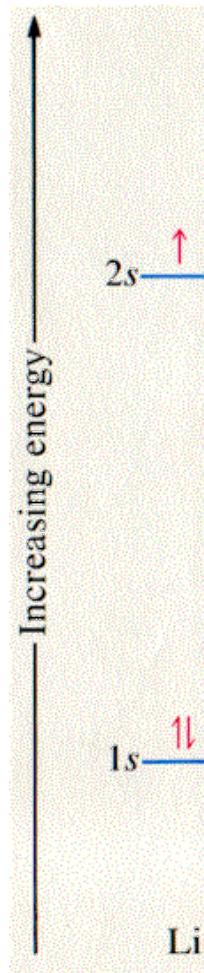
Electron Energy Band Structures [VL]

As atoms interact with their neighbors, isolated states become *waves* of different energy, forming *bands* of electron states



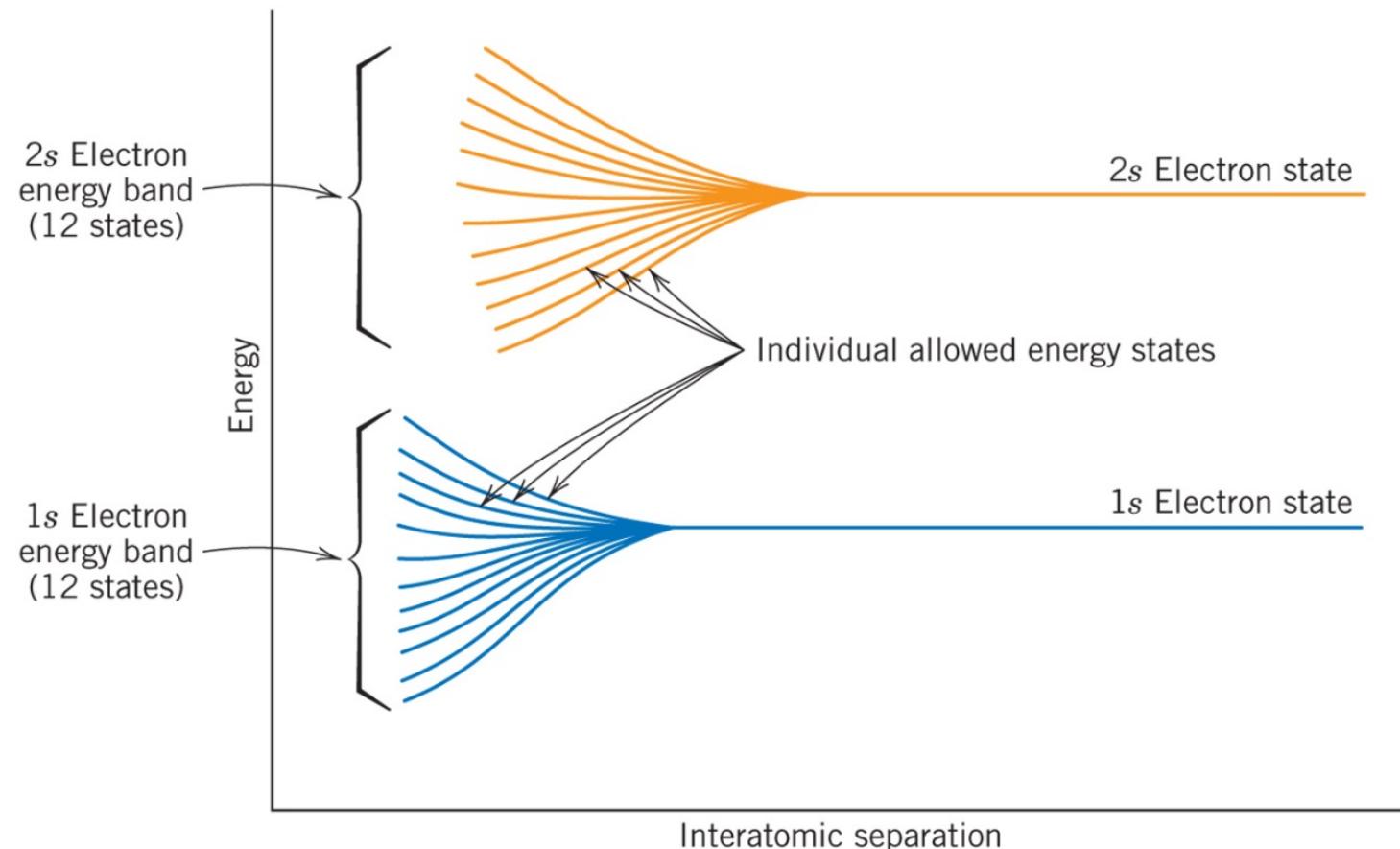
- Each atom contributes 1 state for s , 3 for p , 5 for d ... (m_l)
- For N atoms, a total of Ns states, $3Np$ states, $5Nf$ states.

Electron States in Isolated Atom → Assembly [VL]



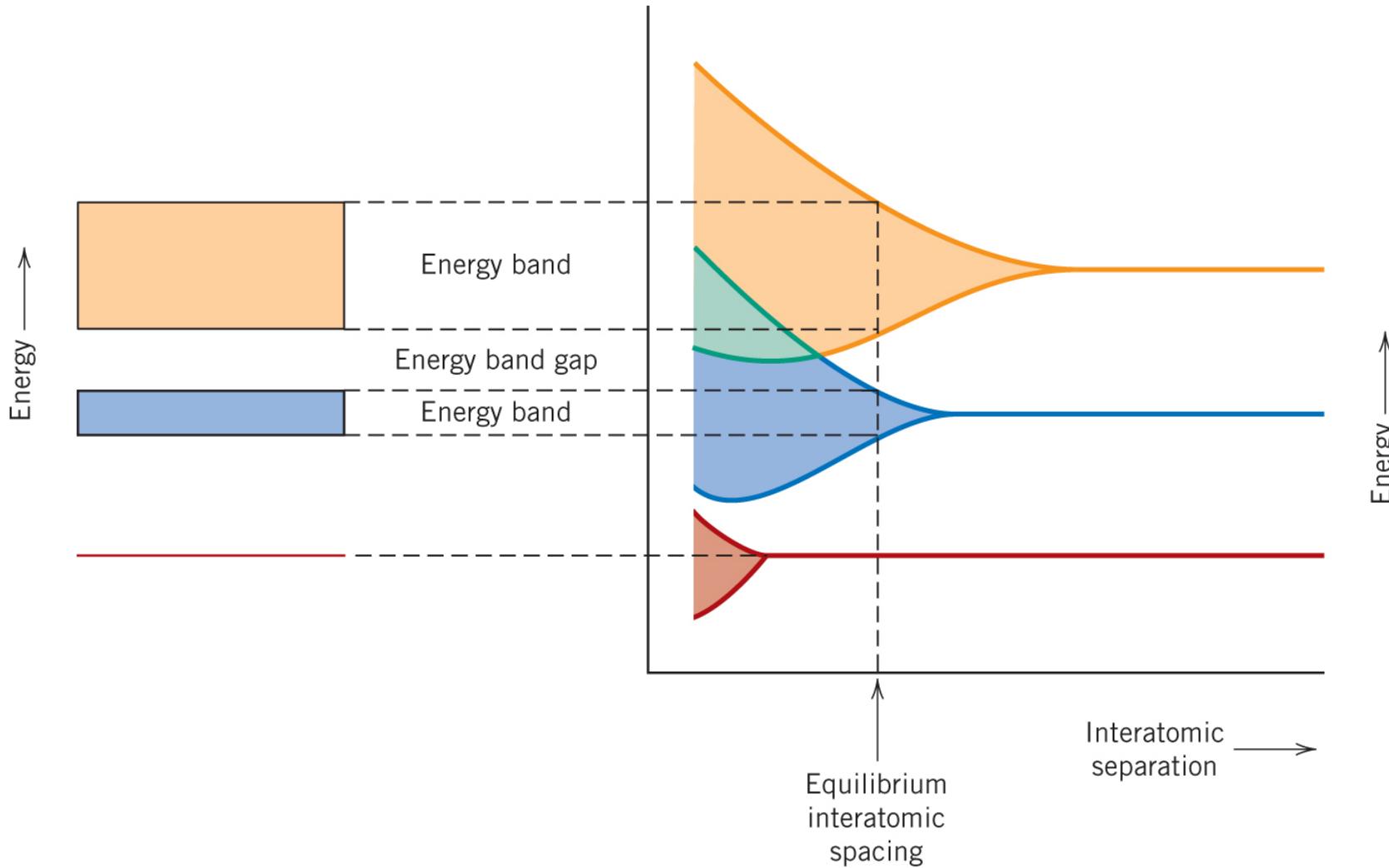
Electron Energy Band Structures [VL]

- The electrical properties of materials are a consequence of the electron band structure
 - In particular it depends on the arrangement of outermost electron bands and if/how electrons occupy those energy states.



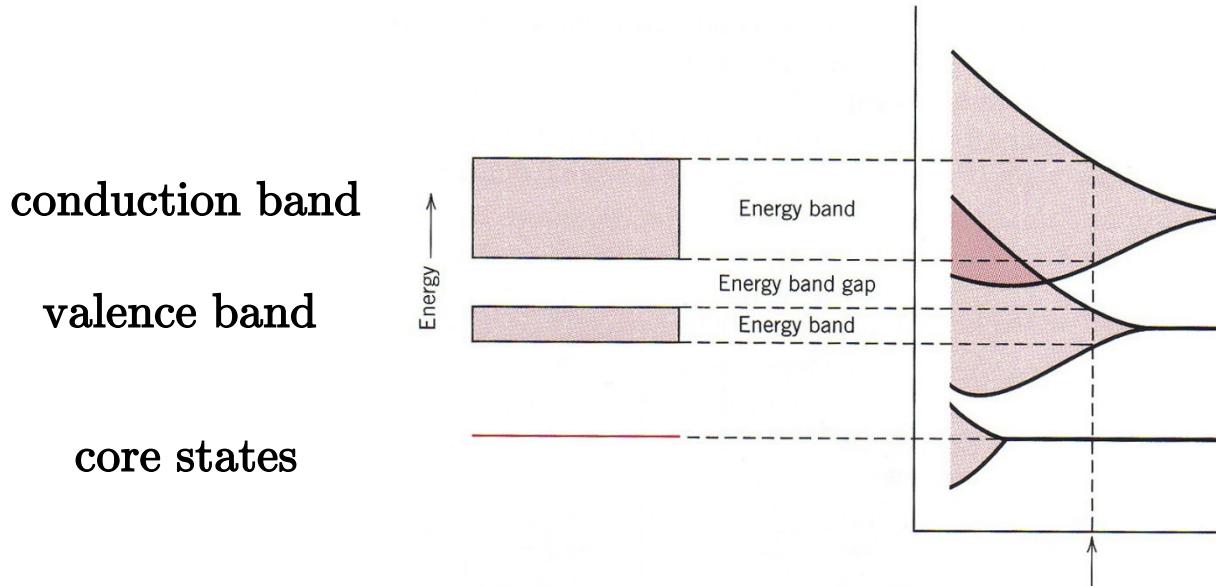
Electron Energy Band Structures [VL]

- As N gets very large individual atomic electron states combine to form continuous electron energy bands



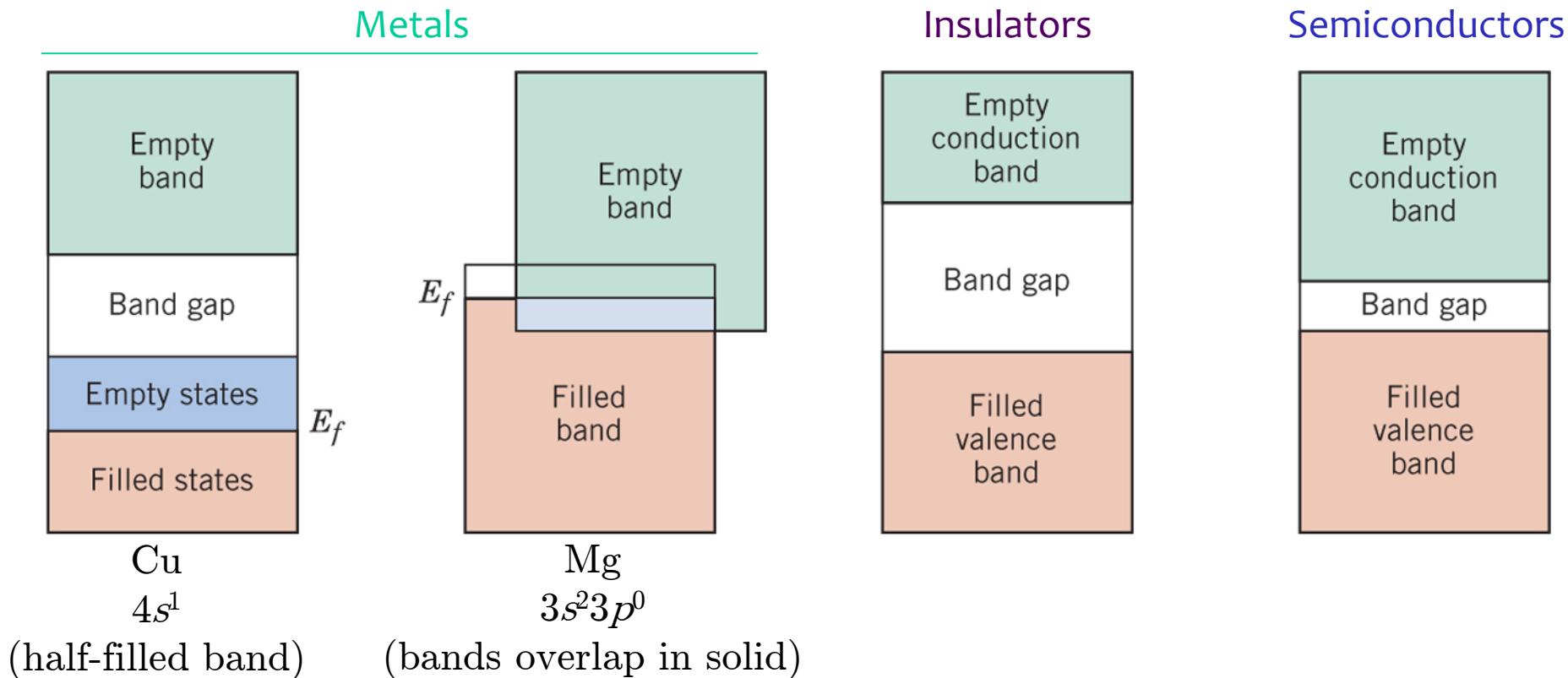
Classification of Energy Bands in a Solid

1. The highest energy band that is *at least partially occupied* is known as the **valence band**
2. All the bands below the valence band are **core bands (states)**. They are fully **occupied bands**, with no net movement of electrons
3. The energy band above the valence band is the **conduction band**
4. The term **band gap** refers to the magnitude of the forbidden energy range between the valence and conduction bands



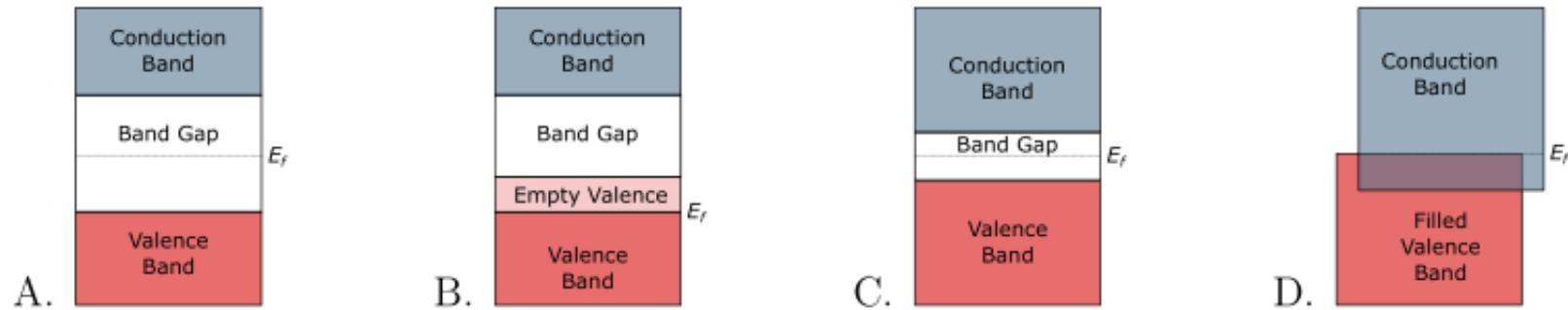
Electron Energy Band Structures [VL]

- Four different types of band structures are possible at 0 K.



Concept Check

1. Mg, Ca, Sr, and Ba are very good conductors of electricity. Which diagram best represents these materials' band structure?



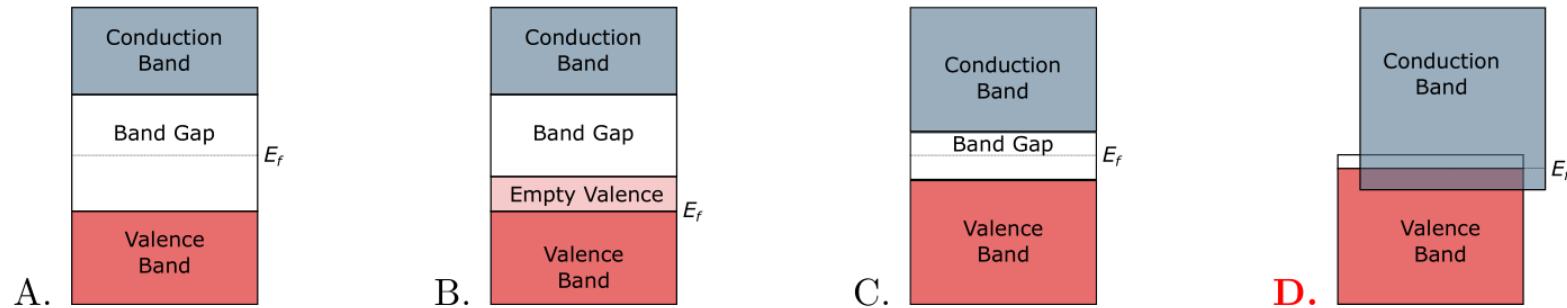
Periodic Table of Elements

A detailed periodic table of elements. The table includes element symbols, atomic numbers, atomic weights, and various properties. It features color-coded groups: Alkali metals (Group 1), Alkaline earth metals (Group 2), Lanthanoids (lanthanides, Group 3), Actinoids (actinides, Group 4), Transition metals (Groups 5-12), Poor metals (Groups 13-15), Other nonmetals (Groups 16-17), Noble gases (Group 18), and a section for Metals (Groups 13-18). The table also includes sections for Solids, Liquids, and Gases. The Fermi level (E_F) is indicated by a blue shaded rectangular box spanning columns 57-71.

Atomic #	Symbol	Name	Atomic Weight
1	H	Hydrogen	1.00794
2	He	Helium	4.002602
3	Li	Lithium	6.941
4	Be	Boron	9.012162
5	B	Carbon	12.0107
6	C	Nitrogen	14.0071
7	N	Oxygen	15.9994
8	O	Fluorine	18.9984032
9	F	Neon	20.1979
10	Ne	Neon	20.1979
11	Na	Sodium	22.98976928
12	Mg	Magnesium	24.305
13	Al	Aluminum	26.981526
14	Si	Silicon	28.03762
15	P	Phosphorus	30.973762
16	S	Sulfur	32.065
17	Cl	Chlorine	35.45
18	Ar	Argon	39.949
19	K	Potassium	39.0983
20	Ca	Calcium	40.078
21	Sc	Scandium	44.95915
22	Ti	Titanium	47.867
23	V	Vanadium	50.9415
24	Cr	Chromium	51.981
25	Mn	Manganese	54.93845
26	Fe	Iron	55.845
27	Co	Cobalt	58.93315
28	Ni	Nickel	58.6934
29	Cu	Copper	63.546
30	Zn	Zinc	65.40
31	Ga	Gallium	69.72
32	Ge	Germanium	72.63
33	As	Antimony	74.9216
34	Se	Selenium	78.961
35	Br	Bromine	79.901
36	Kr	Krypton	83.798
37	Rb	Rubidium	85.4675
38	Sr	Samarium	87.620
39	Y	Yttrium	88.903
40	Zr	Zirconium	91.224
41	Nb	Niobium	91.903
42	Tc	Tantalum	91.707
43	Ru	Ruthenium	91.907
44	Rh	Rhenium	91.707
45	Pd	Palladium	91.707
46	Ag	Silver	96.002
47	Cd	Cadmium	114.41
48	In	Inertium	114.81
49	In	Inertium	114.81
50	Sn	Antimony	118.710
51	Sb	Antimony	121.700
52	Te	Tellurium	127.60
53	I	Iodine	126.9047
54	Xe	Xenon	131.293
55	Cs	Cesium	132.904519
56	Ba	Boron	137.327
57-71			
72	Hf	Hafnium	178.49
73	W	Tungsten	183.54
74	Os	Osmium	187.237
75	Ir	Iridium	192.23
76	Hs	Hassium	204.971
77	Mt	Moscovium	210.934
78	Pt	Platinum	209.505
79	Au	Aurum	209.505
80	Hg	Mercury	209.505
81	Tl	Thallium	204.3633
82	Pb	Lead	208.6054
83	Bi	Bismuth	208.6054
84	Po	Polonium	208.6054
85	At	Astatine	208.6054
86	Rn	Radon	222.0176
87	Fr	Francium	223
88	Ra	Radioustronium	226
89-103			
104	Db	Dubnium	262
105	Sg	Destungium	268
106	Bh	Berkelium	264
107	Hs	Hassium	277
108	Mt	Moscovium	289
109	Mt	Moscovium	277
110	Ds	Darmstadtium	277
111	Rg	Rutherfordium	272
112	Cn	Curium	260
113	Fm	Fermium	254
114	Uup	Ununpentium	255
115	Lv	Ununhexium	252
116	Uus	Ununseptium	253
117	Uuo	Ununoctium	254

Concept Check - Solution

Mg, Ca, Sr, and Ba are very good conductors of electricity. Which diagram best represents these materials' band structure?



Solution:

We can immediately eliminate the fully filled band diagrams with Fermi Levels in the gaps. These are semiconductors (small gap) and insulators (large gaps). The other two are metals. From the periodic table, we know that Mg, Ca, Sr, and Ba have *s* subshells - therefore we must have band overlap to get conduction. This is best represented by the overlapping band diagram.

Periodic Tab

1	2	3	4	5	6	7	8
1 H Hydrogen 1.00794	2 Li Lithium 6.941	3 Na Sodium 22.98976928	4 Mg Magnesium 24.3050	5 Ca Calcium 40.078	6 Sc Scandium 44.955912	7 Ti Titanium 47.867	8 V Vanadium 50.9415
9 K Potassium 39.0985	10 Ca Calcium 40.078	11 Sr Strontium 87.62	12 Y Yttrium 88.9068	13 Zr Zirconium 91.224	14 Nb Niobium 92.90638	15 Mo Molybdenum 95.96	16 Mn Manganese 54.938045
17 Rb Rubidium 85.4676	18 Cs Cesium 132.904519	19 Fr Francium (223)	20 Ba Barium 137.327	21 Hf Hafnium 178.49	22 Ta Tantalum 180.94786	23 W Tungsten 183.84	24 Cr Chromium 51.9861
25 Fe Iron 55.845	26 Ru Ruthenium 101.07	27 Os Osmium 190.23	28 Rh Rhodium 106.207	29 Re Rhenium 186.207	30 Hg Mercury 200.59	31 Pb Lead 207.2	32 Bi Bismuth 210.0
33 Te Tellurium 127.6	34 Po Polonium (209)	35 At Astatine (85)	36 Rb Radium (226)	37 Hg Rutherfordium (261)	38 Db Dubnium (262)	39 Sg Seaborgium (265)	40 Bh Bohrium (254)
41 Tc Technetium (97.9072)	42 Mo Molybdenum (95.96)	43 Ru Technetium (97.9072)	44 Fe Ruthenium (101.07)	45 Os Osmium (190.23)	46 Hg Mercury (200.59)	47 Pb Lead (210.0)	48 Bi Bismuth (207.2)
49 Fr Francium (223)	50 Rb Radium (226)	51 Hg Rutherfordium (261)	52 Db Dubnium (262)	53 Sg Seaborgium (265)	54 Bh Bohrium (254)	55 Hg Bismuth (207.2)	56 Hg Mercury (200.59)
57-71	72-74	75-77	78-80	81-83	84-86	87-89	90-92
89-103	104-106	107-109	110-112	113-115	116-118	119-121	122-124

Conductivity and Band Gap



Summary

- Electrical conductivity and resistivity are:
 - Material parameters
 - Geometry-independent
 - In metals, influenced by defects.
- For metals, mobility is decreased by
 - Increasing temperature
 - Addition of imperfections
 - Plastic deformation
 - Any distortion/deviation from a perfect lattice.
- Band structure
 - As atoms converge, electronic states broaden/split to form bands
 - Simple band structure representations communicate conduction models:
- Conductors, semiconductors, and insulators...
 - Differ in range of conductivity values
 - Differ in availability of electron excitation states

Outcomes

- Classical Electron Conduction
 - Apply classical definitions for electronic properties (e.g., voltage and current (Ohm's Law), current density, etc.).
 - Differentiate between resistivity/conductivity (intrinsic material property) and resistance/conductance (extrinsic materials property). Calculate intrinsic material properties based on measured quantities.
- Electronic Properties and Materials Structure
 - For metals, analyze the effect of various structural features/processing conditions on electronic properties (mobility, drift velocity, scattering frequency, conductivity)
- Band Structure
 - Describe the source of schematic band structure based on interactions between atoms as a function of interatomic separation.
 - Construct a schematic band structure from first principles and distinguish conducting, semiconducting, and insulating band diagrams.