

2.002 MECHANICS & MATERIALS II

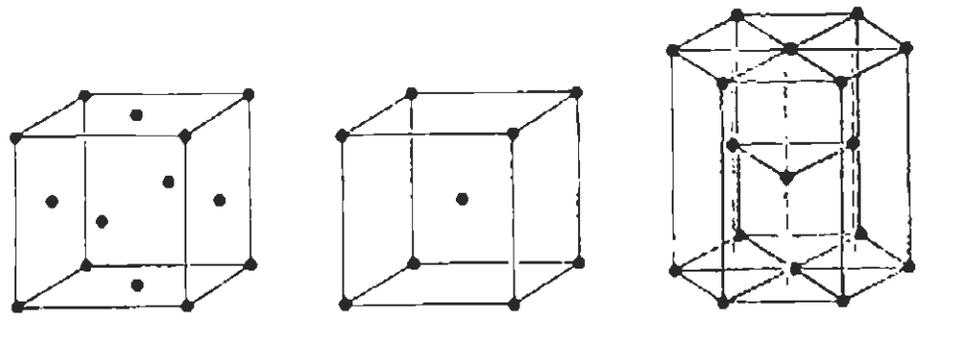
**PHYSICAL BASIS OF PLASTICITY OF
CRYSTALS AND POLYCRYSTALS**

© L. Anand

PHYSICAL BASIS OF PLASTICITY IN METALS AND CERAMICS

- Metals and ceramics in their usual form are **polycrystalline aggregates**. They are composed of a large number of **grains** separated by **grain boundaries**. The interiors of the grains each have a structure which is essentially that of a **single crystal**.

- The most common crystal structures in metals are
 1. Face-centered cubic, FCC; e.g. Al, Cu, Ni, Ag, γ -Fe
 2. Body-centered cubic, BCC; e.g. Nb, Mo, Cr, α -Fe
 3. Hexagonal closed-packed, HCP; e.g. Ti, Mg, Zn, Cd



- In a single crystal plastic deformation occurs by slip on preferred **slip planes**, $\{\mathbf{n}^{(\alpha)}, \alpha = 1, \dots\}$, in preferred **slip directions**, $\{\mathbf{m}^{(\alpha)}, \alpha = 1, \dots\}$.
- The slip planes are most often the planes with the highest density of atoms, and the slip directions in the slip planes are the directions in which the atoms are most closely packed.
- A slip plane and a slip direction is said to form a **slip system**, $\{(\mathbf{m}^{(\alpha)}, \mathbf{n}^{(\alpha)}), \alpha = 1, \dots\}$.

INDICES OF LATTICE PLANES

A plane in a rectangular (x, y, z) -cartesian coordinate system satisfies the equation

$$\frac{x}{a} + \frac{y}{b} + \frac{z}{c} = 1,$$

where (a, b, c) are the **intercepts** of the plane on the x , y , and z -axes respectively.

The **Miller Indices** (hkl) of a plane are the **reciprocals of the intercepts reduced to the smallest integers**:

$$h = \frac{1}{a}, \quad k = \frac{1}{b}, \quad l = \frac{1}{c}.$$

The reciprocals are used simply to avoid infinities when planes are parallel to axes.

INDICES OF LATTICE DIRECTIONS

The **indices of a direction** are simply the vector components of the direction resolved along each of the coordinate axes and reduced to the smallest integers.

Note that for the directions we do not use reciprocals because infinities do not crop up here.

- **Resolved shear stress** on a slip system $(\mathbf{m}^{(\alpha)}, \mathbf{n}^{(\alpha)})$:

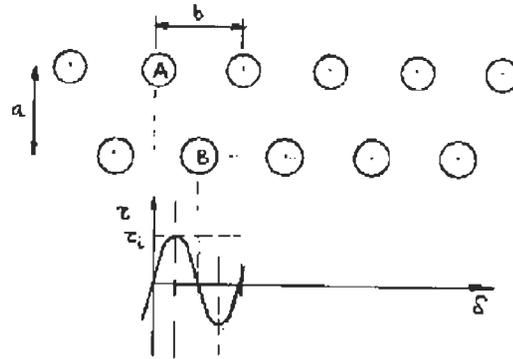
$$\tau^{(\alpha)} \equiv \mathbf{m}^{(\alpha)} \cdot \boldsymbol{\sigma} \mathbf{n}^{(\alpha)}.$$

- **Schmid's Law:**

Slip in a single crystal is initiated when the resolved shear stress on some slip system, $\tau^{(\alpha)}$, reaches a critical value, $\tau_c^{(\alpha)}$, called the **critical resolved shear strength** for the α th slip system:

$$|\tau^{(\alpha)}| \leq \tau_c^{(\alpha)}$$

- **Ideal Shear Strength:**



$$\tau = \tau_i \sin \left(2\pi \frac{\delta}{b} \right), \quad \tau = \tau_i \left(2\pi \frac{\delta}{b} \right), \quad \frac{\delta}{b} \ll 1$$

$$\tau = G\gamma = G \frac{\delta}{a} \approx G \frac{\delta}{b}, \quad \text{since } b \approx a$$

$\tau_i \approx \frac{G}{2\pi}$	Ideal Shear Strength
---------------------------------	-----------------------------

- The ideal shear strength, τ_i , **is much greater** than the measured critical resolved shear strengths, τ_c , of high purity well-annealed single crystals.

Material	G, GPa,	τ_i , MPa	τ_c , MPa	τ_c/τ_i
Aluminum	27	4,297	1	2×10^{-4}
Iron	82	13,051	40	3×10^{-3}
Diamond	505	121,000	25,000	0.21

- Real crystals have line defects called **dislocations**, which move easily.
- When the dislocations move, the crystal deforms plastically.
- It is the presence of dislocations that cause a crystal to plastically deform at a stress level $\tau_c \ll \tau_i$.
- Dislocations are the **carriers of plastic deformation**, much as electrons are carriers of charge.
- This was suggested independently by Taylor, Orowan, and Polanyi in 1934.

Motion of an Edge Dislocation Produces Plastic Strain

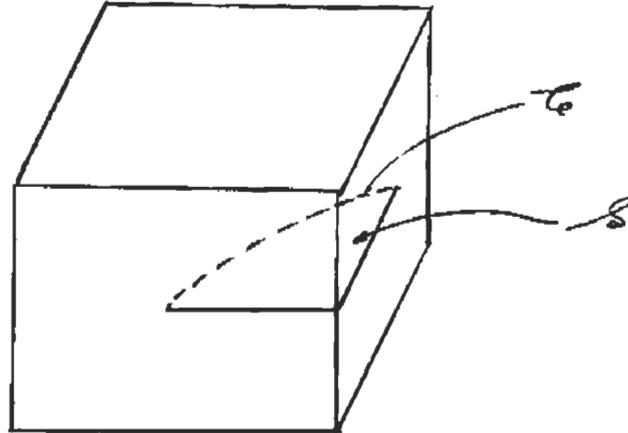
Image removed due to copyright considerations. See Figure 9.4, 9.6, and 9.7 in [Ashby].

Motion of a Screw Dislocation Also Produces Plastic Strain

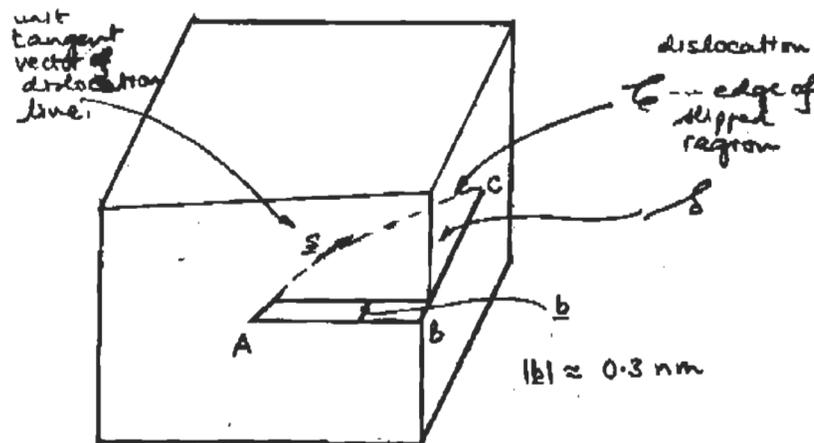
Image removed due to copyright considerations. See Figure 9.8, 9.9, and 9.10 in [Ashby].

- A circuit around a dislocation line with a right-handed screw sense in the direction of the unit tangent vector s of the dislocation line is known as the **Burgers circuit**. The closure failure of such a circuit is called the **Burgers vector**, and denoted by b .

Fig. 1 Schematic of a continuum model of a dislocation.



(a) Cut over a planar surface S .
 C_0 denotes the bounding curve of the cut.



(b) The two faces of the cut are given a small constant relative displacement $\frac{1}{2}$ equal to a lattice vector and the faces of the cut are welded together.

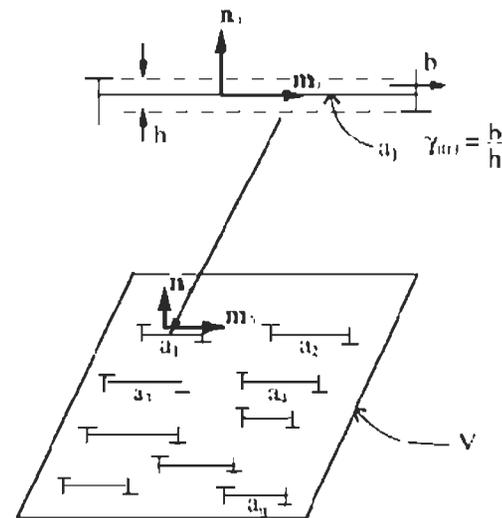
Plastic Shear Strain Increment

$$\Delta\gamma^p = \tan \theta = \frac{Nb}{\delta x} = \frac{Nb\Delta x}{(\delta x)^2} = \rho_d b \Delta x, \quad \rho_d \equiv \frac{N}{(\Delta x)^2} \text{ disl. density}$$

N number of dislocations, b magnitude of burgers vector,
 Δx incremental distance travelled by each dislocation.

$$\boxed{\Delta\gamma^p = \rho_d b \Delta x \quad \text{Orowan Relation}}$$

More Generally:



$$v_{\text{slip}} = h \times \sum_{k=1}^n a_k, \quad \gamma_{\text{tr}} = \frac{b}{h}$$

$$\Delta v_{\text{slip}} = h \times \sum_{k=1}^n \Delta a_k = h \times \Delta A$$

$$\Delta \gamma^p = \frac{\Delta v_{\text{slip}}}{V} \gamma_{\text{tr}} = \frac{b \Delta A}{V}$$

- The average **plastic strain increment**, $\Delta\gamma$, in a representative volume V , due to dislocations with Burgers vector of magnitude b , sweeping out an incremental area ΔA on the slip planes corresponding to a given slip system, is given by

$$\Delta\gamma^p = \frac{b\Delta A}{V}$$

- Let

$$\Delta A = l_m \Delta\bar{x},$$

where l_m is the length of “mobile dislocations” per unit volume, and $\Delta\bar{x}$ is the average distance moved by the dislocations.

- Let

$$\rho_m \equiv \frac{l_m}{V}, \quad \text{mobile dislocation density.}$$

Dislocation density is measured in line-length per unit volume, or number per unit area.

- Then

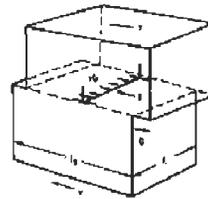
$$\Delta \gamma^p = \frac{b \Delta A}{V} = \rho_m b \Delta \bar{x}$$

or

$$\dot{\gamma}^p = \rho_m b \bar{v} \quad \text{Orowan relation,}$$

where \bar{v} is the average velocity of the mobile dislocation segments.

Force on a Dislocation



External work = $(\tau l_1 l_2) \times b$, Internal dissipation = $f \times l_1 \times l_2$

f – resistive force per unit length offered by material to dislocation motion. The resistance is due to intrinsic friction opposing dislocation motion, plus contributions from alloying and work-hardening.

External work = Internal dissipation $\Rightarrow \tau b = f$

$$\tau \leq \tau_c, \quad \tau_c = \frac{f}{b}$$

Line Tension of a Dislocation

- The atoms near the core of a dislocation are displaced from their proper positions, and thus have a higher energy.
- In order to keep the total energy as low as possible, the dislocation tries to be as short as possible, it behaves as if it had a line tension T .



A diagram showing a horizontal line representing a dislocation. At each end of the line, there is a double-headed arrow pointing outwards, labeled with the letter 'T', representing tension forces. In the center of the line, there is a label $T = \frac{Gb^2}{2}$.

- Roughly:

$$\text{Strains at the core of a dislocation} \approx \frac{1}{2}$$

$$\text{Stresses at the core of a dislocation} \approx \frac{G}{2}$$

$$\text{Strain energy per unit volume of core} \approx \frac{G}{8}$$

$$\text{Core radius} \approx b$$

$$\text{Volume of dislocation core per unit length} \approx \pi b^2$$

$$\text{Strain energy per unit length of core} \approx \frac{\pi}{8} G b^2 \approx \frac{G b^2}{2}$$

$T \approx \frac{G b^2}{2} \quad \text{line tension}$

Yield strength of a crystal

$$\tau \leq \tau_c, \quad \tau_c \equiv \frac{f}{b}$$

The major contributions to the resistance to plastic flow, τ_c , or the resistive force per unit length for dislocation motion, f , of a single crystal are

$$\tau_c \equiv \frac{f}{b} = \frac{f_l}{b} + \frac{f_{ss}}{b} + \frac{f_o}{b} + \frac{f_{sh}}{b}$$

or

$$\tau_c = \tau_l + \tau_{ss} + \tau_o + \tau_{sh}$$

- τ_l – **intrinsic lattice resistance**
- τ_{ss} – **solid solution hardening**
- τ_o – **obstacle (precipitate and dispersion) hardening**
- τ_{sh} – **strain hardening**

- $\tau_l = \frac{f_l}{b}$ is the contribution due to **intrinsic lattice resistance** to dislocation motion. It is also called the **Peierls stress**.

It depends on the nature of the interatomic bonds, and the crystal structure.

Covalent bonding gives a high value of τ_l . It is this that causes the high strength and hardness of diamond, carbides, oxides, and intermetallic compounds.

Pure metals are soft because the non-localized metallic bond does little to prevent dislocation motion, and thus they have a low lattice resistance.

The resistance to plastic flow of a crystal, τ_c , of a material with low intrinsic lattice resistance, τ_l , may be increased by

- Solid solution hardening.
- Dispersion hardening.
- Strain-hardening.

- τ_{SS} is the contribution due to **solid solution strengthening** of the lattice. It is found that

$$\tau_{SS} \approx \epsilon_s^{3/2} c^{1/2},$$

where ϵ_s is the mismatch dilational strain between the solute atoms and the matrix, and c is the concentration of the solute.

Image removed due to copyright considerations. See [Ashby] Fig. 10.1.

- τ_o is the contribution due to **obstacle or precipitate/particle strengthening**.

It is found that for non-shearable particles

$$\tau_o \approx \frac{2T}{bL} = \frac{Gb}{L},$$

where L is the mean interparticle spacing on the slip planes.

Image removed due to copyright considerations. See [Ashby] Fig. 10.2.

$$\text{Critical config.: } \tau b L = 2T \Rightarrow \tau = \frac{2T}{bL} = \frac{2 \times (Gb^2)/2}{bL} = \frac{Gb}{L}$$

$$\tau_o = \frac{Gb}{L}$$

The greatest hardening is produced by strong, closely spaced particles.

- As plastic deformation occurs, dislocations multiply, the dislocation density increases, and the resistance to further plastic flow increases. This phenomenon is known as **strain hardening**, and the contribution due to the resistance to dislocation motion offered by this increased dislocation density which hinders dislocation motion is denoted by τ_{sh} .

Image removed due to copyright considerations. See [Ashby] Fig. 10.3.

Yield in Polycrystals

- An “isotropic” polycrystalline material element is usually considered to be composed of a collection of a few hundred single crystals or grains, in which the lattices are randomly oriented.

Image removed due to copyright considerations. See [Ashby] Fig. 10.5.

Shear yield strength of polycrystal:

$$\tau_{y,\text{polycrystal}} \approx 1.5 \times \tau_{c,\text{single crystal}}$$

Tensile yield strength of polycrystal:

$$\sigma_{y,\text{polycrystal}} \approx 2 \times \tau_{y,\text{polycrystal}} \approx 3 \times \tau_{c,\text{single crystal}}$$

$$\boxed{\sigma_y \approx 3 \times \tau_c}$$

All the statements we have made about increasing τ_c also apply to increasing σ_y .

- This relation does not take the size of grains into account. It is found experimentally that σ_y increases as the grain size d of the polycrystal decreases:

$$\sigma_y \approx \sigma_o + k d^{-1/2} \quad \text{Hall-Petch Relation}$$

where σ_o is approximately the yield strength of a large grained polycrystal.

SUMMARY

- Elastic strain in a single crystal is the strain related to the stretching of the crystal lattice under the action of applied stress.

Elastic strain is recoverable . It disappears on removal of applied stress; it is non-dissipative .

- Since the production of plastic strain requires the breakage of interatomic bonds, plastic deformation is dissipative .

- Crystals contain dislocations.
- When dislocations move, the crystal deforms plastically.
- Plastic strain is incompressible because dislocation motion produces a shearing type of deformation.
- Upon application of a sufficiently large resolved shear stress, dislocations will move, but upon removal of the applied stress they remain at the positions to which they have moved to.

Plastic strain remains upon removal of applied stress. that is, plastic strain produces a permanent set.

- Elastic and plastic strains are additive:

$$\gamma = \gamma^e + \gamma^p \quad \Rightarrow \quad \epsilon = \epsilon^e + \epsilon^p$$

Metallic materials can undergo deformations in which the magnitude of the plastic strains far exceeds those of the elastic strains.

- The current resolved shear stress determines which dislocations will move to produce a plastic strain increment. The current stress does not determine which dislocations have moved in the past to produce prior plastic strain.

The current resolved shear stress governs the plastic strain increment, and not the total strain as in elasticity.

- Hydrostatic pressure has a negligibly small effect on the plastic flow of metals.
- The yield strength of crystals, τ_c , depends very strongly on the intrinsic lattice resistance. For materials with low intrinsic lattice resistance, the yield strength may be increased by solid solution hardening, obstacle (precipitate and dispersion) hardening, and strain hardening:

$$\tau_c = \tau_l + \tau_{ss} + \tau_o + \tau_{sh}$$

- The yield strength of polycrystals in tension is approximately three times the yield strength of a single crystal in shear:

$$\sigma_y \approx 3 \times \tau_c$$

- The yield strength σ_y increases as the grain size d decreases:

$$\sigma_y \approx \sigma_o + k d^{-1/2} \quad \text{Hall-Petch Relation}$$

where σ_o is approximately the yield strength of a large grained polycrystal.