Chapter 6. Morphological Basis for Mechanical Response.

Metals:
In metals and crystalline ceramics mechanical response is intimately tied to crystalline defects and to crystalline grain structure. Grain structure can be considered in the context of a composite structure or as a locus for crystalline defects and this will be discussed later. The formation and propagation of crystalline defects serve as a mechanism to absorb energy in plastic deformation of a crystalline material. Defects in crystals can be categorized as point defects, such as a misplaced atom or void, line defects, such as a dislocation, and surface defects, such as a twin plane, or a collection of line defects at a grain boundary. The most important of defect structures for mechanical properties are line defects and the most important of line defects is the dislocation that is related to slip planes in metals. Slip planes are the mechanism by which metals plastically deform. *Slip dislocations* can be *edge or screw dislocations*. The *edge dislocation* is called a *Taylor-Orowan dislocation*. In the figure below a plane of atoms has slipped in the direction of the slip vector resulting in a perfect crystallographic alignment of the atoms except along a line, line AD, which is the edge dislocation. Specific planes in a crystal are subject to this type of slip. The crystallographic planes across the slip plane have been displaced by the Burgess vector, **b**, and for edge dislocations the Burgess vector is always normal to the edge dislocation, AD.

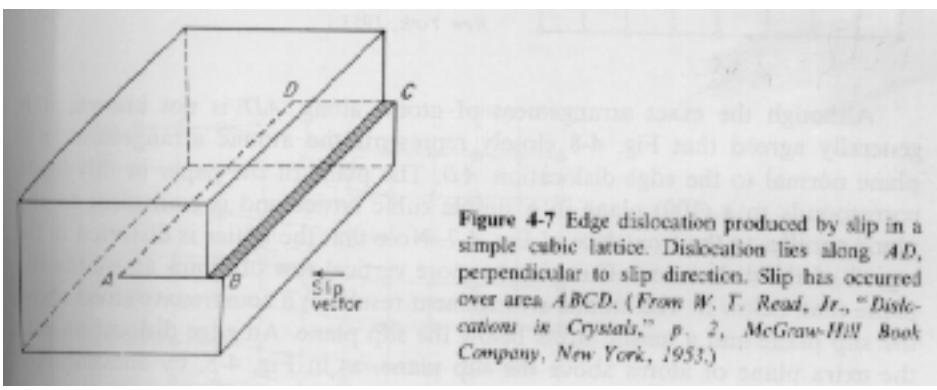

Figure 4-7 Edge dislocation produced by slip in a simple cubic lattice. Dislocation lies along *AD*, perpendicular to slip direction. Slip has occurred over area *ABCD*. (*From W. T. Read, Jr., "Dislocations in Crystals," p. 2, McGraw-Hill Book Company, New York, 1953.*)

The figure below shows how the edge dislocation might appear on an atomic scale normal to the dislocation line, AD above. The region immediately near the dislocation is disordered. The edge dislocation shown is called positive and is represented by an inverted T since the extra plane of atoms is above the dislocation. A negative dislocation would be represented by T and would have the extra plane of atoms below the dislocation.

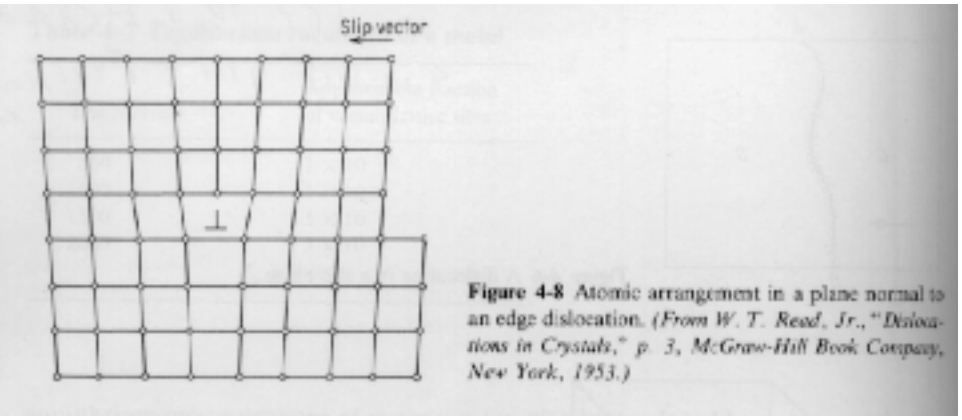

Figure 4-8 Atomic arrangement in a plane normal to an edge dislocation. *(From W. T. Read, Jr., "Dislocations in Crystals," p. 3, McGraw-Hill Book Company, New York, 1953.)*

The edge dislocation can slip in the direction of the slip vector in the first figure. I can also glide in a direction normal to the slip direction and normal to the axis of the edge dislocation.

Motion and formation of edge dislocations are the primary mechanism of plastic deformation in metals and many other crystalline materials.

Screw dislocations, or Burgess dislocations, result from displacement of two planes of atoms as shown in the figure below with the Burgess vector parallel to the dislocation line.

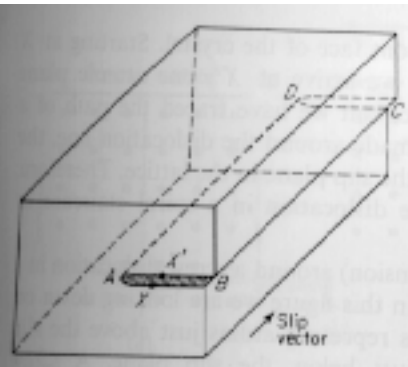

Figure 4-9 Slip that produces a screw dislocation in a simple cubic lattice. Dislocation lies along *AD*, parallel to slip direction. Slip has occurred over the area *ABCD*. *(From W. T. Read, Jr., "Dislocations in Crystals," p. 15, McGraw-Hill Book Company, New York, 1953.)*

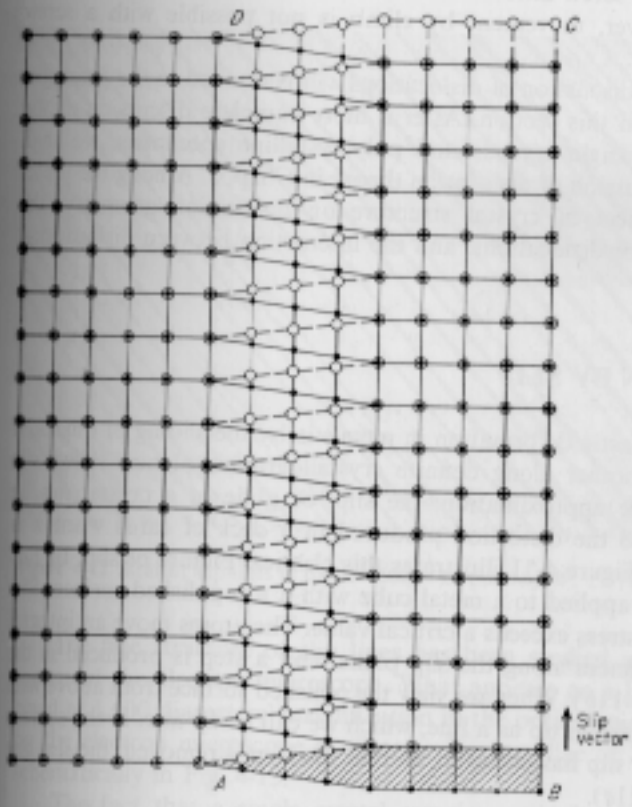

Figure 4-10 Atomic arrangement around the screw dislocation shown in Fig. 4-9. The plane of the figure is parallel to the slip plane. *ABCD* is the slipped area, and *AD* is the screw dislocation. Open circles represent atoms in the atomic plane just above the slip plane, and the solid circles are atoms in the plane just below the slip plane. *(From W. T. Read, Jr., "Dislocations in Crystals," p. 17, McGraw-Hill Book Company, New York, 1953.)*

In metals plastic deformation occurs for the most part through the formation of slip planes that occur on the most densely packed planes ({111} for FCC) since these planes have the largest spacing. Slip occurs in the <110> direction of which there are 12. The slip plane and the slip direction is called the *slip-system*. BCC crystals can slip along {110}, {112} and {123} planes, which are equally close packed, but always in the <111> direction giving 48 possible slip systems. HCP crystals slip along the {0001} plane and in the <1120> directions of which there are 3.

Slip of an atomic plane can be visualized as a deck of cards, which is the same analogy used in simple shear flow. It is shear stress that causes plastic deformation in metals. Then simple models based on the energy required to shear planes of atoms can be formulated to model plastic deformation in metals. As before, we can consider the energy associated with an atom displaced from its equilibrium position in a crystal as a sine wave, yielding the shear stress for slip of an atomic plane,

$$\tau = \tau_m \sin\frac{2\pi x}{b} \approx \tau_m \frac{2\pi x}{b}$$

where the latter equality is for small displacements.

We can also write Hooke's law for small displacements in terms of the shear modulus,

$$\tau = G\gamma = G\frac{x}{a} = \tau_m \frac{2\pi x}{b}$$

Which yields,

$$\tau_m \approx \frac{G}{2\pi} \approx \text{ 3 to 30 GPa for metals}$$

This is 100 to 1000 times the observed yield stress for metals.

Dislocations can explain this discrepancy since it takes much less energy to move a dislocation through a crystal than to move an entire crystallographic plane since a dislocation is a localized defect. The figure below shows such a motion of an edge dislocation by slip. To consider the motion of such a dislocation we consider that the presence of a dislocation introduces an elastic strain energy to the crystal. The dislocation has physical dimensions and since it is a disordered region it introduces an interfacial energy associated with its length and width. The width also controls the extent of elastic deformation of the neighboring crystal planes. The narrower the dislocation the larger is the elastic strain energy but the smaller the surface energy associated with the "interface". Then the energy of a dislocation could be minimized through a balance of surface and bulk strain energies both of which have a functional dependence on the width of the dislocation, w. The width of a dislocation determines the "*Peierls-Nabarro force*" or the force required to move the dislocation through the crystal.

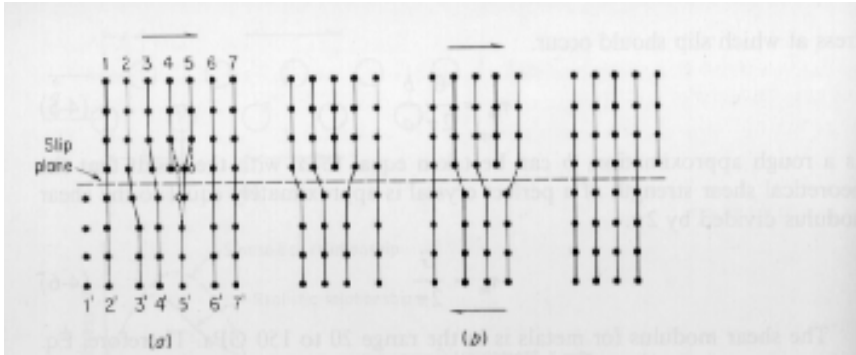

Figure 4-15 (*a*) Atom movements near dislocation in slip; (*b*) movement of an edge dislocation.

The Peierls stress is given by,

$$\tau_p \approx \frac{2G}{1-\nu} e^{-2\pi w/b} = \frac{2G}{1-\nu} e^{-2\pi a/((1-\nu)b)}$$

where a is the distance between slip planes and b is the distance between atoms in the slip direction. The Peierls equation is based on a sinusoidal elastic strain force and other approximations so is not of great use in predicting the yield stress for metals but the general functionality on the width of dislocations and atomic spacing explains why ceramics, with narrow dislocations due to ionic bonding and high surface energy have a higher energy to yield than metals where w is approximately 10 atomic spacings.

In a real metal or ceramic many dislocations are present to account for plastic deformation. These dislocations are randomly placed (with excluded volume) in the crystal. The macroscopic strain is expressed in terms of average features of the many dislocations,

$$\gamma = b\rho_d \bar{x}$$

where b is the slip distance associated with one dislocation, i.e. one atomic spacing, ρ_b is the density of dislocations, number times length per volume or number per area normal to the dislocations. x bar is the average distance a dislocation has moved. This approach assumes all dislocations are parallel to each other. It is much easier to measure the speed of motion of an average dislocation, v bar, rather than the average distance a dislocation has moved. Using this average velocity the bulk shear strain rate is calculated,

$$\dot{\gamma} = b\rho_d \bar{v}$$

<v> and ρ_b depend on the applied shear stress, the rate of deformation, temperature and sample history. For example,

$$v = A\tau^m \quad \text{m varies from 1.5 to 40}$$

Additionally, dislocation motion requires a critical stress below which there is no motion and plateaus at an upper limiting velocity. This critical stress is called the *critical resolved shear stress for slip*, this is like a yield stress except that it is defined for a single crystal.

Twinning:
In addition to dislocations and line defects crystals can deform through the formation of a twin plane. Twinning may involved a coordinated deformation of a large number of atoms and can lead to serrations in mechanical deformation curves and "tin cry" or loud clicks on formation of twins. (Creaking of metal prior to failure). A twin is a mirror plane in a crystal along a low index plane. Shear stress along the twin plane causes atoms to move a distance that is proportional to the distance from the twin plane. Atom motion in twinning is less than an atomic spacing. Twinning can occur due to shear stress or during annealing after mechanical deformation. Mechanical twins occur usually in HCP or BCC crystals but may occur in some FCC crystals. Twins usually occur in response to rapid loading. Martensitic transformations, change in crystal structure due to stress, parallel the mechanical behavior or twinning.

Strain Hardening:
The shear stress required to initiate slip, *critical resolved shear stress*, is a function of the thermomechanical history, as noted above. This shear stress increases with cumulative strain. This behavior is known as *strain hardening* or *work hardening*. The mechanism for strain hardening is interaction between dislocations and between dislocations and impurities or defects in the crystal. The dislocation density, ρ_r, increases with cumulative strain by a variety of mechanisms. Since dislocations can move only in specific crystallographic directions and with specific applied shear stresses, the combination of dislocations can lead to unfavorable dislocation orientations that can not move. This is termed a *sessile dislocation*. Strain hardening is a rich area of research in metals and the interested student is referred to Dieter and books on physical metallurgy.

Grains:
Most metals and ceramics used in engineering applications are composed of many small (10-1000 μm) crystallites called grains. These grains are connected by a grain boundary which is a few atomic-spacings in thickness. The grain boundary can vary from complete mis-match of crystallographic orientation, high-angle grain boundary, to a grain boundary composed of a regular array of dislocations, low-angle grain boundary. High-angle grain boundaries are disordered, amorphous, and are the normal condition. High-angle grain boundaries display high surface energy. Impurities tend to segregate at grain boundaries due to this high surface energy.

For a polycrystalline material the crystallographic orientation of grains have limited relationship with each other. Then all possible orientations of crystals exist. A given deformation such as tensile strain will result in all possible crystallographic orientations of strain, however there are only 6 independent components of strain as shown previously. For a material that is incompressible the sum of the dilatometric components is 0 resulting in five independent strain components. If the crystal has five or more independent slip systems the polycrystalline material will be ductile. This is true for cubic metals. If the crystal has less than five slip systems (plane and direction), such as for HCP and low symmetry crystals, the polycrystalline material will have low ductility, especially at low temperatures.

Hall-Petch Relationship:
The Hall-Petch relationship associates grain size and yield stress for a polycrystalline material, derived in the early 1950's. It has recently been used as the argument for research into nano-scale grains in polycrystalline materials.

$$\sigma_{yield} = \sigma_i + \frac{k}{D^{1/2}}$$

where σ_i is the friction stress that reflects resistance to dislocation movement in the crystal, k is the locking parameter reflecting how grains contribute to strain hardening and D is the diameter of an average grain.

Yield-Point Elongation/Lueders bands:
Materials that display localized yielding sometimes display a peak in the stress strain curve followed by a plateau where elongation occurs at constant stress and finally a terminal plastic or elastic elongation. In metals this behavior occurs in conjunction with the presence of Lueders bands which appear as 45° lines across the sample in a localized region. The formation of the initial Lueders bands corresponds with the peak in the stress-strain curve and the plateau corresponds with expansion of the banded region until all of the sample is contains these bands and the terminal region is seen in the stress-strain curve. The peak of the stress-strain curve is sometimes called an upper yield point, while the plateau stress is sometimes called the lower yield point. The plateau region in metals is sometimes choppy due to the formation of multiple Lueders bands.

This type of stress strain behavior is very common in semi-crystalline polymers as will be discussed below.

Alloy Composite Systems:
Precipitation of a second phase in a metal or ceramic can lead to reinforcement. For example, aging of an Al-Cu alloy can lead to composition fluctuations called Guinier-Preston zones. Locally these crystalline zones have a higher strain, associated with composition fluctuations. If the metal is aged platelet precipitates of $CuAl_2$ appear. The hardness of the alloy reaches a peak just before the formation of discrete precipitates. The discrete precipitates act as stress concentration regions, as if small holes were made in the alloy. Dislocations can pass directly through GP zones, while discrete precipitates can act as traps for dislocations, concentrating stress locally and eventually, leading to failure of the precipitate particle.

Fiber Composite Moduli and Strength:
High strength fibers, such as boron, graphite or alumina, are sometimes added to low strength metals such as aluminum to reinforce the low weight metal for applications such as aircraft manufacture. This uniaxial reinforcement is directly linked to the fiber-matrix interfacial interaction. The stress distribution in a fiber is complex and dominated by interfacial shear stress at the fiber tips and tensile stress in the fiber center if good bonding between the matrix and fiber is achieved. Under the assumption of equal strain for the matrix and fiber, the composite modulus is given by a rule of mixtures,

$$E_c = fE_f + (1-f)E_m$$

where E_c is the composite modulus, E_f is the fiber modulus and E_m is the matrix modulus. f is the volume fraction fibers. If plastic deformation occurs in the matrix, then E_m is replaced by the tangent to the stress strain curve at a given extent of strain, the apparent modulus of the composite. Generally, the apparent modulus is much smaller than the first term so the composite modulus, under plastic deformation of the matrix is given by just the fiber term.

The ultimate strength of the matrix is give by,

$$\sigma_{composite,u} = \sigma_{f,u} f + \sigma_{m,uf}(1-f)$$

where $\sigma_{m,uf}$ is the matrix stress at the fibers ultimate strain. For fiber reinforcement this ultimate stress must be greater than the strain-hardened matrix stress, $\sigma_{matrix,u}$, yielding a critical volume fraction of fibers, f*,

$$f^* = \frac{\sigma_{matrix,u} - \sigma_{m,uf}}{\sigma_{f,u} + \sigma_{matrix,u} - \sigma_{m,uf}}$$

Since the ends of fibers are subject to shear, while the center of the fiber is subject to tension, a minimum fiber length for reinforcement can be determined,

$$L_{\min} = \frac{\sigma_{fiber} d}{2\tau_0}$$

where τ_0 is the yield stress of the matrix, σ_f is the axial stress in the fiber and d is the fiber diameter. This describes a critical aspect ratio for the fiber, L/d.