

Material Science

Prof. Satish V. Kailas

Associate Professor
Dept. of Mechanical Engineering,
Indian Institute of Science,
Bangalore – 560012
India

Chapter 3. Imperfections in Solids

3.1 Theoretical yield strength, Point defects, Line defects and Dislocations

3.1.1 Theoretical strength

Atoms are orderly arranged without any disruptions in ideal solids. Under mechanical loads, all solids tend to reshape themselves. This occurs usually by process called slip, the translation of one plane of atoms over another under implied shear stresses.

Consider two planes of atoms subjected a shear stress under applied load. Let's assume, as shown in *figure-3.1*, distance between atoms in slip direction is b , and spacing between the two planes is a .

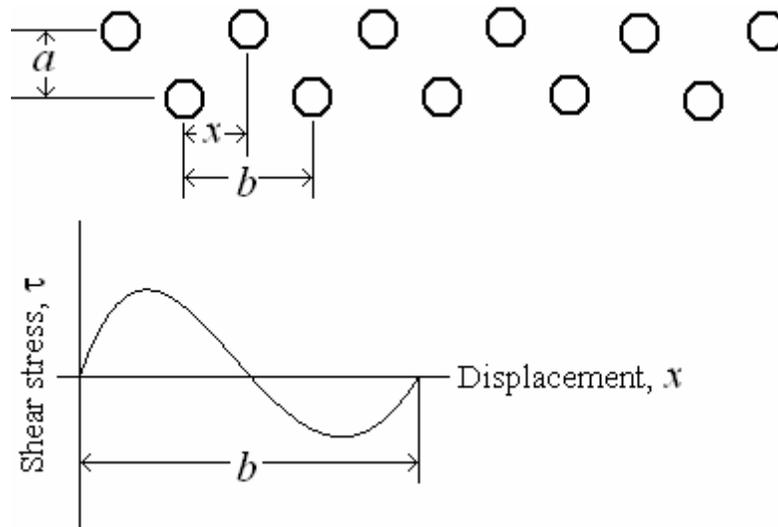


Figure-3.1: Shear displacement of atom planes and variation of shear stress.

The shear stress is zero initially and also once planes moved one identity distance, b . In between, it can be said that shear stress is a periodic function of displacement as each

atom is attracted toward the nearest atom of the other row. Thus the relation of shear stress with displacement can be expressed as follows:

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

where x is the amplitude of sine wave, and b is the period. For small values of x/b , after simplification,

$$\tau \approx \tau_m \frac{2\Pi x}{b}$$

It is safe to approximate at small values of displacement Hooke's law is applicable. Thus,

$$\tau = G\gamma = \frac{Gx}{a}$$

Combining the above two equations, maximum shear stress at which slip should occur is

$$\tau_m = \frac{G}{2\Pi} \frac{b}{a}$$

If it is assumed as $b \approx a$, approximate value of shear stress needed for initiation of slip is

$$\tau_m = \frac{G}{2\Pi}$$

Shear modulus, G , of solids is in the range of 20-150 GPa, and thus theoretical shear strength could be in range 3-30 GPa. However, actual values of the shear stress required for plastic deformation is only about 0.5-10 MPa i.e. about 100 times less than the theoretical value. Because of this discrepancy, it must be said that a mechanism other than shearing of planes must be operative under application of loads thus causing plastic deformation.

3.1.2 Point defects

Defects exist in all solid materials. For ease of their characterization, defects are classified on the basis of their geometry, which is realistic as defects are disrupted regions in a volume of a solid. Defects are:

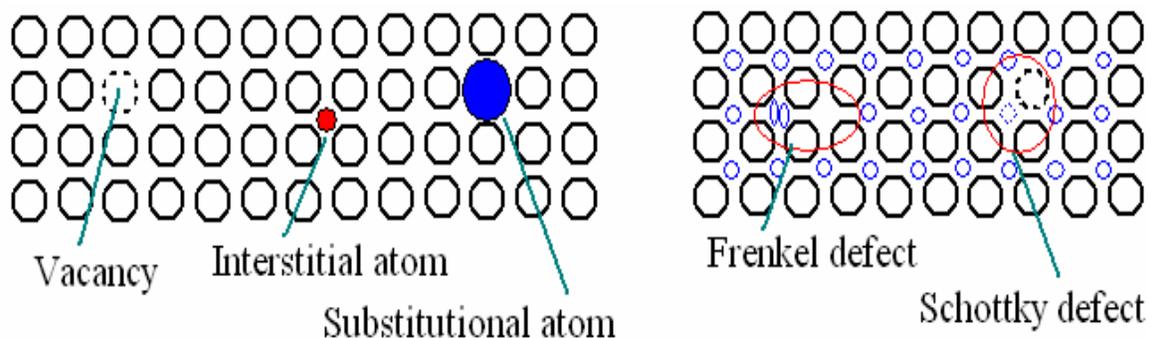
- a. Point defects (zero-dimensional)
- b. Line defects (single dimensional)
- c. Surface defects (two dimensional)
- d. Volume defects (three dimensional)

Point defects, as the name implies, are imperfect point-like regions in the crystal. Typical size of a point defect is about 1-2 atomic diameters. Different point defects are explained in the following paragraphs. *Figure-3.2* depicts various point defects.

A *vacancy* is a vacant lattice position from where the atom is missing. It is usually created when the solid is formed by cooling the liquid. There are other ways of making a vacancy, but they also occur naturally as a result of thermal excitation, and these are thermodynamically stable at temperatures greater than zero. At equilibrium, the fraction of lattice sites that are vacant at a given temperature (T) are:

$$\frac{n}{N} = e^{-Q/kT}$$

where n is the number of vacant sites in N lattice positions, k is gas or Boltzmann's constant, T is absolute temperature in kelvins, and Q is the energy required to move an atom from the interior of a crystal to its surface. It is clear from the equation that there is an exponential increase in number of vacancies with temperature. When the density of vacancies becomes relatively large, there is a possibility for them to cluster together and form voids.



Figur-3.2: Schematic depiction of various point defects

An *interstitial atom* or *interstitialcy* is an atom that occupies a place outside the normal lattice position. It may be the same type of atom as the rest surrounding it (self interstitial) or a foreign impurity atom. Interstitialcy is most probable if the atomic packing factor is low.

Another way an impurity atom can be fitted into a crystal lattice is by substitution. A *substitutional atom* is a foreign atom occupying original lattice position by displacing the parent atom.

In the case of vacancies and foreign atoms (both interstitial and substitutional), there is a change in the coordination of atoms around the defect. This means that the forces are not balanced in the same way as for other atoms in the solid, which results in lattice distortion around the defect.

In ionic crystals, existence of point defects is subjected to the condition of charge neutrality. There are two possibilities for point defects in ionic solids.

- when an ion displaced from a regular position to an interstitial position creating a vacancy, the pair of vacancy-interstitial is called *Frenkel defect*. Cations are usually smaller and thus displaced easily than anions. Closed packed structures have fewer interstitials and displaced ions than vacancies because additional energy is required to force the atoms into the interstitial positions.

- a pair of one cation and one anion can be missing from an ionic crystal, without violating the condition of charge neutrality when the valency of ions is equal. The pair of vacant sites, thus formed, is called *Schottky defect*. This type of point defect is dominant in alkali halides. These *ion-pair vacancies*, like single vacancies, facilitate atomic diffusion.

3.1.3 Line defects or Dislocations:

Line imperfections (one-dimensional defects) are also called Dislocations. They are abrupt changes in the regular ordering of atoms along a line (dislocation line) in the solid. They occur in high densities and strongly influence the mechanical properties of material. They are characterized by the Burgers vector (\mathbf{b}), whose direction and magnitude can be determined by constructing a loop around the disrupted region and noticing the extra inter-atomic spacing needed to close the loop. The Burgers vector in metals points in a close packed lattice direction. It is unique to a dislocation.

Dislocations occur when an extra incomplete plane is inserted. The dislocation line is at the end of the plane. Dislocations can be best understood by referring to two limiting cases - Edge dislocation *and* Screw dislocation.

Edge dislocation or *Taylor-Orowan dislocation* is characterized by a Burger's vector that is perpendicular to the dislocation line. It may be described as an edge of an extra plane of atoms within a crystal structure. Thus regions of compression and tension are associated with an edge dislocation. Because of extra incomplete plane of atoms, the atoms above the dislocation line are squeezed together and are in state of compression whereas atoms below are pulled apart and experience tensile stresses. Edge dislocation is considered *positive* when compressive stresses present above the dislocation line, and is represented by \perp . If the stress state is opposite i.e. compressive stresses exist below the dislocation line, it is considered as negative edge dislocation, and represented by \top . A schematic view of edge dislocations are shown in *figure 3.3*.

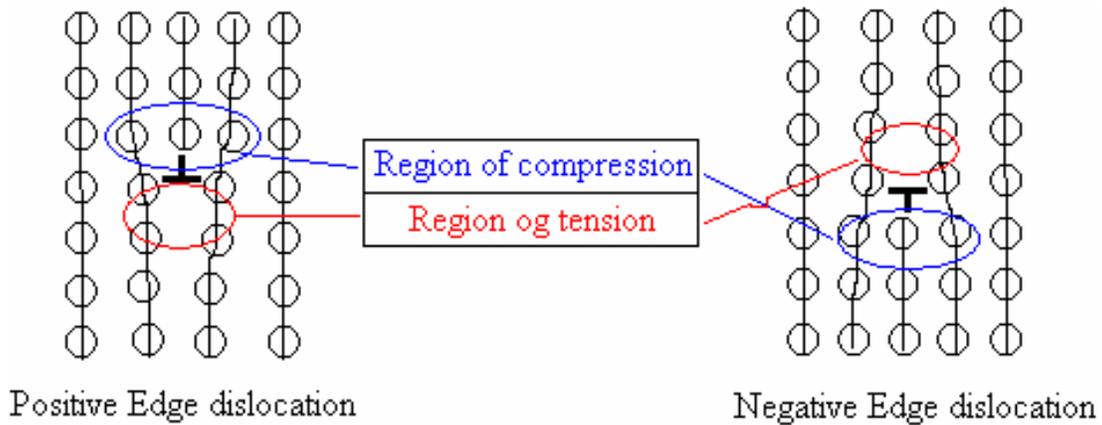


Figure-3.3: Edge dislocations.

A pure edge dislocation can glide or slip in a direction perpendicular to its length i.e. along its Burger's vector in the slip plane (made of \mathbf{b} and \mathbf{t} vectors), on which dislocation moves by slip while conserving number of atoms in the incomplete plane. It may move vertically by a process known as climb, if diffusion of atoms or vacancies can take place at appropriate rate. Atoms are added to the incomplete plane for negative climb i.e. the incomplete plane increases in extent downwards, and vice versa. Thus climb motion is considered as non-conservative, the movement by climb is controlled by diffusion process.

Screw dislocation or *Burgers dislocation* has its dislocation line parallel to the Burger's vector. A screw dislocation is like a spiral ramp with an imperfection line down its axis. Screw dislocations result when displacing planes relative to each other through shear. Shear stresses are associated with the atoms adjacent to the screw dislocation; therefore extra energy is involved as it is in the case of edge dislocations. Screw dislocation is considered positive if Burger's vector and \mathbf{t} -vector or parallel, and vice versa. (\mathbf{t} -vector – an unit vector representing the direction of the dislocation line). A positive screw dislocation is represented by “ \odot ” a dot surrounded by circular direction in clock-wise direction”, whereas the negative screw dislocation is represented by “ \ominus ” a dot surrounded by a circular direction in anti-clock-wise direction”. A schematic view of a negative screw dislocation is shown in *figure 3.4*.

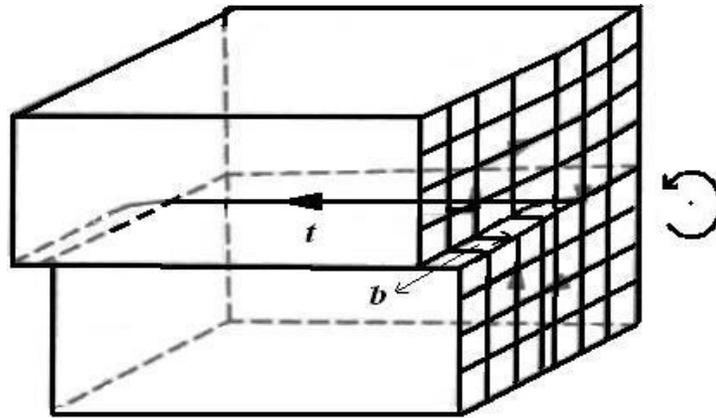


Figure-3.4: *Negative screw dislocation.*

A screw dislocation does not have a preferred slip plane, as an edge dislocation has, and thus the motion of a screw dislocation is less restricted than the motion of an Edge dislocation. As there is no preferred slip plane, screw dislocation can cross-slip on to another plane, and can continue its glide under favorable stress conditions. However, screw dislocation can not move by climb process, whereas edge dislocations can not cross-slip.

Dislocations more commonly originate during plastic deformation, during solidification, and as a consequence of thermal stresses that result from rapid cooling. Edge dislocation arises when there is a slight mismatch in the orientation of adjacent parts of the growing crystal. A screw dislocation allows easy crystal growth because additional atoms can be added to the 'step' of the screw. Thus the term screw is apt, because the step swings around the axis as growth proceeds. Unlike point defects, these are not thermodynamically stable. They can be removed by heating to high temperatures where they cancel each other or move out through the crystal to its surface. Virtually all crystalline materials contain some dislocations. The density of dislocations in a crystal is measures by counting the number of points at which they intersect a random cross-section of the crystal. These points, called etch-pits, can be seen under microscope. In an annealed crystal, the dislocation density is the range of 10^8 - 10^{10} m^{-2} .

Any dislocation in a crystal is a combination of edge and screw types, having varying degrees of edge and screw character. *Figure 3.5* depicts a schematic picture of a common dislocation.

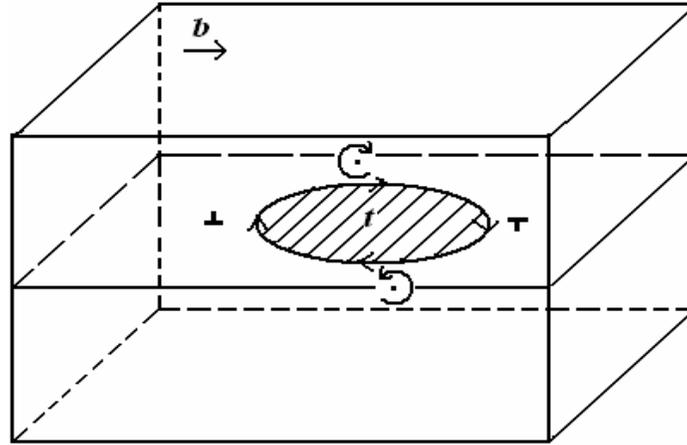


Figure-3.5: Typical dislocation in a crystal.

As shown in *figure 3.5*, the Burger's vector will have the same magnitude and direction over the whole length of dislocation irrespective of the character of the dislocation (edge, screw, or mixed) i.e. Burger's vector is invariant. Other geometrical characteristics of dislocations are:

- vectorial sum of Burger's vectors of dislocations meeting at a point, called node, must be zero.
- t-vectors of all the dislocations meeting at a node must either point towards it or away from it.
- a dislocation line can not end abruptly within the crystal. It can close on itself as a loop, or ends either at a node or at the surface.

Dislocations have distortional energy associated with them as is evident from the presence of tensile/compressive/shear stresses around a dislocation line. Strains can be expected to be in the elastic range, and thus stored elastic energy per unit length of the dislocation can be obtained from the following equation:

$$E \cong Gb^2/2$$

where G – shear modulus and b – Burger's vector.

Dislocations in the real crystal can be classified into two groups based on their geometry – full dislocations and partial dislocations. Partial dislocation's Burger's vector will be a fraction of a lattice translation, whereas Burger's vector is an integral multiple of a lattice translation for full dislocation. As mentioned above, elastic energy associated with a dislocation is proportional to square of its Burger's vector; dislocation will tend to have as small a Burger's vector as possible. This explains the reason for separation of dislocations that tend to stay away from each other!

3.2 Interfacial defects, Bulk or Volume defects and Atomic vibrations

3.2.1 Interfacial defects

Interfacial defects can be defined as boundaries that have two dimensional imperfections in crystalline solids, and have different crystal structures and/or crystallographic orientations on either side of them. They refer to the regions of distortions that lie about a surface having thickness of a few atomic diameters. For example: external surfaces, grain boundaries, twin boundaries, stacking faults, and phase boundaries. These imperfections are not thermodynamically stable, rather they are meta-stable imperfections. They arise from the clustering of line defects into a plane.

External surface: The environment of an atom at a surface differs from that of an atom in the bulk; especially the number of neighbors (coordination) at surface is less. Thus the unsaturated bonds of surface atoms give rise to a surface energy. This result in *relaxation* (the lattice spacing is decreased) or *reconstruction* (the crystal structure changes). To reduce the energy, materials tend to minimize, if possible, the total surface area.

Grain boundaries: Crystalline solids are, usually, made of number of grains separated by grain boundaries. Grain boundaries are several atoms distances wide, and there is mismatch of orientation of grains on either side of the boundary as shown in *figure-3.6*. When this misalignment is slight, on the order of few degrees ($< 10^\circ$), it is called *low angle grain boundary*. These boundaries can be described in terms of aligned dislocation arrays. If the low grain boundary is formed by edge dislocations, it is called *tilt boundary*, and *twist boundary* if formed of screw dislocations. Both tilt and twist boundaries are planar surface imperfections in contrast to high angle grain boundaries. For *high angle grain boundaries*, degree of disorientation is of large range ($> 15^\circ$). Grain boundaries are chemically more reactive because of grain boundary energy. In spite of disordered orientation of atoms at grain boundaries, polycrystalline solids are still very strong as cohesive forces present within and across the boundary.

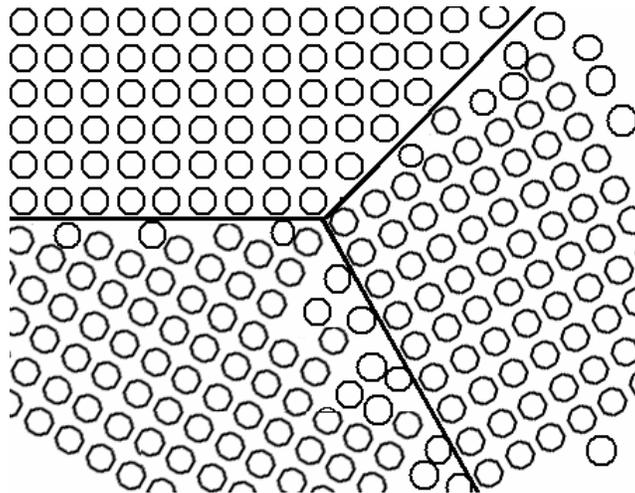


Figure-3.6: Schematic presentation of grain boundaries.

Twin boundaries: It is a special type of grain boundary across which there is specific mirror lattice symmetry. Twin boundaries occur in pairs such that the orientation change introduced by one boundary is restored by the other (*figure-3.7*). The region between the pair of boundaries is called the twinned region. Twins which form during the process of recrystallization are called *annealing twins*, whereas *deformation twins* form during plastic deformation. Twinning occurs on a definite crystallographic plane and in a specific direction, both of which depend on the crystal structure. Annealing twins are typically found in metals that have FCC crystal structure (and low stacking fault energy), while mechanical/deformation twins are observed in BCC and HCP metals. Annealing twins are usually broader and with straighter sides than mechanical twins. Twins do not extend beyond a grain boundary.

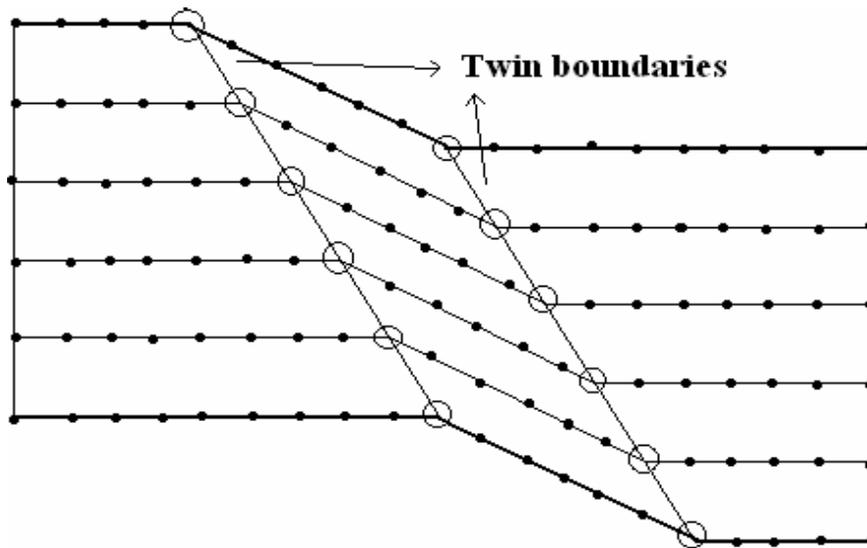


Figure-3.7: A pair of twin boundaries.

Stacking faults: They are faults in stacking sequence of atom planes. Stacking sequence in an FCC crystal is ABC ABC ABC ..., and the sequence for HCP crystals is AB AB AB.... When there is disturbance in the stacking sequence, formation of stacking faults takes place. Two kinds of stacking faults in FCC crystals are: (a) ABC AC ABC... where CA CA represent thin HCP region which is nothing but stacking fault in FCC, (b) ABC ACB CAB is called *extrinsic* or *twin stacking fault*. Three layers ACB constitute the twin. Thus stacking faults in FCC crystal can also be considered as submicroscopic twins. This is why no microscopic twins appear in FCC crystals as formation of stacking faults is energetically favorable. Stacking fault energy varies in range 0.01-0.1 J/m². Lower the stacking fault energy, wider the stacking fault, metal strain hardens rapidly and twin easily. Otherwise, metals of high stacking fault energy i.e. narrower stacking faults show a deformation structure of banded, linear arrays of dislocations.

Phase boundaries exist in multiphase materials across which there is sudden change in physical/chemical characteristics.

3.2.2 Bulk or Volume defects

Volume defects as name suggests are defects in 3-dimensions. These include pores, cracks, foreign inclusions and other phases. These defects are normally introduced during processing and fabrication steps. All these defects are capable of acting as stress raisers, and thus deleterious to parent metal's mechanical behavior. However, in some cases foreign particles are added purposefully to strengthen the parent material. The procedure is called dispersion hardening where foreign particles act as obstacles to movement of dislocations, which facilitates plastic deformation. The second-phase particles act in two distinct ways – particles are either may be cut by the dislocations or the particles resist cutting and dislocations are forced to bypass them. Strengthening due to ordered particles is responsible for the good high-temperature strength on many super-alloys. However, pores are detrimental because they reduce effective load bearing area and act as stress concentration sites.

3.2.3 Atomic vibrations

Atomic vibrations occur, even at zero temperature (a quantum mechanical effect) and increase in amplitude with temperature. In fact, the temperature of a solid is really just a measure of average vibrational activity of atoms and molecules. Vibrations displace *transiently* atoms from their regular lattice site, which destroys the perfect periodicity. In a sense, these atomic vibrations may be thought of as imperfections or defects. At room temperature, a typical vibrational frequency of atoms is of the order of 10^{13} vibrations per second, whereas the amplitude is a few thousandths of a nanometer. Many properties and processes in solids are manifestations of this vibrational atomic motion. For example: melting occurs once the atomic bonds are overcome by vigorous vibrations.

References

1. ASM handbook, Metallography and Microstructures, Vol. 9, ASM International, Materials Park, OH, 1985
2. William D. Callister, Jr, Materials Science and Engineering – An introduction, sixth edition, John Wiley & Sons, Inc. 2004.
3. V. Raghavan, Materials Science and Engineering, third edition, Prentice Hall of India Private Limited, New Delhi, 1990.