
UNIT 5 DEFECTS IN SOLIDS

Structure

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5.1 INTRODUCTION

This unit introduces you to various types of deviation from ideal crystal structures that you have studied in Unit 3. Earlier Unit described the possible crystal structures and also discussed how to grow them. Ideally, most crystalline solids are considered to be a perfect periodic array of atoms whose arrangement conforms to the symmetry of 230 space groups (described in Unit 3). The term defect or imperfection is generally used to describe any deviation from such an orderly structures. Actually no solid can have such perfect order of the atoms in a space as described theoretically. In other words, every solid object has some defect present in the structure. Presence of these defects affect the physical and mechanical properties of engineering materials. These defects also control processes and explain phenomena such as annealing, precipitation, diffusion, sintering, oxidation etc. Most of the structure sensitive properties for example yield strength, fracture strength, thermal conductivity, and electrical conductivity depend on the presence and concentration of defects. Advances in production technologies of materials help in reducing the number of defects, however, they do not eliminate defects completely. For example, in silicon wafer manufacturing, which represents one of the most advanced technologies, zero defect density refers to about 100 defects per square centimeter.

Although, many of the properties mentioned above are profoundly sensitive to deviation from crystalline perfection, the influence is not always adverse, often special characteristics are obtained by the introduction of controlled amount of particular types of defects. In fact controlled number of defects in silicon is essential to produce any solid state electronic device. Similarly, intentional addition of interstitial and substitutional atoms in the structure of material forms the basis for strengthening the material.

Objectives

After studying this unit, you should be able to :

- understand various types of defects,
- know formation/origin of these defects,

- calculate the concentration of point defects, **and**
- find energies of dislocations.

5.2 TYPES OF DEFECTS

All defects and imperfections can be considered under three main **categories** : point defects, line defects and planar defects or interfacial or grain **boundary** defects. If the deviation from periodic arrangement is **localised** to the vicinity of only few atoms it is called point defect. On the other hand; if the deviation extends through microscopic regions in the crystals it is called lattice imperfection, because it produces a discontinuity in the lattice, **used** to describe **the** actual periodicity of **an** atomic array in a crystal. There are essentially two **types** of lattice imperfection that can exist in the **crystals** : line defects, so called because they propagate as lines in a crystal and plane defects which have **an aerial** extent. **Although** described in detail in this unit, they are **summarised** in Table 5.1.

5.2.1 Point Defects

Point defects can be divided into vacancies, **interstitials** and **impurities**. **Whether** vacancies or interstitial defects predominate in a particular crystal will **depend on the relative energies** of **formation** of these defects, which are in turn determined by **geometrical factors**.

5.2.2 Vacancies and Interstitial Atoms

A vacancy is obtained by removing **an** atom from the crystal lattice site where **the atom** is usually present; and **interstitial** atom is an additional atom added in an **interstitial** position. In the presence of these two point defects **an** otherwise regular lattice looks as **shown** in Figure 5.1. In a given crystal, **vacancy** or interstitial defect may predominate **depending** on the energy of formation of **these** defects, which **may further** depend on geometrical factors. The energies of defect formation are discussed **in** next section.

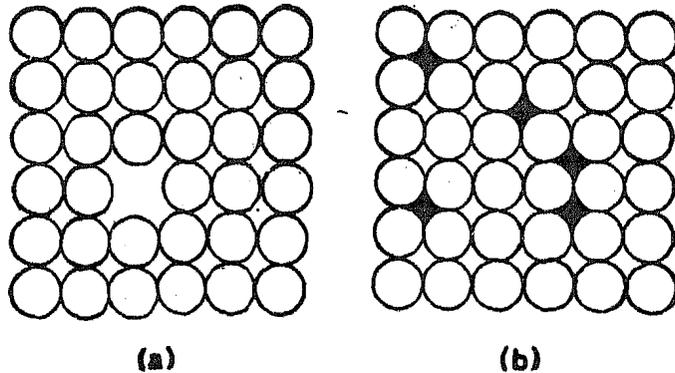


Figure 5.1 : Point Defects in Solids a) Vacancy b) Interstitial

Table 5.1

Type	Name	Description
Point Defects	Interstitial	Extra atom in an interstitial site.
	Schottky defects	Atom missing from correct site
	Frenkel defect	Atom displaced to interstitial site creating nearby vacancy .
Line Defects	Edge dislocation	Row of atoms marking edge of crystallographic plane extending only part way in crystal
	Screw dislocation	Row of atoms about which a normal crystallographic plane appears to spiral.
Plane Defects	Linear	Boundary between adjacent perfect boundary perfect regions in the same crystal that are slightly tilted with respect to each other
	Grain Boundary Stacking fault	Boundary between two parts of closer packing having alternative stacking sequence

We know that point defects disturbs the perfect arrangement of the **surrounding** atoms. **When a vacancy** or a small substitutional atom is present, the surrounding atoms collapse towards the point defect, stretching **the** bonds between the **surrounding** atoms and producing

a tensile stress field. An interstitial or large substitutional atom pushes the surrounding atom together, producing a compressive stress field. In either case effect is widespread. The stress fields are shown in Figure 5.2.

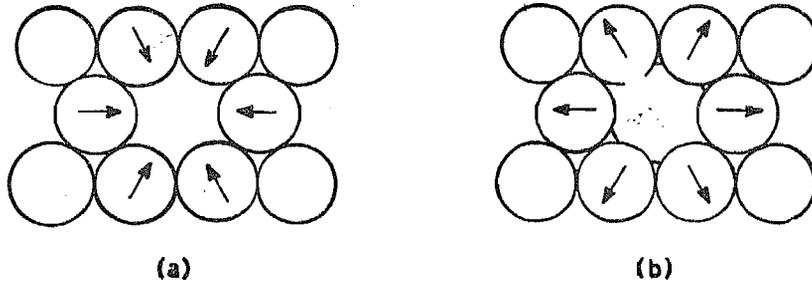


Figure 5.2: a) Representation of Tensile Lattice Strains Produced on Host Atom by Smaller Substitutional Impurity Atom; b) Representation of Compressive Lattice Strains Produced on Host Atom by Larger Substitutional Impurity Atom

5.3 CONCENTRATION OF POINT DEFECTS

Defect such as vacancies and interstitials are internally induced by thermal fluctuation in the material. The presence of defects changes both, the internal energy of the crystal as well as its entropy. Consequently, their equilibrium concentration is a function of energy of formation and the equilibrium temperature. The equilibrium concentration of Schottky defect may be determined as follows. The assumption is that only one type of defect (Schottky defects) is present in the material. Before discussing the calculation let us recollect the definitions of both Schottky and Frenkel defects in an ionic crystal. A Frenkel defect is a vacancy interstitial pair formed when an ion jumps from a normal lattice point to an interstitial site leaving behind a vacancy. The Schottky defect is a pair of vacancies in an ionically bonded material. Schematic of both these defects in ionic crystals are shown in Figure 5.3.

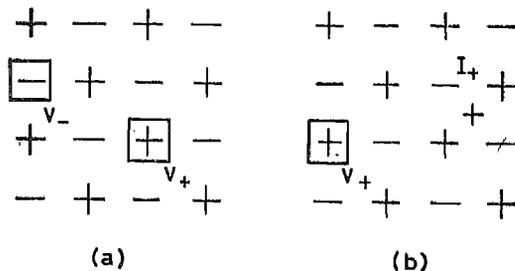


Figure 5.3 : Defect in Ionic Crystals a) Schottky b) Frenkel

Let,

- N = The total number of atoms in a crystal of unit volume
- n = Number of Schottky defect per unit volume.
- E = Energy formation of a Schottky defect i.e. the energy required to move an atom from its lattice site within the crystal to a lattice site on its surface.

The number of ways in which a Schottky defect can occur is given by

$$C_n^N = \frac{N!}{(N - n_s)! n_s!}$$

The entropy associated with this situation, $S = k \ln(\text{number of ways})$, where k is Boltzmann constant.

The energy is given by

$$E = n_s E_s$$

The change in free energy (neglecting volume changes) is given by

$$F = E - TS$$

$$= n_s E_s - kT \left[\ln N! - \ln n! - \ln (N - n_s)! \right]$$

The most probable equilibrium condition is the one, where the free energy is **minimum with** respect to changes in n

i.e.
$$\left(\frac{\partial F}{\partial n_s}\right)_T = \text{constant} = 0$$

Differentiating and setting it to zero

$$E_s = kT \frac{\partial}{\partial n_s} [\ln N! - \ln n_s! - \ln (N - n_s)!]$$

The factorial terms may be simplified using **Stirlings** formula for the factorial of large number.

Thus,
$$\ln X! = X \ln X - X$$

so that

$$\frac{d}{dx} (X!) = \ln X$$

So the equation reduces to

$$E_s = kT \ln \left(\frac{N - n_s}{n_s}\right)$$

hence
$$n_s = \frac{N}{1 + e^{E_s/kT}} \approx N e^{-E_s/kT}$$

The equilibrium concentration of Frenkel defects may be found by analogous approach. Again it is assumed that only these defects are present.

Let,

- N = number of atoms in a crystal of unit volume.
- N' = number of available interstitial sites per unit volume.
- n = number of Frenkel defects (i.e. vacancy interstitial pairs) per unit volume.
- E = Energy of formation of Frenkel defects.

Of all the defects available, a vacancy can occur in $C_{n_v}^N$ ways, and an interstitial in $C_{n_i}^{N'}$ ways. Consequently a **Frenkel** defect can occur in $(C_{n_v}^N C_{n_i}^{N'})$ if the **events** are assumed to be **statistically** independent. The entropy associated with the situation is $S = k \ln y$, y being the number of ways an event occurs. In the present situation

$$S = k \ln C_{n_v}^N C_{n_i}^{N'}$$

The internal energy is given by $E = n_f E_f$

The change in free energy is given by

$$F = E - TS = n_f E_f - kT \ln C_{n_v}^N C_{n_i}^{N'}$$

Minimising and setting to zero
$$\left(\frac{\partial F}{\partial n_f}\right)_T = \text{constant} = 0$$

In thermal equilibrium one can differentiate equation for F and using Sterling formula to get

$$E_f = kT \ln \left[\frac{(N - n_f) (N' - n_f)}{n_f^2} \right]$$

$$n_f = \sqrt{NN'} e^{-E_f/2kT}$$

Above value is the concentration of Frenkel defects in a crystal in thermal **equilibrium**.

Concentration of point defects in excess of the equilibrium value may be obtained by putting **material** to non-equilibrium process.

Let us take an example, When a crystal is heated, a new value higher than the equilibrium value of concentration would exit, usually at the surface, which subsequently spreads throughout the crystal. When this crystal is cooled a lower **concentration** of vacancy is seen

due to sinks in the crystal. The process needs a finite time. However, if the crystal is cooled sufficiently rapidly the vacancies do not get finite time to move and get trapped in the crystal (usually referred to as frozen in) leading to a very high concentration of vacancies.

point defects can be produced in the crystal in various ways

- by irradiation with high energy particles that, when impinging on the solid may produce a cascade of atomic displacements and ionisation,
- plastic deformation,
- quenching, and
- by increasing the temperature so as to increase the amplitude of vibration of atoms thereby increasing the probability of the formation of the defects;

Although these vacancies have atomic dimensions it can affect material properties such as density and in turn one can calculate the concentration of these defects if one knows the density. This is illustrated by following example,

Example 5.1

Iron has a measured density of 7.87 mg/m^3 . The lattice parameters of BCC iron is 2.866 \AA . Calculate the percentage of vacancies in pure Iron.

Solution

$$\rho = \frac{(\text{no of atoms/unit cell}) (55.85 \text{ g/g.mole})}{(2.885 \times 10^{-8})^3 (6.02 \times 10^{23})} = 7.87 \text{ mg/m}^3$$

Thus the number of atoms per unit cell

$$= \frac{(2.885 \times 10^{-8})^3 \times (6.02 \times 10^{23}) \times 7.87}{55.85} = 1.998.$$

There should be 2 atoms/cell in perfect BCC iron crystal. Thus the difference must be due to presence of vacancies.

$$\text{Thus, vacancies} = \frac{(2 - 1.998)}{2} = 0.1\%$$

SAQ 1

The energies of formation of Schottky and Frenkel defect in material are 1 eV/atom ($1.6 \times 10^{-19} \text{ J/atom}$) and 4 eV/atom ($6.4 \times 10^{-19} \text{ J/atom}$) respectively. What are the equilibrium concentration of these defects at 900 K ? Assume that exponential constant, A , is equal to unity.

SAQ 2

The equilibrium vacancy concentration of Schottky defect in copper are 4×10^{-6} , and 14×10^{-5} at temperatures of 1000 K and 1225 K respectively, What are the energy of formation of these defects?

5.4 LINE DEFECTS DISLOCATIONS

Dislocations are an extremely important class of crystal defects. They are responsible for the relative weakness of pure metals and in certain cases (after work hardening) for just the opposite effect of extra hardness.

A dislocation is regarded as a linear disturbance of the atomic arrangements caused by the displacement of one group of atoms in a crystal with respect to another. Dislocations play

as strength and account for the plastic deformation and the ductility in the materials. They arise in crystal due to growth accidents, thermal stresses, external stresses causing plastic flow etc.

5.4.1 Edge Dislocation

The distortion of a crystal structure may also be caused by the insertion of an extra plane of atoms part way into the crystal. Most of the distortion is concentrated about the edge of the extra plane, called the "half plane" of extra atoms and so we speak of dislocations as being #at of line distortion along the end of the plane. So the dislocation is a line defect. For example in Figure 5.4 edge dislocation is perpendicular to the plane of the page and passing through point A.

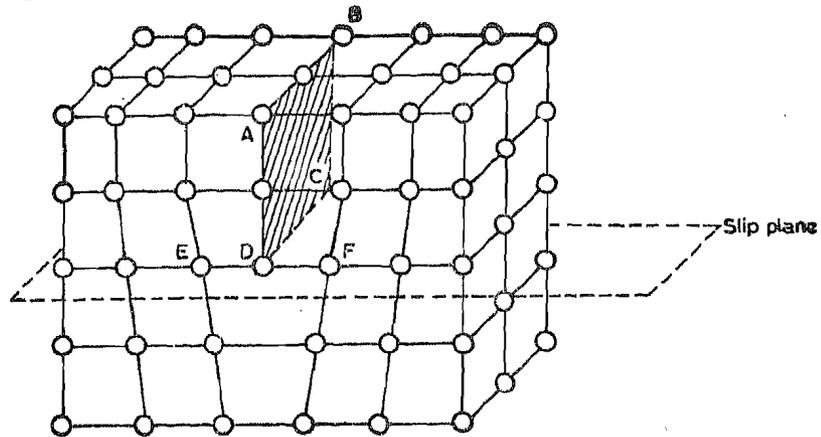


Figure 5.4: Edge Dislocation Introduced due to an Extra Half Plane of Atoms ABCD

All dislocations have the important characteristic that the distortion is severe only in the vicinity of the dislocation line. In fact along the dislocation line the atoms may not even possess the correct number of neighbours, while, not more than a few atom distance away from the center, the distortion may be so small that the crystal is locally nearly perfect.

The region near the dislocation line where distortion is maximum (extremely large) is called the core of the dislocation, here local strain is quite high. Two extreme type of dislocations are possible, the edge dislocation and screw dislocation, which are described in the next sub-section. However any particular dislocation is usually a mixture of these two dislocations. Far away from the core, the strain is small enough to be described by small strain elastic theory, and so it is called the elastic region.

5.4.2 Screw Dislocation

Let a sharp cut be made part way through a perfect crystal; further let the material on one side of the cut be moved up atoms then placed back into contact. The resultant external character of a crystal is that of Figure 5.5,

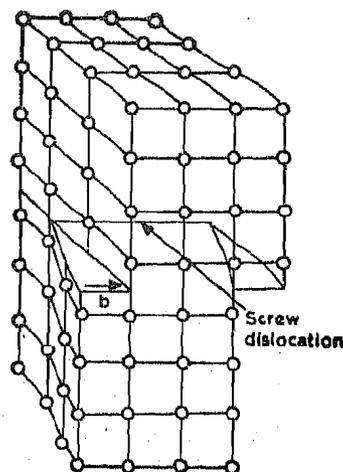


Figure 5.5: Lattice Representation of Screw Dislocation

Clearly a line of dislocation exist along the edge of the cut; the line is called screw dislocation. Important feature of the screw dislocation is the new character of the atom planes. Complete planes of atoms **normal** to the dislocation no longer exist. Rather, all atoms lie on a single surface which spirals from one end of the crystal to another hence the word screw. The pitch of the screw may be either right handed or left handed, and it may also be one or more atom distances per revolution. The simple dislocation just described has a pitch of one atom spacing per revolution. Again, the degree of distortion varies with distance from the center of the dislocation. **Atoms** far away from the screw **dislocation** are in regions of very little local distortion, while **atoms** near the center are in regions highly distorted and the local crystalline symmetry is destroyed.

5.4.3 Mixed Dislocation

The edge and screw dislocations mentioned above are considered to be pure extremes of the linear defects. Most linear defects in the actual **materials** will be mixed as shown in Figure 5.6(c), alongwith edge and screw in Figures 5.6 (a) & (b) respectively.

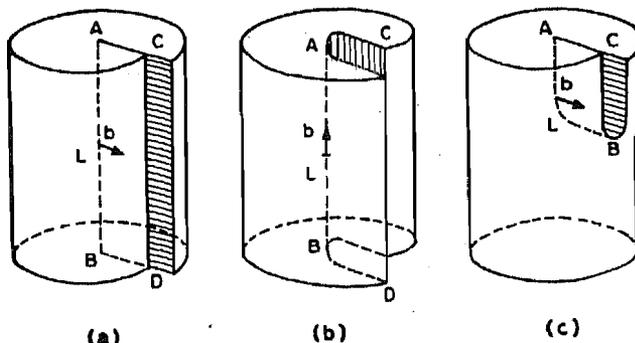


Figure 5.6 : a) Edge b) Screw c) Mixed Dislocation. Note Edge at A and Screw nt B

In **this** general case, the mixed dislocation has both edge and screw characters. The Burgers vector for the mixed dislocation is neither parallel nor perpendicular to the line of dislocation but has a fixed orientation in space that is consistent with our earlier **definitions** for pure dislocations.

5.4.4 Magnitude of Dislocation and Burgers Vectors

The **vector** defining the position of the repeating unit (unit'cell) of a **perfect** single crystal is given by equation

$$\mathbf{r} = n_1 \mathbf{a} + n_2 \mathbf{b} + n_3 \mathbf{c}$$

where n_1, n_2, n_3 are integers and vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ represent the primitive translations of the lattice. With simple lattice structures **e.g.** with most pure metals, the repeating units are single atoms (ions). In this case the vector \mathbf{r} is **simply the** position vector of the atoms, For real crystals equation applies only approximately because of the lattice distortion. If however the atoms are only slightly displaced from their perfect lattice sites, every atom of real **lattice** belong to unambiguously to some ideal lattice site defined by above equation. Thus an ideal crystal may be correlated to the real crystal. The region where this is possible is termed good material, and where it is not possible is termed **as** bad material. This bad material can be **characterised** by Burger Vectors. First let us give closer look to this "bad material" region. It can be enclosed by the path called Burger Circuit,

5.4.5 Burgers Circuit

At large distances from the dislocation L , the crystal is but slightly distorted, and one can set up a local correspondence between the points of the real crystal and their **homologs** in the perfect crystal.

Beginning with three points such **as** ABC in the real crystal and the corresponding in the perfect crystals one can define without ambiguity all neighboring points such as D. All areas where such a **local** correlation is possible will be called zones of good **crystal**. The center L of dislocation, where this operation is not possible **will** be a zone of bad **crystal**. **This** is shown in Figure 5.7.

Starting from a point such as A and moving step by step, one can pass through all points M located in good crystal. But if circuit is large enough, the correlation established is not

unique, it can be a function of the circuit used. Let us consider for instance the closed path AEFGA round a zone of a bad crystal (a) the corresponding circuit AEFED in the perfect crystal does not close. The vector BA which must be added to the path in the perfect crystal in order to close it form evidently be independent of the form and position if the circuit, and be equal to the Burger Vector of, the dislocation. The circuit AEFGA is called Burger Circuit.

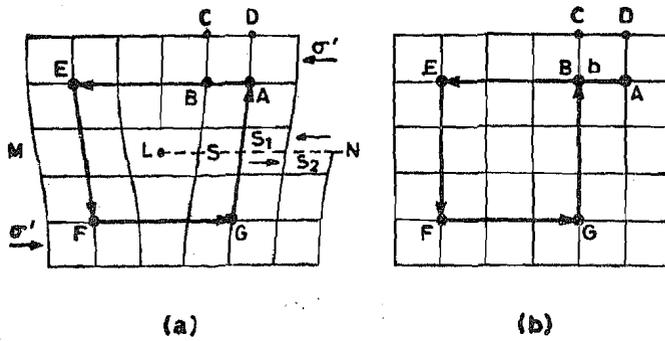


Figure 5.7: Burgers Circuit and Burgers Vector; a) Helical Crystal, b) Perfect Crystal

Three Important properties of Burger Vector are :

- 1) b depends only on the nature of the bad crystal around L, nor evidently on the origin or the form of the circuits if the latter.
- 2) The Burgers vector of a circuit enclosing several dislocation is equal to the sum of the Burgers Vectors of the dislocation.
- 3) If a dislocation ends at a node a displacement of the circuit C_1 to $C_1 + 1$ shows that

$$b_1 = b_2 + b_3.$$

In the general case, if for each dislocation line learning a node such as A, one takes Burgers circuit C_1 circling around each line in the same direction seen from point A one has

$$\sum_i b_i = 0$$

5.4.6 Significance of Burgers Vector

The local expansion, termed the dilatation around the edge dislocation can be described by a simple analytical expression, The dilatation Δ at a point near an edge dislocation is given by

$$\Delta = \frac{\Delta V}{V} = \frac{b}{r} \sin \theta$$

The factor b, the magnitude of the vector is called the Burgers Vectors. It is a measure of the strength of the distortion caused by the dislocation. The quantity r is the radial distance from the point to the dislocation line, and θ is angle defined in Figure 5.8. The sign of dilation, positive for expansion and negative for compression is proper if θ is measured as shown.

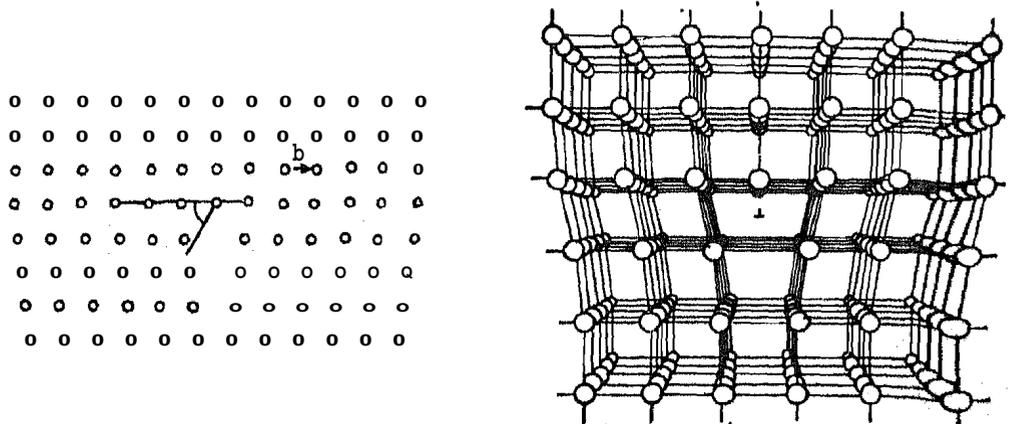


Figure 5.8 : Atomic Arrangement of Atoms in Edge Dislocation Reproduced here to Explain Significance of Burgers Vectors

In contrast to the type of distortion surrounding the edge dislocation, the atoms near the center of the screw dislocation are not in dilatation but are on a twisted or stressed lattice. These atoms being on a spiral ramp, are displaced from their original positions in the perfect crystal according to the equation which describes the spiral ramp

$$u_z = \frac{b}{2\pi} \theta$$

The Z axis is along the dislocation, and u_z is the displacement in the direction. The angle θ is measured from some axis perpendicular to the dislocation; note that as θ increases by 2π , the displacement increases by the factor b . The vector b is again the Burgers Vector and is a measure of strength of the dislocation.

Partial Dislocation : A dislocation having a Burgers Vector which is not a lattice translation.

5.5 ENERGY OF DISLOCATIONS

The energy of a dislocation can be estimated by assuming that the crystal behaves as an elastic solid during the process of creation of the dislocation. Calculation of the energy can easily be performed for a strength screw dislocation, however, the results are similar for an edge dislocation.

Starting with the perfect crystal let it be cut in the way described in sub-section 5.4.2. for a screw dislocation and let the two sides of the cut be displaced with respect to each other by distance b in the prescribed manner. For the displacement to be made, a distribution of forces must be exerted over the surface of the cut and the work done by the forces in making the displacement b is equal to the energy of the dislocation, U_d .

$$U_d = \int F \cdot b \, dA$$

Thus the integral is evaluated over the area of the surface of the cut the force F is the average force over unit area at a point on the surface during the displacement. The average value must be used because the force at a point builds up linearly from zero to maximum value as the displacement is carried out.

To calculate the energy, we must have a quantitative estimate of the magnitude of the force F . This can be understood as follows (Figure 5.9).

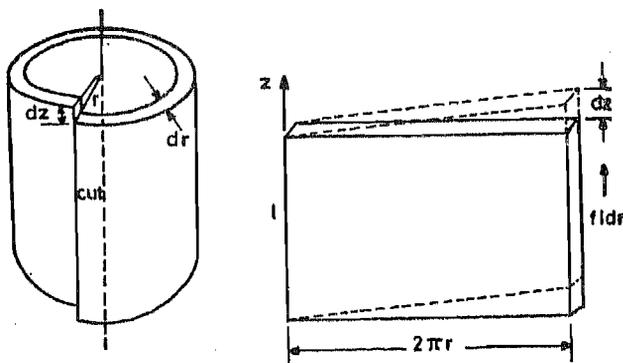


Figure 5.9 : Determination of Dislocation Energy around a Screw Dislocation

Let the crystal be considered as a series of concentric cylindrical shells, with the dislocation in the center. Each shell is cut along its cylindrical length where the cut is then displaced with respect to the other side by a distance b . If the thickness of shell is small then geometrical configuration of the shell is not important for calculating the resistance force during the displacement.

In particular, the force will be the same if the shell is opened out is reduced to consideration of the shearing displacement of a plate. For small shearing displacement, Hooke's law surely holds. Therefore, force per unit area, f , necessary to shear a cylindrical shell a distance r from the center of the dislocation into the final configuration by amount b is just

$$f = \frac{\mu b}{2\pi r}$$

where μ is the shear modulus of the material. In the calculation of the energy needed to displace the cylindrical shell, the average force during the complete displacement to b is used.

The average force $\langle f_{av} \rangle$ is just one half of the final value when the displacement is b .

$$\text{Thus, } F = \langle f_{av} \rangle = \frac{1}{2}f.$$

The energy of dislocation is

$$U_d = \int \frac{\mu b^2}{4\pi r} dA$$

Since $dA = dz dr$, U_d for dislocation of length l is

$$U_d = \int_{r_0}^r \int_0^l \frac{\mu b^2}{4\pi r} dz dr$$

Thus,

$$U_d = \frac{\mu b^2 l}{4\pi} \ln \left(\frac{r_1}{r_0} \right)$$

The energy calculated by using above equation depends on the values taken for the integration limits on r . For a crystal of infinite size, the energy of a single dislocation is infinite.

However, crystals of ordinary size (say 1 cm on an edge) contain many dislocations. These dislocations in a random distribution cancel out each others strain fields at distances approximately equal to the mean distance between them. Experimental observations show that the mean distance of separation of 10^4 atom spacing; hence r_1 is of this order.

As $r \rightarrow 0$, the expression becomes divergent. However, because of the finite size of atoms, we cannot consider any region of atomic dimensions as an elastic continuum and elasticity theory may not be correct. It is reasonable therefore to consider region within about one lattice spacing of the geometric center of the dislocation to be a void and to delete it from consideration. In the region within about two spacings of the center of the dislocation, the core, the discrete nature of the structure is important and displacements are sufficiently large to bring in nonlinear terms in the core effects can be neglected. For example, the energy of the dislocation resides primarily in the strained region well outside the core, because the logarithm is not very sensitive to the size of r . If r_0 is about one or two atom spacings, the ratio $\frac{r_1}{r_0}$ is about 5×10^3 .

Once this ratio is determined the energy U_d can be calculated easily. The Burgers vector b is about 2.5 \AA , μ is about $10^{11} \text{ Newtons/m}^2$. Then U_d is about $4 \times 10^{-9} \text{ Joules/m}$ of dislocation length equivalent to about 10×10^{-19} joules (or about 6 eV) per atom length (2.5 \AA) of dislocation line. Considerable variation in energy can exist for different solids, but the range of energy for screw dislocations should be 3 to 10 eV per atom length. The displacement around edge dislocation is more complicated than for screw. So energy calculations are more difficult. However, energy in this case is about the same. One of the important characteristics of dislocation is the fact that unlike point defects particularly vacancies which exist at equilibrium in significant numbers given by Boltzmann factor $e^{-E_v/KT}$, the dislocations in solids seem to have nearly zero equilibrium densities. The reason is that the formation of energy of dislocation is very high. With elastic energy of about 8 eV per atom length, the Boltzmann factor is insignificant at room temperatures. Thus, the dislocation densities experimentally observed depend upon the previous treatment, of the crystal, the method of growth, previous mechanical treatment, thermal history etc.

5.6 PLANAR DEFECTS/SURFACE IMPERFECTIONS

Surface imperfections in a crystal arise from a change in the stacking of atomic planes across the boundary. The change may be one of the orientation or the stacking sequence of the planes. Following are the major imperfections:

5.6.1 Grain Boundaries

Those surface imperfections which separate crystals of different orientations in a polycrystalline aggregate are shown in Figure 5.10.

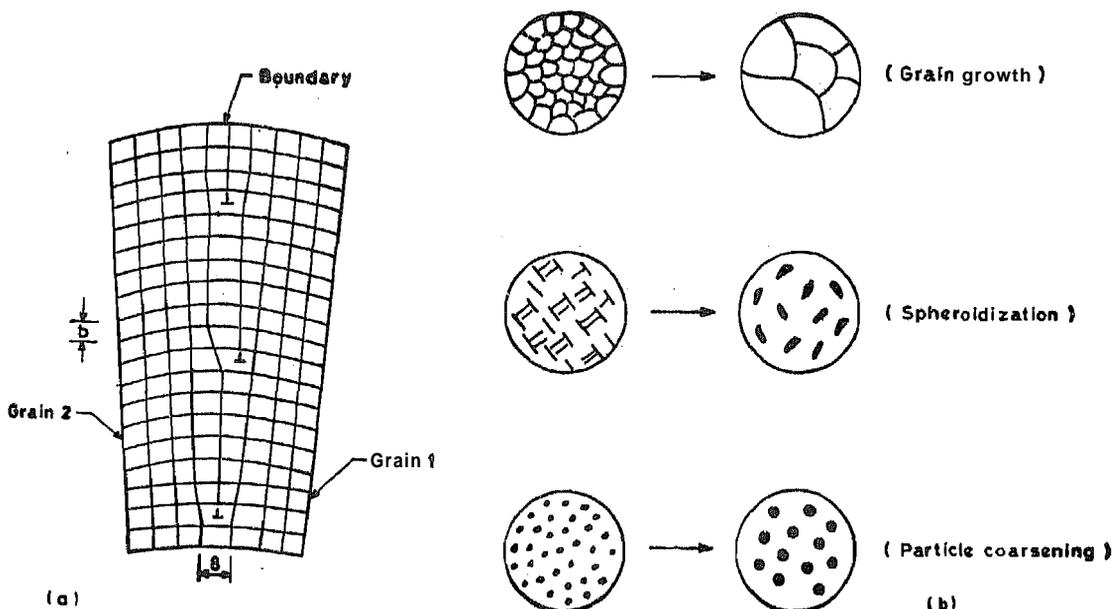


Figure 5.10 : a) Grain Boundaries in a Polycrystalline Solid, b) Process of Grain Growth for Reduction in Grain Boundary Area to Reduce Energy

The lattice of each grain is identical but lattice are oriented differently. Thus a grain boundary is surface that separates the individual grains and is a narrow zone in which the atoms are not properly spaced. The atoms are too close at some locations in the grain boundary causing a region of compression, while the other areas the atoms are far apart, causing a region of tension. We can control the properties of the material by grain size strengthening, this is discussed in the next unit. All grain boundaries have a relatively high energy, typically 0.2–1 J/m and as a result they are non-equilibrium defects. Thus the crystals will always try to reduce the total grain boundary area in order to reduce the free energy. This is illustrated in the Figure 5.10.

5.6.2 Twin Boundaries

Surface imperfections which separate two orientations in such a manner that they are mirror images of one another are called twin boundaries. The volume of the material which has an orientation that is an mirror image of a matrix orientation is called twin. This is shown in Figure 5.11.

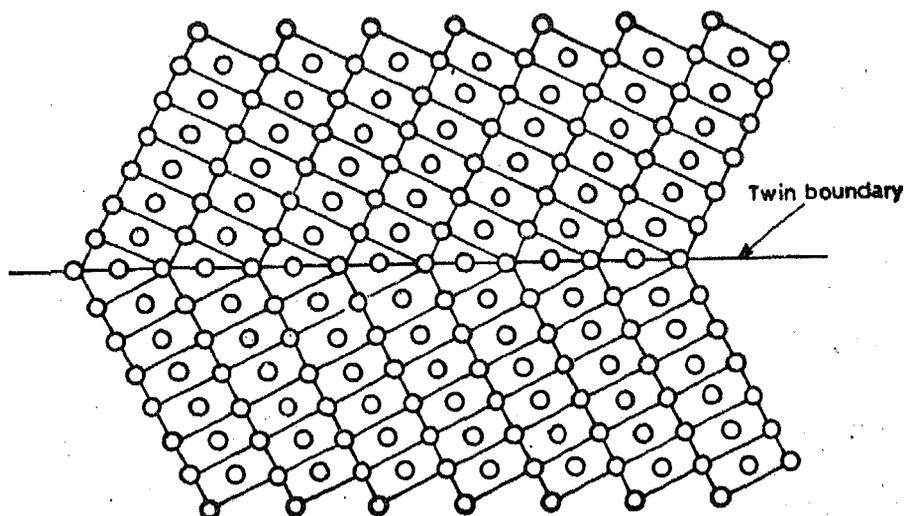


Figure 5.11: A Twin Boundary Separates Two Crystalline Regions that are, Structurally, Mirror Images of Each Other

5.6.3 Stacking Fault

A stacking fault is a surface imperfection that results from the stacking of one atomic plane out of sequence on another while the lattice on either side of fault is perfect. For example the stacking sequence of an ideal FCC crystal may be described as ABC, ABCABC. A stacking fault might change the sequence ABC ABABABC... The stacking fault in this case is due to the A plane of atoms after the second B. This may be described as a very thin region of stacking fault in a FCC crystal.

SAQ 3

Draw a Burger Circuit for an edge dislocation in a primitive cubic crystal. In certain crystal the Burger vector for an edge dislocation is 2.5×10^{-10} . Calculate the force per unit length on the v dislocation with shear of 350 N/m^2 is applied.

5.7 BULK OR VOLUME DEFECTS

In the earlier sections we considered defects which are of atomic dimensions. Other defects also exists in all solid materials that are much larger than those discussed. The defects include pores, cracks, foreign inclusions and other phases. They are normally introduced during processing and fabrication steps. These defects affect mechanical properties, electrical properties, thermal properties and so on.

5.8 SUMMARY

All solid materials contain large number of defects. The several types of defects are classified on the basis of their geometry and size. Point defects are those associated with one or two atomic positions, including vacancies, interstitials and impurity atoms.

Dislocations are one-dimensional defects of which edge and screw are pure in nature. the magnitude and direction of lattice distortion associated with a dislocation is specified by its Burgers vector. The relative orientations of Burgers vector and dislocation line are perpendicular for edge, parallel for screw and neither perpendicular nor parallel for mixed. There are other imperfections which include grain boundaries, twin boundaries, volume defects such as cracks and pores. We have also discussed the formation of these defects and how to calculate the concentration of these defects.

5.9 KEY WORDS

Burgers Vector	:	The direction and distance that a dislocation moves in each step.
Dislocation Edge Dislocation	:	A line imperfection in the lattice of a crystalline material.
Edge Dislocation	:	A dislocation introduced into the lattice by adding an "extra half plane" of atoms.
Frenkel Defect	:	A pair of point defects produced when an ion moves to create an interstitial site.
Grain Boundary	:	A planar defect which represents the boundary between two grains.
Interstitial Defect	‡	A point defect introduced in the lattice when the atoms leaves the original site and is present at a site which is not a regular position in the lattice.
Schottky Defect	:	A pair of point defect in ionic solids both cation and anion vacancy form in the solid.

- Screw Dislocation** : A dislocation produced in the crystal when atomic plane produces a spiral ramp about the dislocation.
- Stacking Fault** : A surface defect in materials caused by the improper stacking sequence of closed packed planes.
- Twin Boundary** : A surface defect across which there is a mirror image misorientation of the lattice.
- Vacancy** : Vacancy is created when an atom is missing from a lattice position.

5.10 ANSWERS TO SAQs

SAQ 1 & 2

Use equations derived in section 5.3 for concentration and energies of formation of Schottky and Frenkel defects, substitute the values given in SAQs 1 & 2 to get the answers.

SAQ 3

$$8.75 \times 10^{-8} \text{ N/m.}$$

Use equation for force on the dislocation; substitute the values given in the problem to get the answer.

FURTHER READINGS

- 1) Askeland, D. R., 1989, *The Science and Engineering of Materials*, 2nd Edition, PWS-Kent Publishing Company, Boston.
- 2) Van ~~Vl~~ack, L. H., 1989, *Elements of Materials Science and Engineering*, 6th Edition, Addison-Wesely Publishing Company, Reading MA.
- 3) **Shackelford**, J. F., 1988, *Introduction to Materials Science for Engineers*, 2nd Edition, **Macmillian** Publishing Company, New York.
- 4) Narula, G. K., **Narula**, K. S., Gupta, V. K., 1988, *Materials Science*, Tata **McGraw Hill** Publishing Company Ltd., New Delhi.
- 5) **Pollock**, D. D., 1990, *Physics of Engineering Materials*, **Prentice Hall**, USA.
- 6) Keer, H. V., 1993, *Principles of the Solid State*, Wiley Eastern, Delhi.
- 7) **Smith**, W. F., 1993, *Foundations of Materials Science & Engineering*, **McGraw-Hill**.
- 8) Anderson, J. C., **Leaver**, K. D., Rawlings, R. D., and Alexander, J. M., 1990 *Materials Science*, 4th Edition, Chapman & Hall, Madras.
- 9) **Polyakov**, A. M., 1985, *Science for Everyone; Semiconductors Made Simple*, Mir Publishers, Moscow.