CHAPTER 2

DEFECTS IN CRYSTALS AND DISLOCATIONS

2.1-POINT AND LINE DEFECTS

All real crystals contain imperfections which may be point, line, surface or volume defects, and which disturb locally the regular arrangement of the atoms. Their presence can significantly modify the properties of crystalline solids. Furthermore, for each material there can be a specific defect which has a particular influence on the material properties. In this work are presented point and line defects.

2.1.1-Point defects

All the atoms in a perfect lattice are at specific atomic site, if the thermal vibration is ignored. In a pure metal two types of point defects are possible, namely a “vacant atomic site” or “vacancy”, and a “self-interstitial atom”. These intrinsic defects are schematically shown in figure 2.1

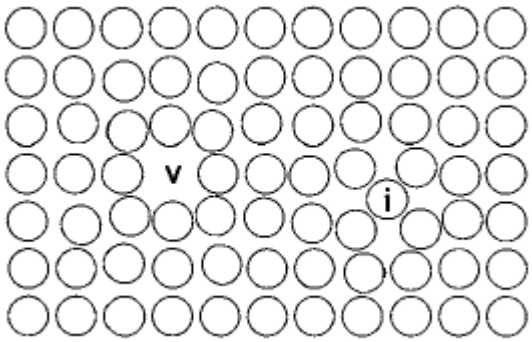


Figure 2.1 - *Vacancy and self-interstitial atom in an (001) plane of a simple cubic lattice*

The vacancy has been formed by the removal of a single atom from its lattice site in the perfect crystal. The interstitial has been formed by the introduction of an extra atom into an interstice between perfect lattice sites. Vacancies and interstitial can be produced in materials by plastic deformation and high-energy particle irradiation. Furthermore, intrinsic point defects are introduced into crystals simply by virtue of temperature, for at all temperatures above 0 K there is a thermodynamically stable condition. The equilibrium concentration of defects, given by the ratio of the number of defects to the number of atomic sites, corresponding to the condition of minimum free energy is

(2.1)

Where K is the Boltzmann's constant, T is the temperature expressed in deg Kelvin, and Ef is the energy of formation of one defect.

For the vacancy, the formation energy Ef, is that required to remove one atom from its lattice site to a place on the surface of the crystal. The self-interstitial is created by removing one atom from the surface and inserting it into an interstitial site, and the formation energy is tipically two to four times the formation energy for vacancies. Thus, the concentration given by equation (2.1) is many orders of magnitude smaller for interstitials, and so in metals in thermal equilibrium the concentration of interstitials may be neglected in comparison with that of vacancies.

As atoms vibrate randomly due to thermal fluctuations, these point defects can occasionally jump from one lattice site or interstice to another. For large numbers of atoms under equilibrium conditions, these random jumps produce no net effect, as there are as many jumps in one direction as in any other. However, under any driving force, such as an applied stress or temperature gradient, more of these jumps will occur in a preferred direction. For example, interstitials may move preferentially from regions of high stress to region of law stress.

Impurity atoms in a crystal can be considered as extrinsic point defects and they play a very important role in the physical and mechanical properties of all materials. Impurity atoms can take up two different types of site, as illustrated (figure 2.2) :

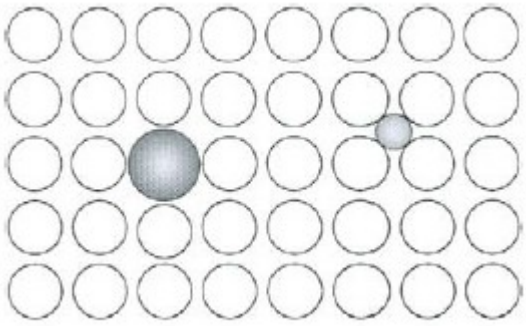


Figure 2.2 - *Substitutional and interstitial impurity atoms*

- Substitutional impurity atom, in which an atom of the parent lattice lying in a lattice site is replaced by the impurity atom.
- Interstitial impurity atom, in which the impurity atom is at a non-lattice site similar to the self-interstitial atoms referred to above.

All the point defects mentioned produce a local distortion in the otherwise perfect lattice. The amount of distortion and hence the amount of additional energy in the lattice due to the defects depends on the amount of "*space*" between the atoms in the lattice and the "*size*" of the atoms introduced.

The interstice sites between atoms generally have volumes of less than one atomic volume, and the interstitial atoms therefore tend to produce large distortions among the surrounding atoms. That's why the formation energy for interstitial atoms takes large volumes, and can result in crystal volume increases as large as several atomic volumes per interstitial atom.

Additional effects are important when the removal of addition of atoms changes the local electric charge in the lattice.

2.1.2-Experimental evidence of existence of dislocations.

From the perspective of mechanical properties, the dislocation is perhaps the most important crystalline defect. These are essentially lines through a crystal along which there is a systematic error in the way the atoms are arranged. Although there are many techniques now available for the direct observation of dislocations, the existence of these line defects was deduced by inference in the early stages of dislocation study. Strong evidence arose from attempts to reconcile theoretical and experimental values of the applied shear stress required to plastically deform a single crystal. This deformation occurs by atomic planes sliding over each other. In a perfect crystal, in the absence of dislocations, the sliding of one plane past and adjacent plane would have to be a rigid co-operative movement of all the atoms from one position of perfect registry to another. The shear stress required for this process was first calculated by Frenkel in 1926. The situation illustrated in the following scheme (figure 2.3) :

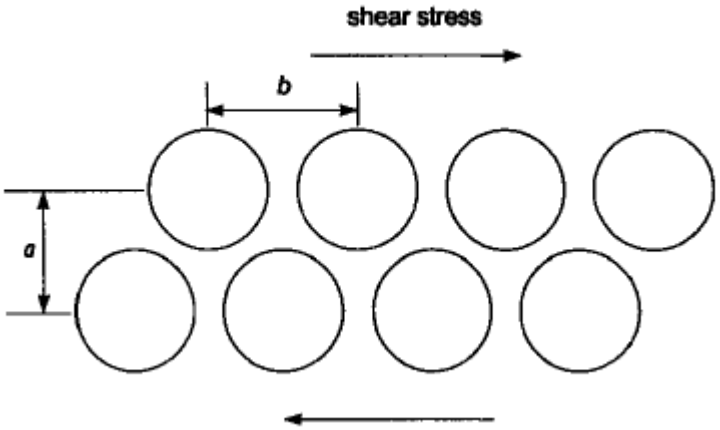


Figure 2.3 - *Representation of atom position used to estimate the theoretical shear stress for slip*

It is assumed that there is a periodic shearing force required to move the top row of atoms across the bottom row which is given by the sinusoidal relation:

$$\tau = \frac{Gb}{2\pi a}\sin\frac{2\pi x}{b} \qquad (2.2)$$

Where τ is the applied shear stress, G is the shear modulus, b the spacing between atoms in the direction of the shear stress, a the spacing of the rows of atoms and x is the shear translation of the two rows away from the low-energy equilibrium position.

The maximum value of τ is then the theoretical critical shear stress and is:

$$\tau_{th} = \frac{b}{a}\frac{G}{2\pi} \qquad (2.3)$$

Since b ≈ a, the theoretical shear strength is a sizeable fraction of the shear modulus. Using more realistic expressions for the force as a function of shear displacement, values of $\tau_{th} \approx G/30$ have been obtained. Although these are approximate calculations, they show that τ_{th} is many orders of magnitude greater than observed values (10^{-4} to 10^{-8} G) of the resolved shear stress for slip measured in real, well-annealed crystals. This striking difference between prediction and experiment was accounted for by the presence of dislocations independently by Orowan, Polanyi and Taylor in 1934.

Dislocations are now recognized as the primary carriers of plastic deformation in crystalline solids, giving rise to the ductility that makes metals workable and, through their manipulation and entanglement, to the work hardening that makes those same metals strong.

2.2- GEOMETRY OF DISLOCATION.

The basic geometries of dislocations are the edge and screw dislocation.

Edge dislocation

An edge dislocation is a defect where an extra half-plane of atoms is introduced mid way through the crystal, distorting nearby planes of atoms. When enough force is applied from one side of the crystal structure, this extra plane passes through planes of atoms breaking and joining bonds with them until it reaches the grain boundary.

A schematic example of an edge dislocation is showed below (figure 2.4) :

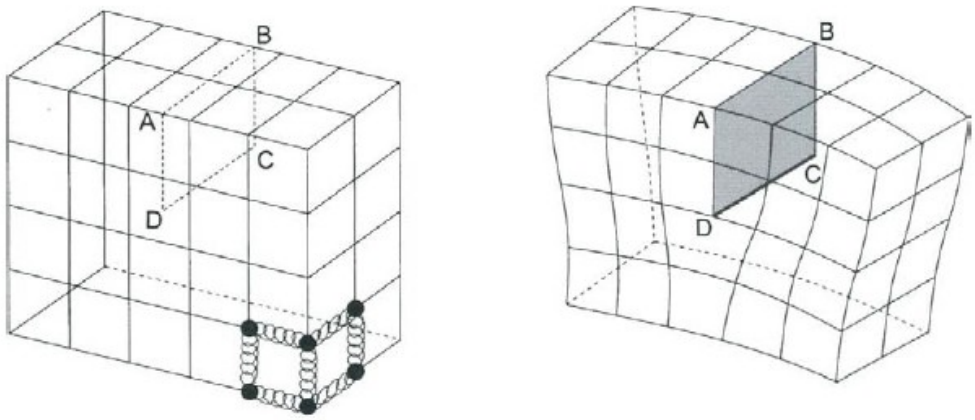


Figure 2.4 - *Model of a simple cubic lattice and representation of an edge dislocation*

The arrangement of atoms around an edge dislocation can be simulated by the following sequence of operations. Suppose that all the bonds across the surface *ABCD* are broken and the faces of the crystal are separated so that an extra half-plane of atoms can be inserted in the slot, as illustrated in figure 2.4. The faces of the slot will be displaced by one atom spacing, but the only large disturbance of the atoms from their normal position relative to their neighbors is close to the line *DC*. The deflection and distortion of the interatomic bonds decrease with increasing distance from the line. This line *DC* is called a *positive edge dislocation*. A *negative edge dislocation* would be obtained by inserting the extra plane of atoms below plane *ABCD*.

Screw dislocation

A screw dislocation is much more harder to visulaize.

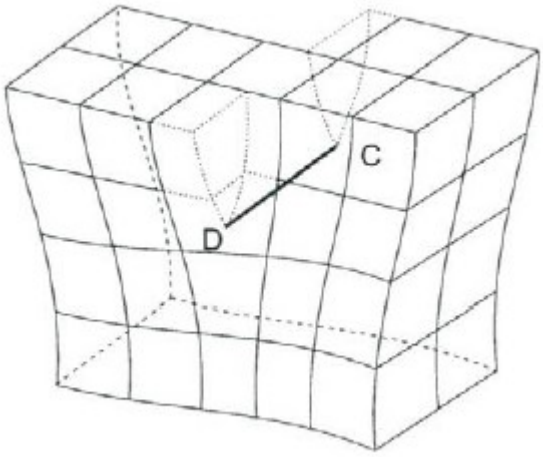


Figure 2.5 - *Left-handed screw dislocation*

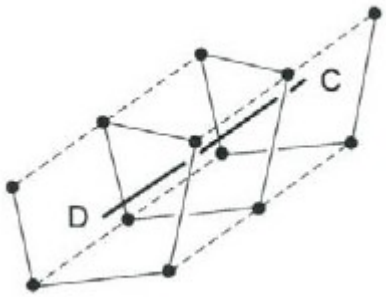


Figure 2.6 - *Spiral of atoms adjacent to the line DC*

The arrangement of atoms round a screw dislocation can be simulated by displacing the crystal on one side of ABCD relative to the other side in the direction AB as in figure 2.6. The set of parallel planes initially perpendicular to *DC* have been transformed into a single surface, and the spiral nature is clearly demonstrated by the atom position shown in Figure 2.6. In this figure DC is a screw dislocation. Looking down the

dislocation line, if the helix advances one plane when a clockwise circuit is made around it, it is referred to as a right-handed screw dislocation, and if the reverse is true it is left-handed.

Actually, edge and screw dislocations are just extreme forms of the possible dislocation structures that can occur. Most dislocations are a hybrid of the edge and screw forms.

2.3- BURGUERS VECTOR AND BURGERS CIRCUIT

The most useful definition of a dislocation is given in terms of the Burgers circuit. A burgers circuit is any atom-to-atom path taken in a crystal containing dislocations which forms a closed loop. Such a path, *MNOPQ*, is illustrated in the following figure (figure 2.7) :

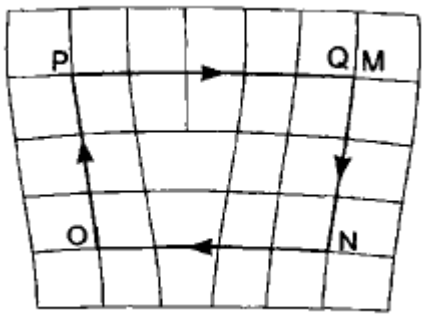


Figure 2.7 - *Burger circuit round an edge dislocation*

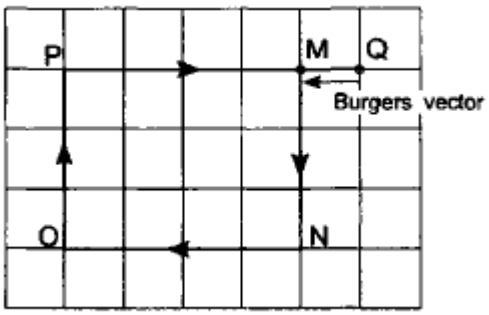


Figure 2.8 - *The same circuit of figure 2.7 in a perfect crystal*

If the same atom-to-atom sequence is made in a dislocation-free crystal, as in figure 2.8, and the circuit does not close, then the first circuit, the one showed in figure 2.7, must enclose one or more dislocations. The vector required to complete the circuit is called the Burgers vector.

- The Burgers vector of an edge dislocation is normal to the line of the dislocation.
- The Burgers vector of a screw dislocation is parallel to the line of the dislocation.

In the most general case the dislocation line lies at an arbitrary angle to its Burgers vector and the dislocation line has a mixed edge and screw character. However, the Burgers vector of a single dislocation has fixed length and direction, and is independent of the position and orientation of the dislocation line.

Burgers circuit taken around other defects, such as vacancies and interstitials, do not lead to closure failures. Two roles are used defining Burgers vectors and Burger circuits.

First, when looking along the dislocation line, which defines the positive line sense or direction of the dislocation, the circuit is taken in a clockwise fashion. Second, the Burgers vector is taken to run from the finish to the star point of the reference circuit in the perfect crystal. This defines the right-hand/finish-start (RH/FS) convention. Reversing the line sense reverses the direction of the Burgers vector for a given dislocation.

Furthermore, dislocations with the same line sense but opposite Burgers vectors (or alternatively with opposite line senses and the same Burgers vector) are physical opposites. Dislocations which are physical opposites of each other annihilate and restore perfect crystal if brought together. The Burgers vector b is conveniently described using Miller's indices.

Dislocations lines can end at the surface of a crystal and at grain boundaries, but never inside a crystal. Thus, dislocations must either form closed loops or branch into other dislocations. When three or more dislocations meet at a point, or node, it is a necessary condition that the Burgers vector is conserved.

A schematic example of this condition is shown (figure 2.9) :

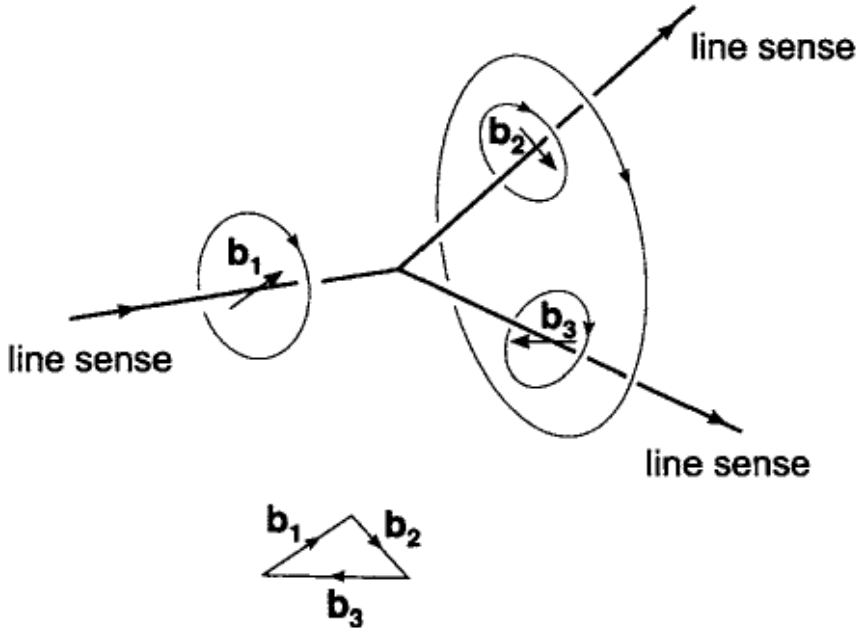


Figure 2.9 - *Three dislocations forming a node and Burgers' conservation condition*

The mathematical expression of this condition can be expressed :

$$b_1 = b_2 + b_3 \qquad (2.4)$$

The dislocation density ρ is defined as the total length of dislocation line per unit volume of crystal. An alternative definition, which is sometimes more convenient to use, is the number of dislocations intersecting a unit area, again measured in units of m^{-2}. If all the dislocations are parallel, the two density values are the same, but for a completely random arrangement the volume density is twice the surface density.

The average distance between dislocations in a network of density ρ is of the order of $1/\sqrt{\rho}$.

2.4-MOVEMENT OF DISLOCATIONS

There are two basic types of dislocation movement. Glide or conservative motion occurs when the dislocation moves in the surface which contains both its line and Burgers vector. Climb or non-conservative motion occurs when the dislocation moves out of the glide surface, and thus normal to the Burgers vector.

2.4.1-Concept of slip

Glide of many dislocations results in slip, which is the most common manifestation of plastic deformation in crystalline solids. It can be envisaged as sliding or successive displacement of one plane of atoms over another on so-called slip planes. This is uniquely defined as the plane which contains both the line and the Burgers vector of the dislocation.

Further deformation occurs either by more movement on existing slip planes or by the formation of new slip planes.

The slip planes are normally the planes with the highest density of atoms, and the direction of slip is the shortest lattice translation vectors. Often, this direction is one in which the atoms are most closely spaced.

A slip plane and a slip direction in the plane constitute a slip system.

Slip results in the formation of steps on the surface of the crystal. The slip direction is necessarily always parallel to the Burgers vector of the

dislocation responsible for slip. The movement of one dislocation across the slip plane to the surface of the crystal produces a surface slip step equal to the Burgers vector.

A characteristic shear stress is required for slip. It can be schematically shown (figure 2.10) :

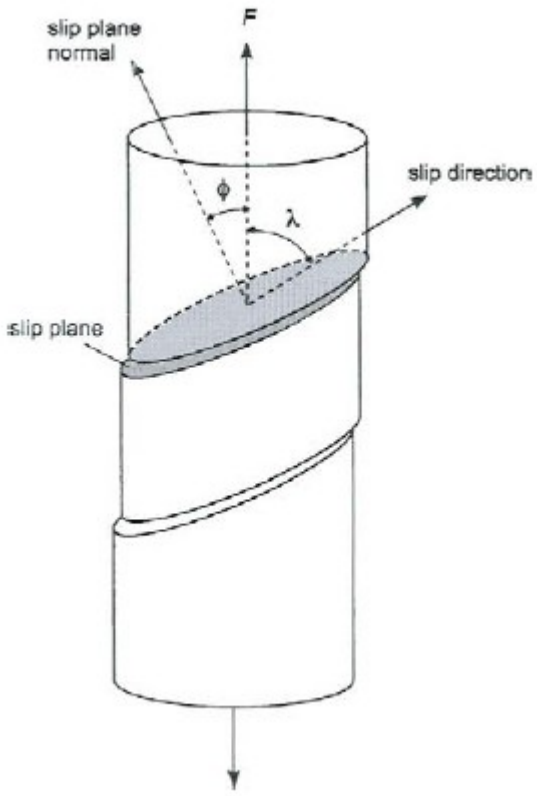


Figure 2.10 - *Illustration of the geometry of slip in crystalline materials*

The illustrated crystal is being deformed in tension by an applied force F along the axis of the cylindrical crystal. The cross sectional Area is A and so the tensile stress parallel to F is :

$$\sigma = \frac{F}{A} \qquad (2.5)$$

The force has a component $F\cos\lambda$ in the slip direction, where λ is the angle between F and the slip direction. This force acts over the slip surface which has an area $A/\cos\phi$, where ϕ is the angle between F and the normal to the slip plane. Thus the *shear stress* τ, resolved on the slip plane in the slip direction, is :

$$\tau = \frac{F}{A}\cos\phi\cos\lambda \qquad (2.6)$$

If F_c is the tensile force required to start slip, the corresponding value of the shear stress τ_c is called the critical resolved shear stress for slip. It has been found in some crystals which deform on a single slip system that τ_c is independent of the orientation of the crystal.

2.4.2- DISLOCATIONS AND SLIP.

With the concept of slip just introduced, dislocation can be defned as the boundary between the slipped and unslipped parts of the crystal. As showed in chapter 2.1.2, the theoretical shear stress for slip was many times greater than the experimentally observed stress. The low value can be accounted for by the movement of dislocations.

Only a relatively small applied stress is required to move the dislocation along the slip plane, as it is demonstrated in the following scheme for an edge dislocation (figure 2.11) :

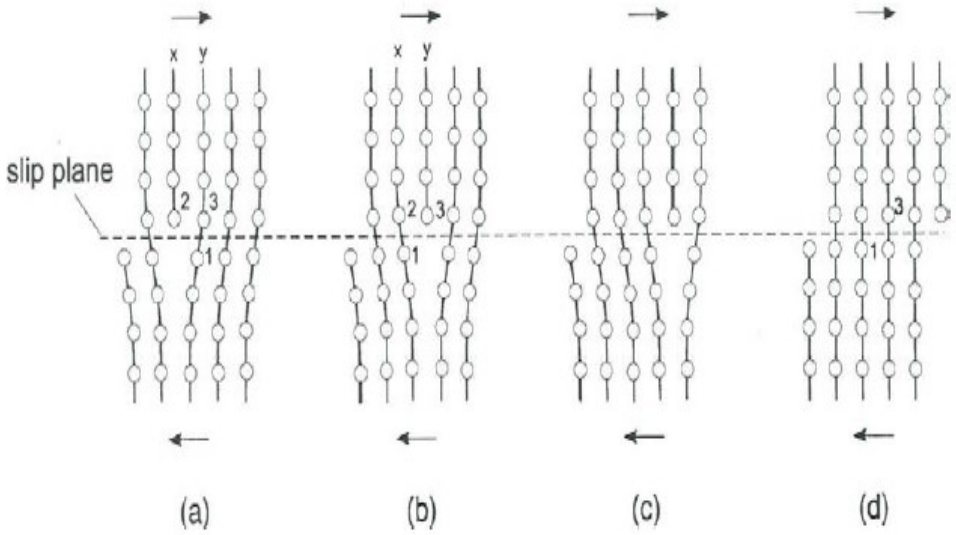


Figure 2.11 - *Movement of an edge dislocation*

where the arrow indicate the applied shear stress.

Well away from the dislocation, the atom spacing are close to the perfect crystal values, and a shear stress as high as the theoretical value (2.3) would be required to slide them all past each other. Near the dislocation line itself, some atom spacing are far away from the ideal values, and small relative changes in position of only a few of atoms are required for the dislocation to move. Thus the applied stress required to overcome the lattice resistance to the movement of the dislocation is much more smaller than the theoretical shear stress of a perfect lattice, due to the successive glide of the extra half-plane.

It is also possible to see that two neighbouring atoms on sites adjacent across the slip plane, like the atoms "1" and "3" in figure 2.11, are displaced relative to each other by the Burgers vector when the

dislocation glides past. The global effect of many thousands of such dislocations is a surface step on the material (figure 2.12) :

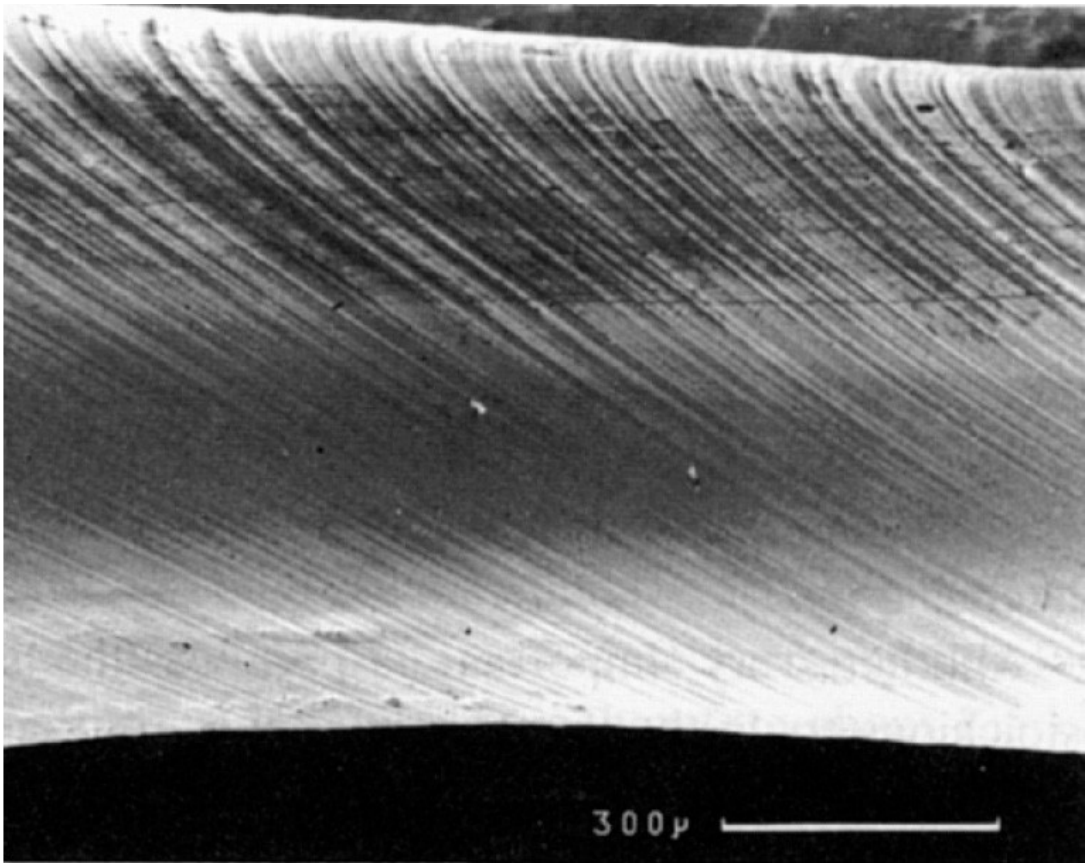


Figure 2.12 - *Single crystal of cadmium deforming by dislocation slip, forming steps on the surface*

It is important to remark two particular rule for dislocation glide :

- dislocations of opposite sign glide in opposite directions under the same stress

- for dislocation glide a shear stress must act on the slip plane in the direction of the Burgers vector, irrespective of the direction of the dislocation line

Those properties are schematically shown for an edge and screw dislocation (figure 2.13 and 2.14) :

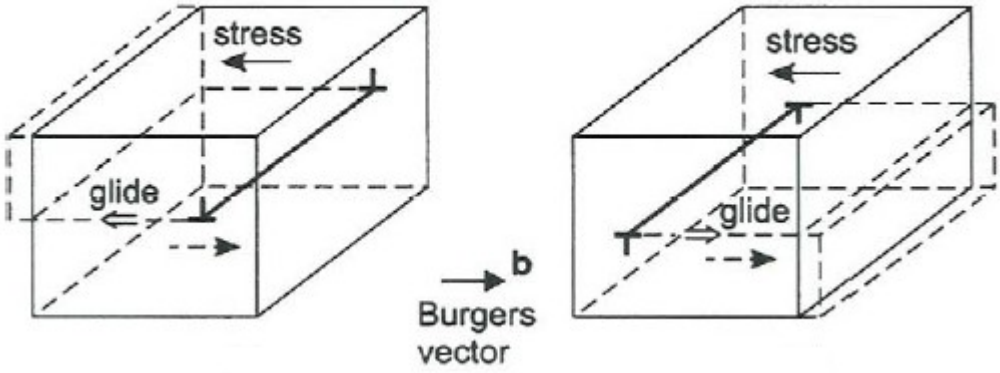


Figure 2.13 - *Plastic deformation by glide of edge dislocation under the applied shear stress*

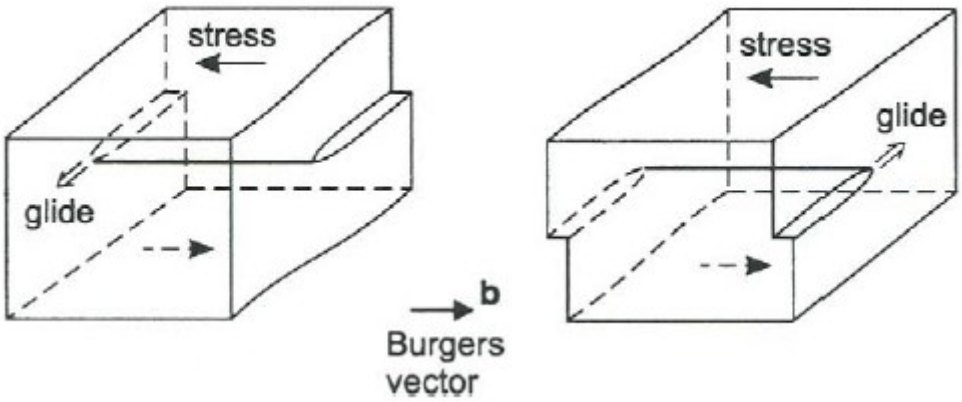


Figure 2.14 - *Plastic deformation by glide of screw dislocation under the applied shear stress*

2.5-CLIMB

At low temperatures where diffusion is difficult, and in the absence of a non-equilibrium concentration of point defects, the movement of dislocations is restricted almost entirely to glide. However, at higher temperatures and edge dislocation can move out of its slip plane by a process called climb (figure 2.15) :

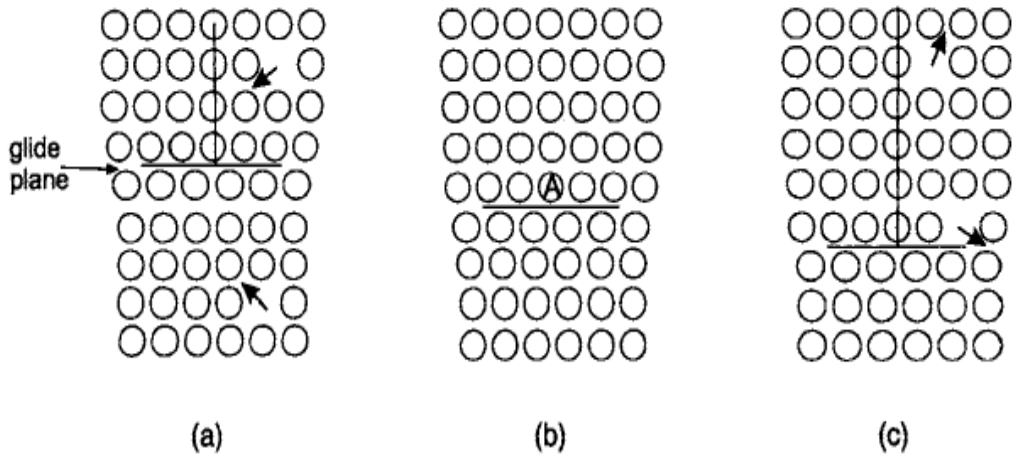


Figure 2.15 - *Positive and negative climb of an edge dislocation*

The row of atoms *A* normal to the plane of the diagram is removed, the dislocation line moves up one atom spacing out of its original slip plane: this is called positive climb. Similarly, if a row of atoms is introduced below the extra half-plane the dislocation line moves down one atom spacing, negative climb. For this kind of movements, volumes

are not conserved. The mass transport involved occurs by diffusion and therefore climb requires thermal activation.

It has been implied above that a complete row of atoms is removed simultaneously, whereas in practice individual vacancies or small clusters of vacancies diffuse to the dislocation. The effect of this is that the climb of a short section of a dislocation line results in the formation of two steps called jogs (figure 2.16) :

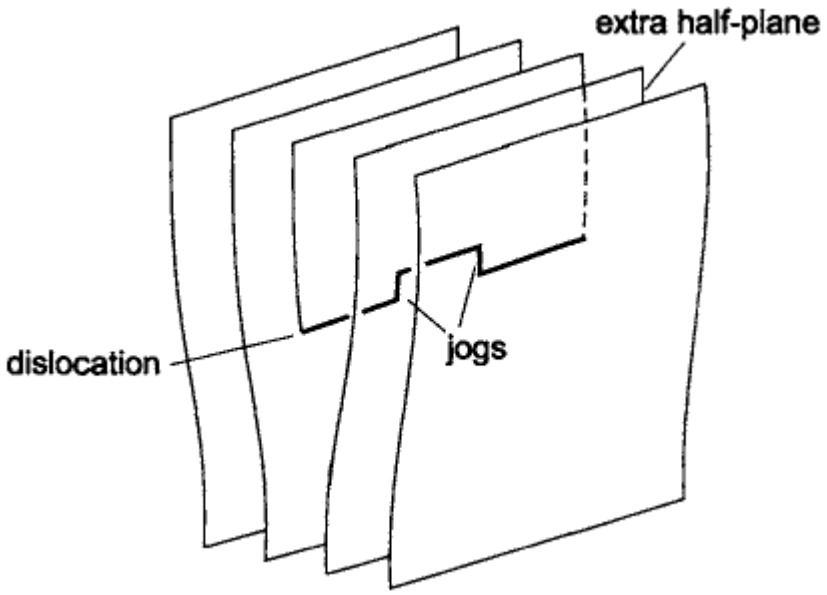


Figure 2.16 - *Single jogs on an edge dislocation*

Both positive and negative climb proceeds by the nucleation and motion of jogs. Conversely, jogs are sources and sinks for vacancies.

Jogs are steps on the dislocation which move it from one atomic slip plane to another. Steps which displace it on the same slip plane are

called kinks. The two are distinguished below for and edge and screw dislocation (figure 2.17 and 2.18) :

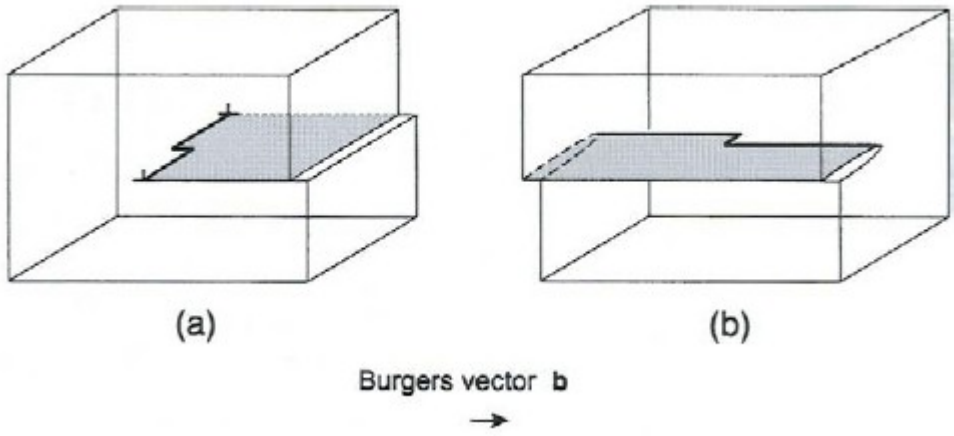


Figure 2.17 - *Kinks in edge (a) and screw(b) dislocation*

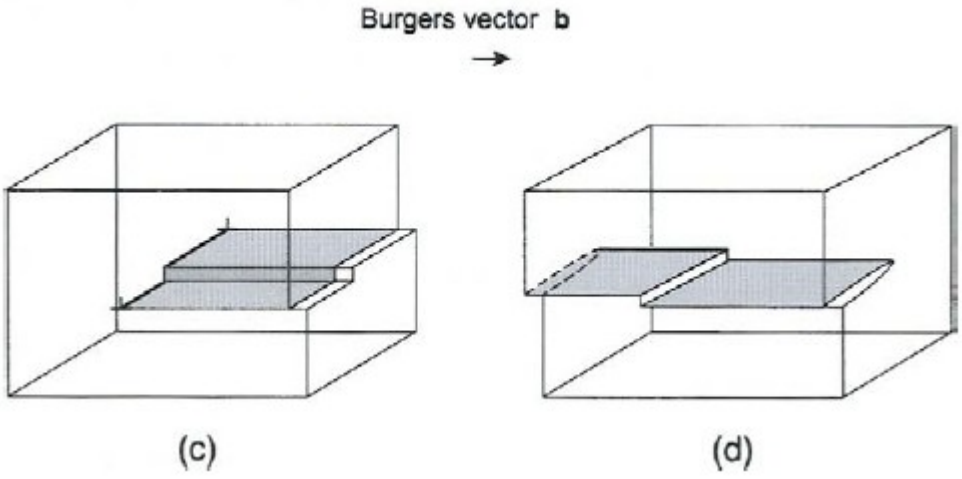


Figure 2.18 - *Jogs in edge (c) and screw (d) dislocation*

Jogs and kinks are short elements of dislocation with the same Burgers vector as the line on which they lie, and the usual rules apply for their conservative and non-conservative movements.