DEFECTS IN CRYSTALS

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Defects in Crystals-II

The Frenkel defect and Schotkey defects together are called as intrinsic defects

77.13.3 Impurities

Impurities give rise to compositional defects. Impurities may be small particles (such as slag inclusions in metals) embedded in the structure, or foreign (metal) atoms in the lattice. Foreign atoms generally have atomic radii and electronic structures differing from those of the host atoms and therefore act as centres of distortion. Impurities may considerably distort the lattice.

There are two types of impurity defects.

(*i*) **Substitutional impurity.** A substitutional impurity refers to a foreign atom that substitutes for or replaces a parent atom in the lattice (Fig. 77.*29*).

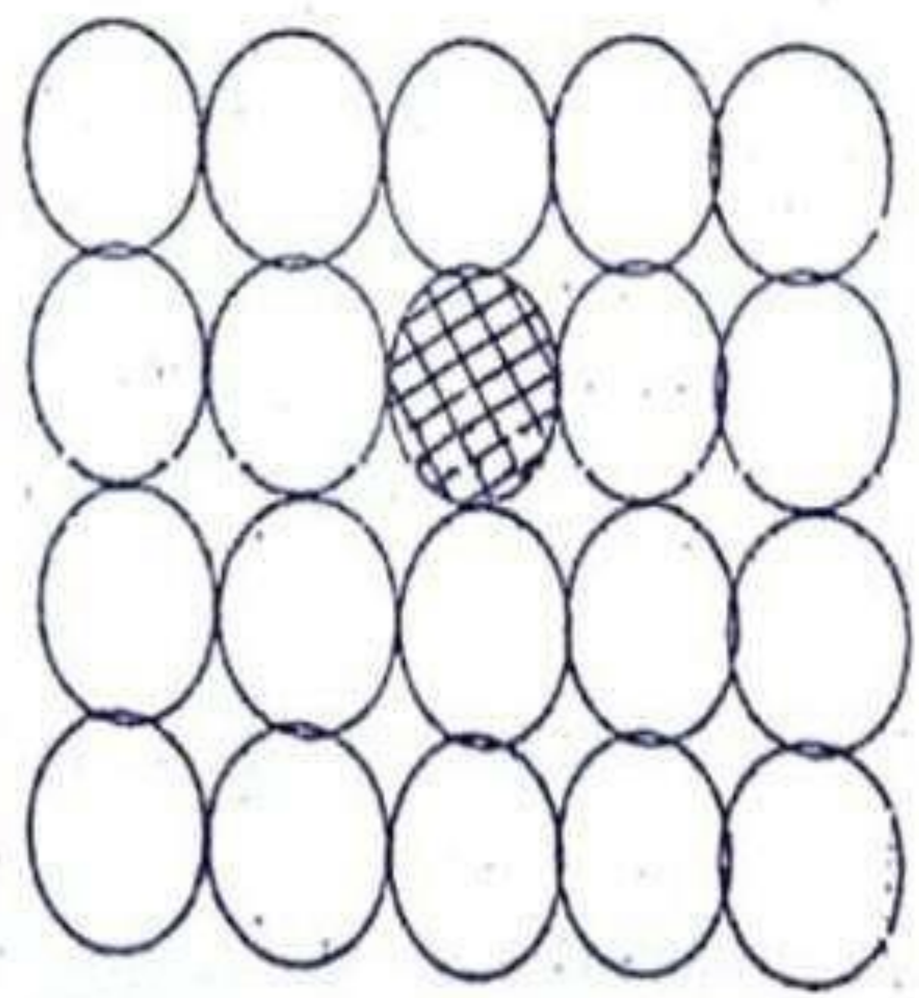


Fig. 77.29

EXAMPLES. 1. In ionic solids (e.g., in NaCl), the substitution of Na^+ by Li^+ produces a substitutional impurity.

2. In semiconductor technology, aluminium and phosphorus doped in silicon are substitutional impurities in the crystal.

A controlled addition of impurity to a very pure crystal is the basis of producing many electronic devices.

(ii) Interstitial impurity

An interstitial impurity is a small sized atom occupying the void space in the parent crystal, without dislodging any of the parent atoms from their sites (Fig. 77.30).

An atom can enter the interstitial or void space only when it is substantially smaller than the parent atom.

EXAMPLE. In FCC iron, the atomic radius of iron atom is 0.225 nm. Carbon atoms with atomic radius 0.0777 nm can occupy the octahedral void spaces in FCC lattice as interstitial impurities.

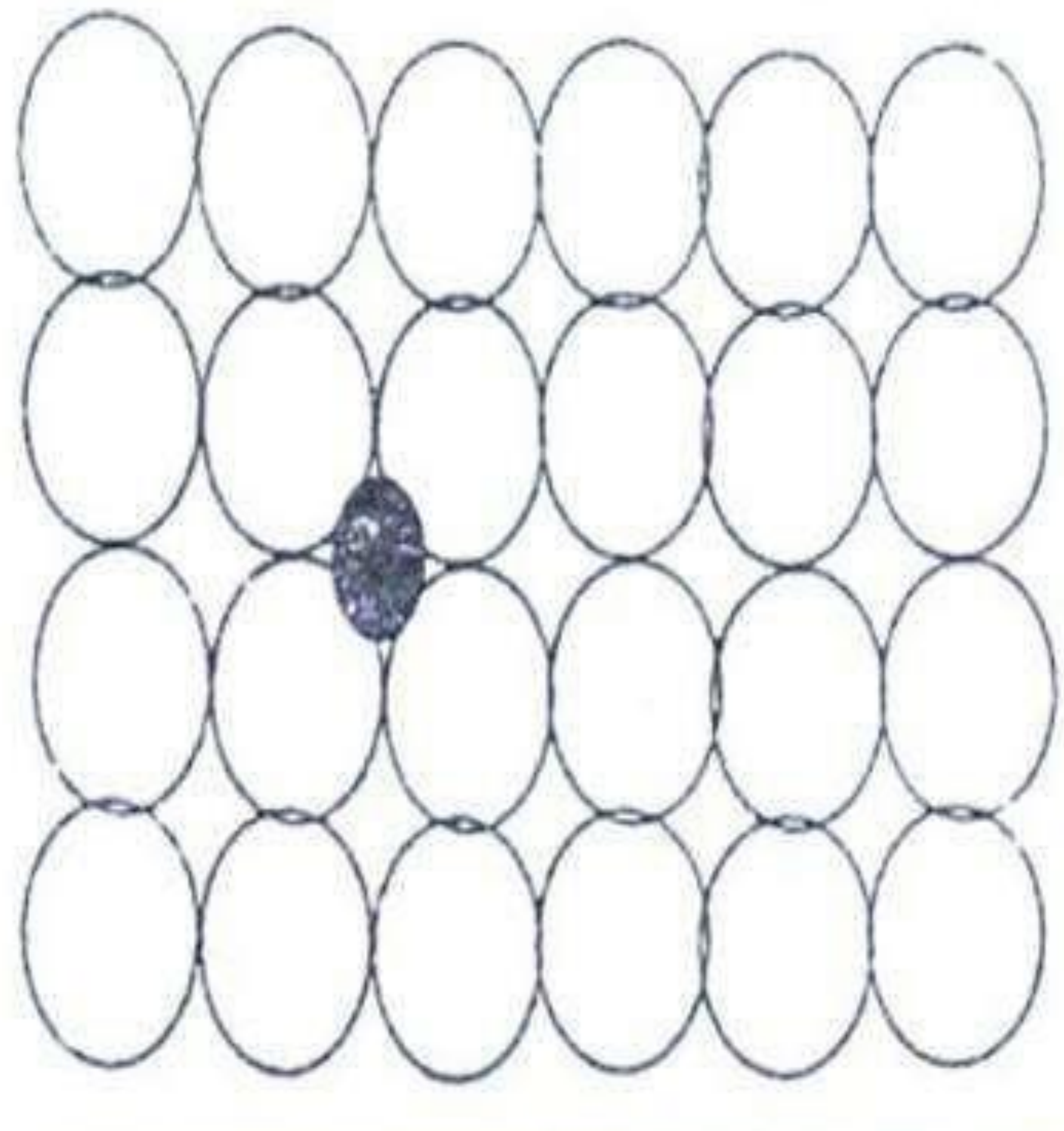


Fig. 77.30

77.13.4 Electronic Defects

Electronic defects are the result of errors in charge distribution in solids.

These defects are free to move in the crystal under the influence of an electrical field. This accounts for some electronic conductivity of certain solids and their increased reactivity.

EXAMPLE. In zinc oxide (ZnO), the zinc ions occupy interstitials. This leads to a large number of positive charges at interstitials. Suppose in some places zinc ions are missing. Then, at these places, there is a gain of negative charges due to loss of positive charges. Thus a vacancy or an interstitial impurity may produce an excess or deficiency of positive or negative charges.

77.17 Line Defects

Line defects are called dislocations. These are one-dimensional imperfections in the geometrica sense. A *dislocation* may be defined as a disturbed region between two substantially perfect parts c a crystal (Fig. 77.33).

Dislocation is a line defect in a crystal structure whereby a part-plane of atoms is displaced fror its symmetrically stable positions in the array. It is surrounded within the structure by an extensiv elastic strain field and its associated stresses.

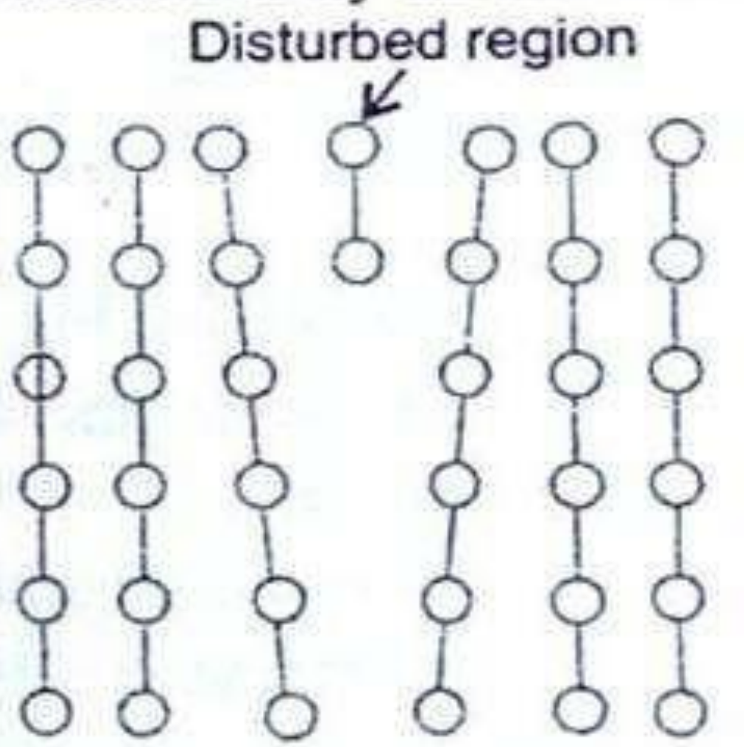


Fig. 77.33

There are two basic types of dislocations :

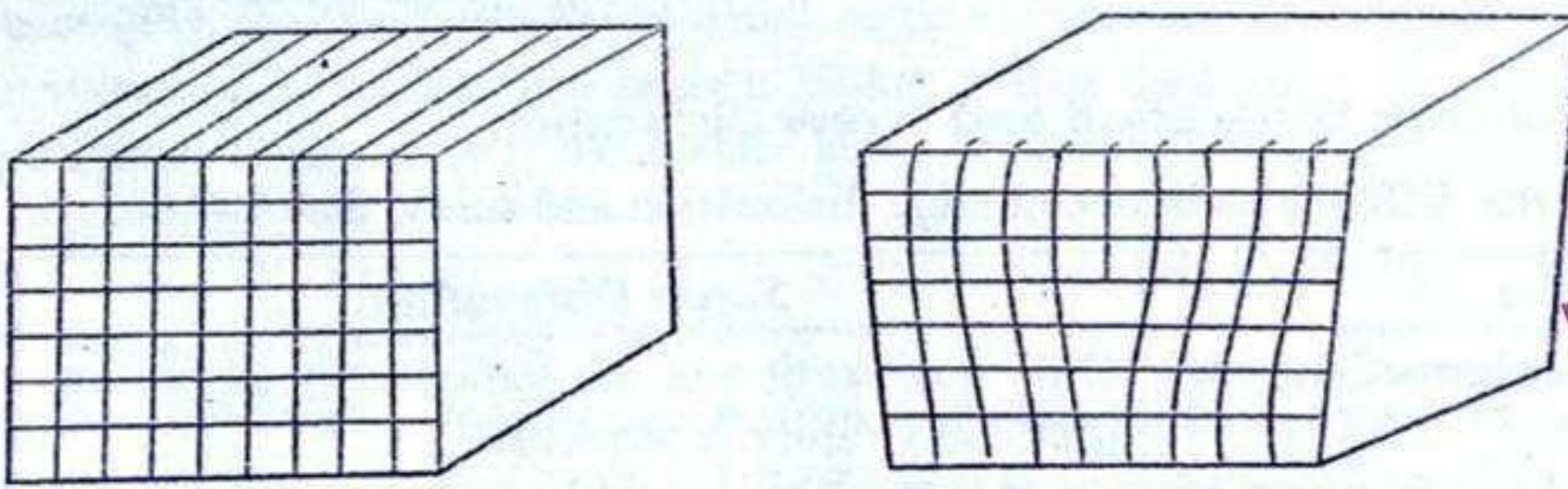
1. Edge dislocation, and
2. Screw dislocation

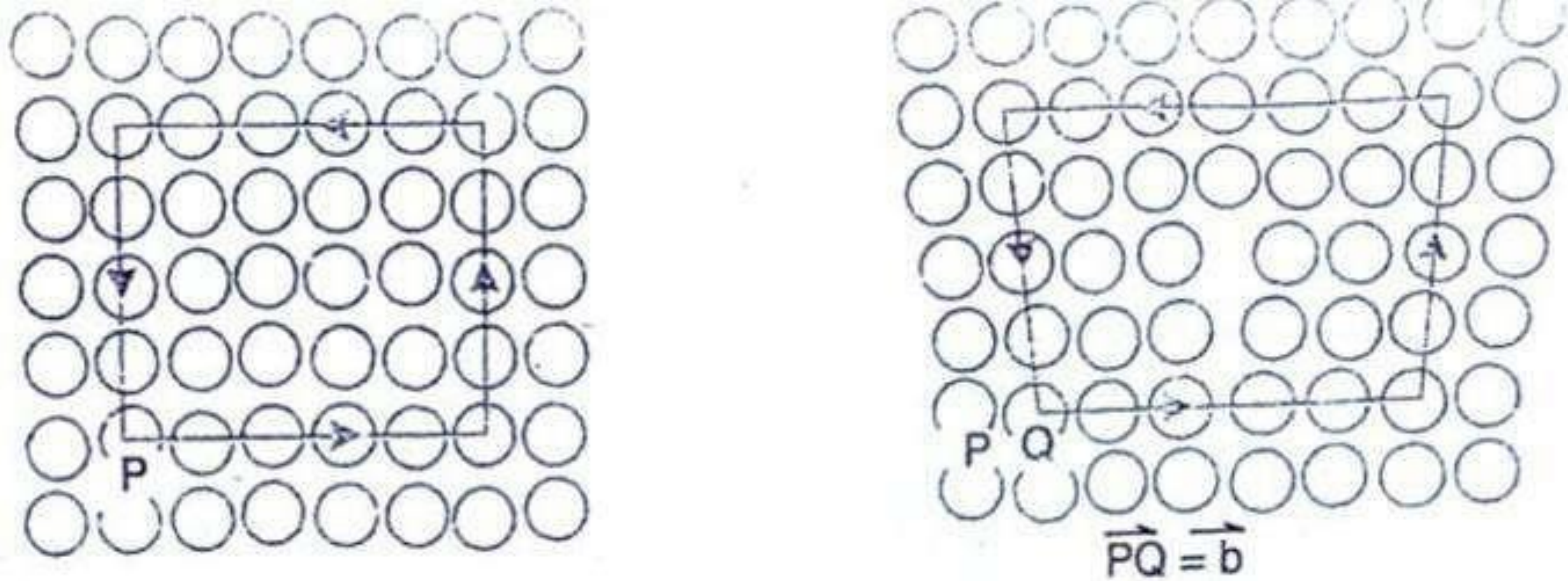
77.17.1 Edge Dislocation

Fig. 77.34 (a) shows a perfect crystal.

The top sketch shows a three dimensional view of a perfect crystal.

The bottom sketch shows the arrangement of atoms on its front face.





(a) (b)

Fig. 77.34

Fig. 77.34 (b) shows an imperfect crystal.

The top sketch shows a three dimensional view of an imperfect crystal with an edge dislocation.

The bottom sketch shows the arrangement of atoms on its front face. The atoms above the edge of the extra plane are squeezed together and are in a state of compression. The bond lengths have been compressed to smaller than the equilibrium value. Just below the edge of the extraplane, the atoms are pulled apart and are in a state of tension. Here the bond lengths have been stretched to above the normal values. This distorted configuration extends all along the edge into the crystal. There is an extra energy due to the distortion in the region immediately surrounding the edge of the incomplete plane. As the region of maximum distortion is centred around the edge of the incomplete plane, this distortion represents a line imperfection and is called an *edge dislocation*.

The vector $\vec{b} = \overline{PQ}$ connecting the end point Q with the starting point P is the Burgers vector of the dislocation.

Defects in Crystals-III

Edge dislocation can be classified as *positive edge dislocation* and *negative edge dislocation*.

An edge dislocation involves an extra row of atoms, either above (positive sign) or below (negative sign) the slip plane (Fig. 77.35).

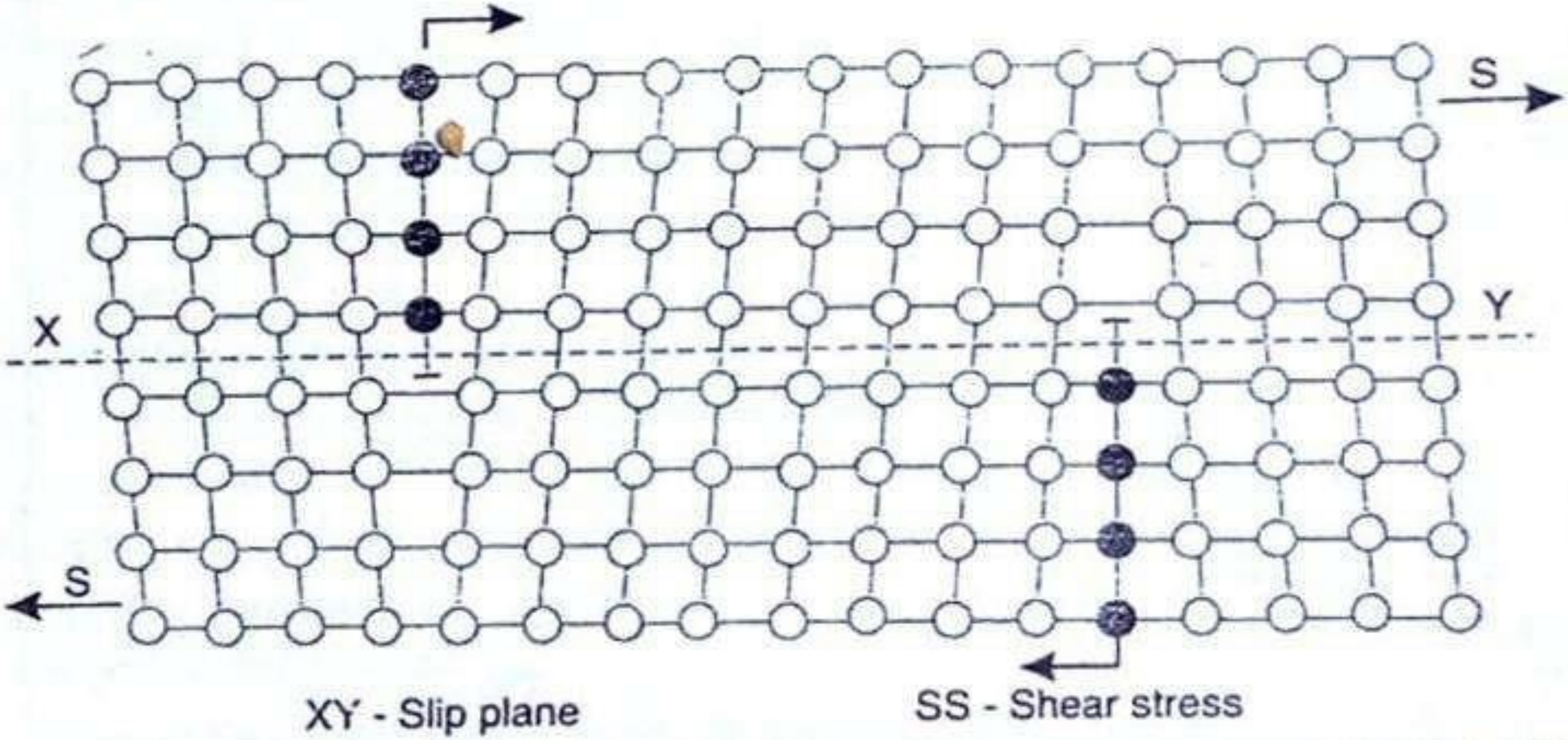


Fig. 77.35

The horizontal line *XY* is called the slip plane.

(i) Positive dislocation

If an extra plane of atoms is above the line *XY*, the edge dislocation is said to be positive. It is denoted by the symbol ⊥ .

(ii) Negative dislocation

If an extra plane of atoms is below the line *XY*, the dislocation is said to be negative. It is denoted by the symbol *T*.

The presence of an extra plane of atoms means that adjacent atoms are displaced elastically. Consequently, from both sides elastic forces are exerted on the dislocation. These forces balance out, so that it is easy to move the dislocation from one position to another.

Under a shear stress sense $\rightleftharpoons$ a positive dislocation ($\perp$) moves to the right and a negative dislocation (T) to the left (Fig. 77.35).

Slip caused by the movement of edge dislocation

Fig. 77.36 shows how edge dislocation (*D*) gets glided along the slip plane under the action of shear stress (*S*) and how the slip is caused by the movement of an edge dislocation.

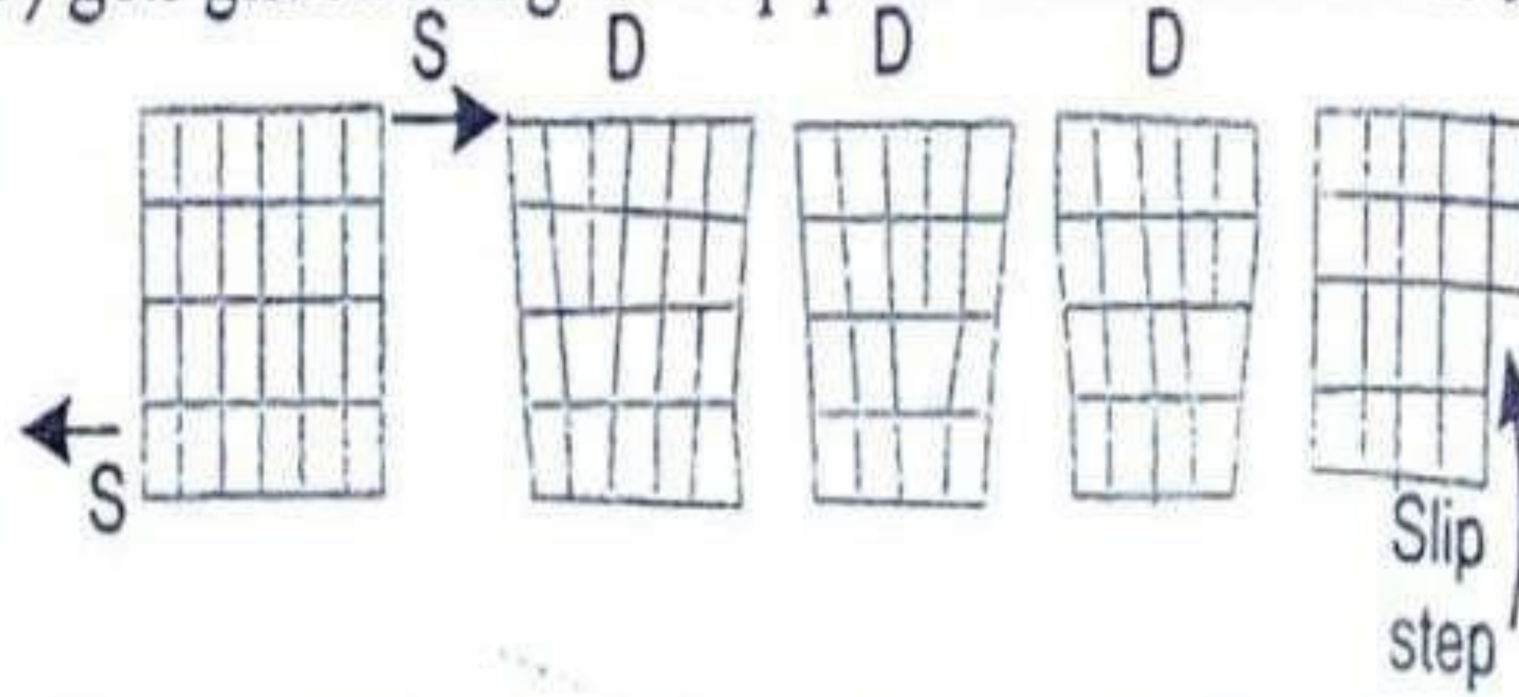


Fig. 77.36

As the dislocation glides out of the crystal completely, it produces a *slip step* of one atom width at the edge of the crystal.

The edge dislocation is particularly useful in explaining slip in plastic flow during mechanical working.

77.17.3 Burger's Vector

The Burger's vector indicates how much and in what direction the lattice above the slip plane appears to have been shifted with respect to the lattice below the slip plane. The Burger's vector is perpendicular to the edge dislocation.

Burger's Vector marks the magnitude and direction of the strain component of dislocation.

Method of determining Burger's Vector for Edge Dislocation

Fig. 77.37 shows the method of determining the Burger's Vector.

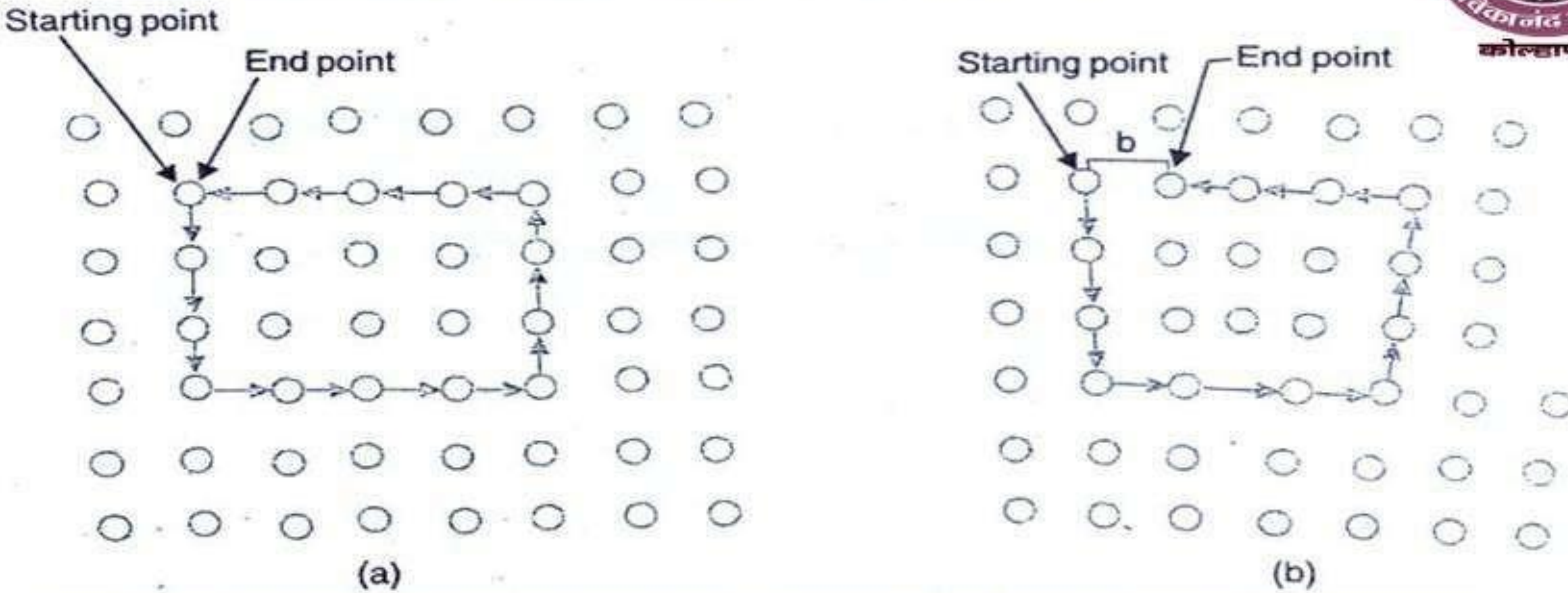


Fig. 77.37

The Burger's circuit is formed by proceeding through the undisturbed region surrounding a dislocation in steps which are integral multiples of a lattice translation. The loop is completed by going an equal number of translations in a positive sense and negative sense in a plane normal to the dislocation line.

(*i*) The Burger's loop closes upon itself if it does not enclose a dislocation [Fig. 77.37 (a)].

(*ii*) The Burger's circuit surrounding an edge dislocation is shown in Fig. 77.37 (b). The end point does not coincide with the starting point.

77.17.4 Screw Dislocation

Screw dislocation results from a displacement of the atoms in one part of a crystal relative to the rest of the crystal, forming a spiral ramp around the dislocation line.

Fig. 77.38 shows what happens when one part of the crystal is displaced relative to the rest of the crystal and the displacement terminates within the crystal.

The row of atoms marking the termination of the displacement is the screw dislocation. $E F$ indicates the dislocation line.

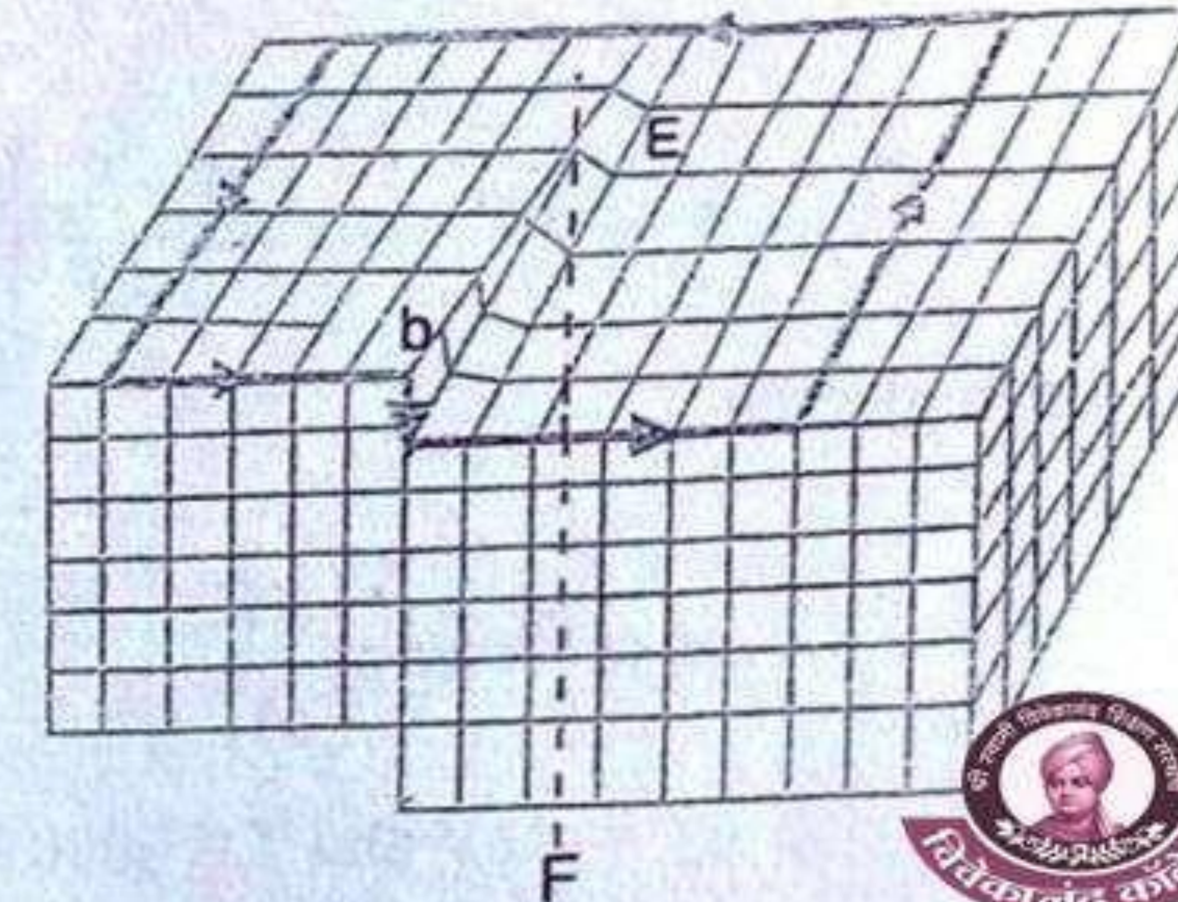


Fig. 77.38

In screw dislocation, the Burger's vector lies *parallel* to the dislocation line along the axis of a line of atoms in the same plane. The Burger's vector (Fig. 77.39) determines the magnitude and direction of the screw dislocation. The screw dislocation may be thought of as produced by cutting the crystal partway through with a knife and shearing it parallel to the edge of the cut by one atom spacing. A screw dislocation transforms successive atom planes into the surface of a helix.

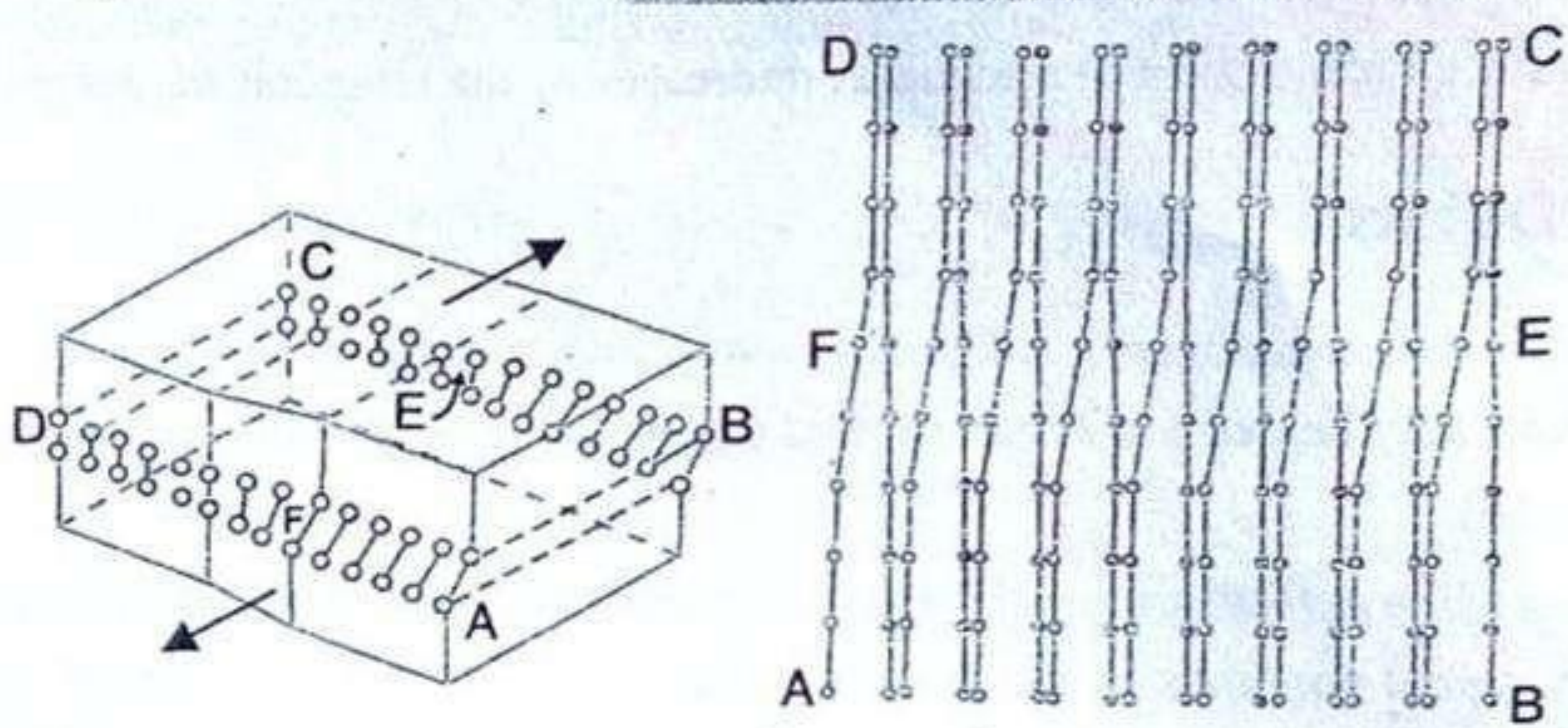


Fig. 77.39