9.6 Dislocations

The small critical shearing strains observed are due to the linear defect of structure, which is called the **dislocation.** Taylor, Arvin, and Pauline proposed concept of dislocations in 1934. They assumed that the sliding is the motion of dislocations.

9.6.1 Edge Dislocations

There are two ideal kinds of dislocations: the edge dislocation and the screw dislocation. The real dislocation is a superposition of those ones. The geometric properties of a dislocation can be easily described when the concepts of ideal dislocations are used. The atomic structure of an edge dislocation is shown in Fig.9.6. The space order of atoms near the edge dislocation in a crystal of a simple cubical structure is shown in Fig.9.7. A glance at the Fig.9.7 shows that the structural distortion is due to the additional atomic plane. The distortion is mainly located hear the low edge of the additional plane. The distortion line along the edge of additional plane is supposed to be a **dislocation.** Thus the dislocation is a linear defect. All strong distortions are concentrated in closest vicinity of a **dislocation line.** At a distance of about several atomic diameters, the distortions are so small that the properties of a crystal at those points can be considered as ideal.

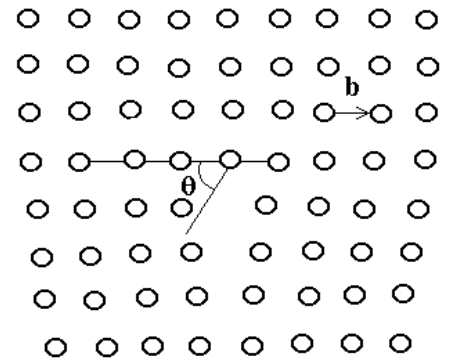


Fig.9.6. Cross-section of a crystal with dislocation

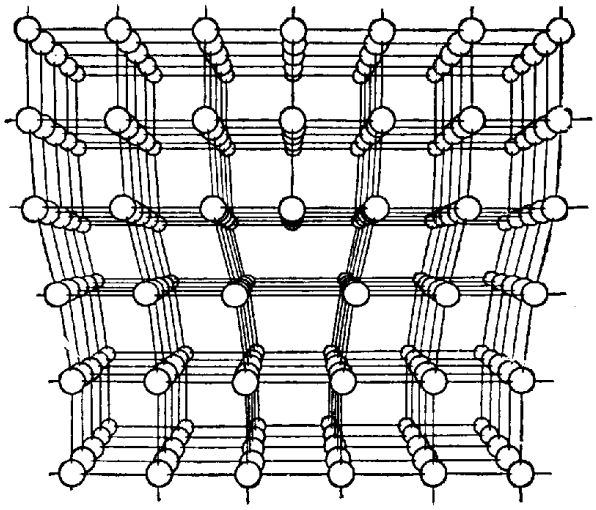


Fig.9.7. The space atomic structure near an edge dislocation in a simple cubical crystal

The dislocation line region where distortions are great is called the **dislocation nucleus.** In that region, the local deformations are great too. At a far distance from the nucleus, the deformations can be considered as small and treated by the theory of elastic deformation. The region far off the nucleus is called the **elastic region.**

The atoms located above the edge of additional plane undergo the action of constricting strains. Two atomic rows (from the left and right of additional plane) are pressed together. In close vicinity above the additional plane, the atomic structure is

lengthened. The local lengthening is called the **dilatation.** The dilatation Δ at a point near the edge dislocation is defined as follows:

$$\Delta = \frac{\Delta V}{V} = \frac{b}{r}\sin\theta. \qquad (9.54)$$

Parameter *b* is a module of the Burgers vector. That quantity characterizes the distortions produced by a dislocation. The quantity *r* is the distance between the given point and dislocation.

9.6.2 Screw Dislocations

The screw dislocation is shown in Fig.9.8. The screw dislocation is a border between the initial and displaced region of a crystal. The border is parallel to the direction of sliding.

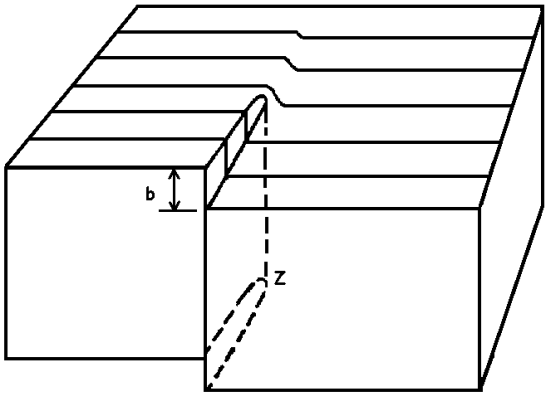


Fig.9.8 A screw dislocation. The height of the step on the upper surface usually is equal to the lattice parameter. The atomic rows that are perpendicular to the dislocation are located on a screw surface.

In order to understand the properties of a screw dislocation let us use the following speculations. Assume that a thin cut of a certain depth is made in crystal. Assume that we shifted one side of the cut upward at one atomic distance and the again unite the cut sides (Fig.9.8). A glance at the figure shows that the distortion line coincides with the cut edge. That line is called the **screw dislocation.**

Thus the structure of atomic planes is changed. There are no more the fully filled planes perpendicular to the dislocation. All atoms are located on the same screw surface, which begins from one edge of a crystal and ends at the other edge. The screw can be of a clockwise or opposite type. The screw step can be from one up to several inter-atomic distances. The step of the dislocation described is one inter-atomic distance.

Analogues to edge dislocations, the distortions depend on the distance from the dislocation center.

The screwing and shearing of the lattice are produced. Atoms located upon a screw surface are displaced from its natural position of an ideal crystal. The displacement correspond to the screw surface equation:

$$u_z = \frac{b}{2\pi}\theta. \qquad (9.54)$$

In Fig.9.8, the z-axis is directed along the dislocation, the quantity u_z is a displacement along that direction. The angle is measured from the axis, which is perpendicular to dislocation. We remind that the vector ***b*** is the Burgers vector.

9.6.3 The Burgers Vector

Let us imagine two crystalline lattices: ideal and with defects. If in a real crystal there are point defects we can establish reciprocal correspondence between atoms of both crystals. In some places of the real lattice there can be no atoms, in some places exec atoms would appear, but in other parts it coincides with the ideal one. The region of a real crystal where reciprocal correspondence can be established is called the

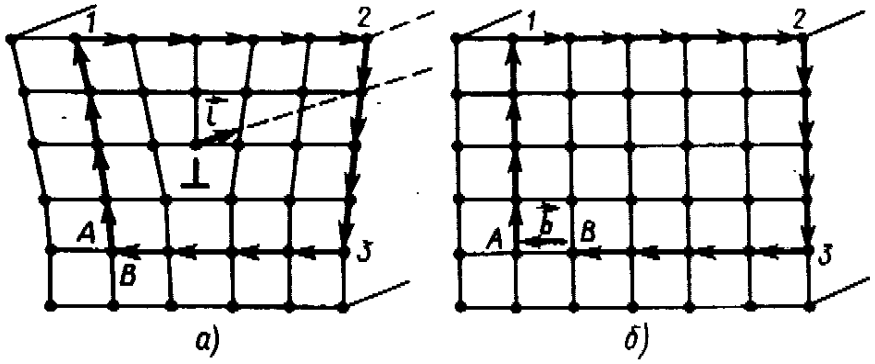


Fig.9.9. the Burgers contour in a real (a) and in ideal (b) crystal. I is the ort tangential to the dislocation line

region of a **good crystal.** The region where it is impossible is called the region of a **bad crystal.**

An arbitrary contour in a real crystal build in the region of a good crystal is called the **Burgers contour.** Using the reciprocal correspondence we can build analogues contour in the ideal crystal. If in the real crystal, the contour is build around a dislocation (Fig.9.9a), the corresponding contour in the ideal crystal would not be closed (Fig.9.9b).

In order to close that contour, a vector ***b*** is needed. That vector is called the **Burgers vector** and represents the vector of shearing. The Burgers contour of a

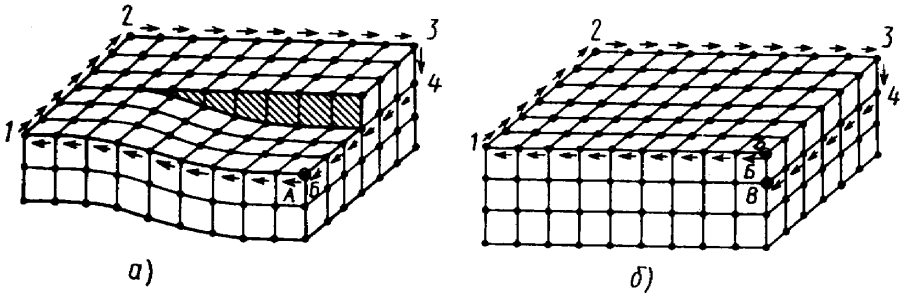


Fig.9.10. the Burgers contour of a screw dislocation: a – real crystal, b – ideal crystal

screw dislocation is shown in Fig.9.10

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

The contour can be displaced, lengthened, or constricted in the direction perpendicular to the dislocation line. The Burgers vector dies not change.

The vector can change if while displacing the contour intersects the ‘bad” region. Thus the Burgers vector of a dislocation is constant and the dislocation can not break inside a crystal. The dislocation can break only on the surface of a crystal, inter-

crystallite border, or the other dislocation. Very often dislocations form close loops or nets inside a crystal.

The Burgers vector of a contour surrounding several dislocations is the sum of vectors of separate dislocations.

$$\vec{b} = \vec{b}_1 + \vec{b}_2 + \vec{b}_3 + \cdots + \vec{b}_n. \tag{9.55}$$

Sometimes that vector can be zero:

$$\sum_1^n \vec{b}_i = 0. \tag{9.56}$$

The others linear defects can be present in a crystal: for example the chains of vacancies or inter-node atoms. The Burgers contour about those point defects is identical to that one of the "good" region, the Burgers vector is zero.

The Burgers vector represents one of the lattice translation vectors. Its module and direction is discrete.

9.6.4 The Strains Needed to Produce a Dislocation in an Ideal Crystal

In order to produce a dislocation, it is necessary to make a shift in a sliding plane.

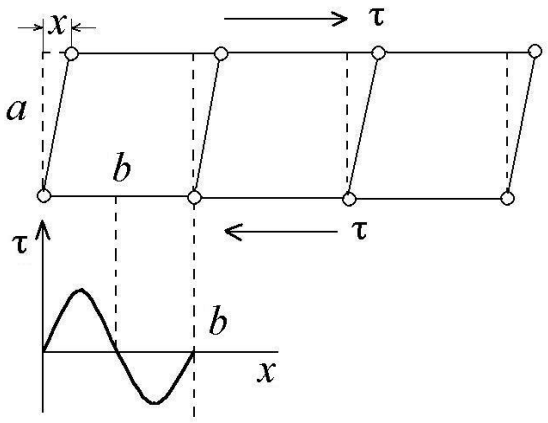


Fig.9.11. **The shearing of a plane relative another plane in a uniformly deformed crystal. The dependence of strain on the plane displacement from their equilibrium position**

Hence, to find the strains needed to build a dislocation, we are to calculate the shearing stability in an ideal crystal.

A simple rectangular lattice is shown in Fig.9.11. While displacing the atomic planes, the shearing strain τ tries to re-establish the equilibrium. The lattice is symmetrical and at $x = nb/2 \quad (n = 0,1,2,\cdots), \quad \tau = 0.$

When $0 < x < b/2, \quad \tau > 0;$ *if* $\quad b/2 < x < b, \quad \tau < 0.$ The following function holds that condition:

$$\tau = k \sin \frac{2\pi x}{b}. \tag{9.57}$$

When displacements are small:

$$\tau = k \frac{2\pi x}{b}. \tag{9.58}$$

In accordance with the Gook law:

$$\tau = G \frac{x}{a} \tag{9.59}$$

G is the shearing module. Hence:

$$k\frac{2\pi x}{b} = G\frac{x}{a}. \tag{9.60}$$

$$k = \frac{b}{a}\cdot\frac{G}{2\pi}. \tag{9.61}$$

Comparing (9.57) and (9.61) we see that the coefficient is a maximal strain of the lattice when $x = b/4$. thus:

$$\sigma_{theoretical} = \frac{bG}{2\pi a}. \tag{9.62}$$

We can write:

$$\sigma_{theoretical} \approx \frac{G}{10}. \tag{9.63}$$

More accurate calculation leads to:

$$\sigma_{theoretical} \approx \frac{G}{30}. \tag{9.64}$$

The experiments show that the shearing in crystals begins at smaller strains: $\sigma = (10^{-4} - 10^{-5})G$. It is due to the fact that the shearing is produced not by displacement of atomic planes relative each other but by sliding of dislocations.

Dislocations are being generated when the crystal grows (for example while hardening the melt). The generation of dislocations is initiated by residual of vacancies while cooling of crystals. When crystals are saturated with vacancies, the cavities and dislocations can form.

The manufacturing of crystals without dislocations is a very difficult task. The dislocation density (the number of dislocation lines, winch intersect a unit square) is $(10^2 - 10^3)\,cm^2$ in qualitative crystals of silicon and germanium and $(10^{11} - 10^{12})\,cm^2$ in strongly deformed metallic crystals.

9.6.4 Energy of Dislocation

Assume that in the process of dislocation generation, the crystal is like an elastic body. Imagine that we make a cutting inside an ideal crystal (analogues to 9.6.3). Let us shift both sides of the cutting relative each other at a distance *b*. The mechanic work done is the energy of dislocation:

$$U_d = \int \vec{F}\vec{b}dS. \tag{9.65}$$

The quantity *dS* is the elementary square of the cutting, $\vec{F}$ is a mean force (per a unit square) acting upon the cutting side while shearing.

Assume that the crystal is a set of coaxial cylinders (Fig9.12).

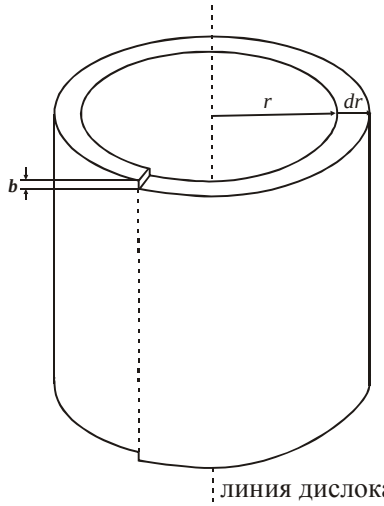


Fig.9.12 **The cylindrical envelope about a dislocation: l– the length, dr – thickness, dz – an elementary shift, a force fldr is applied to the cross-section, ldr – the elementary square, f – the force per a unit square.**

For small shearing deformation, the Gook law is true:

$$\vec{f} = \frac{G\vec{b}}{2\pi r}. \tag{9.66}$$

It is assumed that the force time dependence is linear. Hence:

$$\vec{F} = \left\langle \vec{f}_{av} \right\rangle = \frac{1}{2}\vec{f}_{\max} \tag{9.67}$$

$$\vec{F} = \frac{G\vec{b}}{4\pi r}. \tag{9.68}$$

The dislocation energy:

$$U_d = \int \frac{Gb^2}{4\pi r} dA. \tag{9.69}$$

The energy of a dislocation with the length *l*:

$$U_d = \int_{r_0}^{r_1} \int_0^l \frac{Gb}{4\pi r} dz dr. \tag{9.70}$$

$$U_d = \frac{Gb^2 l}{4\pi} \ln \frac{r_1}{r_0}. \tag{9.71}$$

The interaction between dislocations leads to reciprocal compensation of elastic strains. The deformations diminish at a distance about an average interval between dislocations Experiments show that is about 10^4 inter-atomic intervals. Thus the quantity r_1 is of the same order.

Table 9.2 Elastic modules and dislocation energy

Material	Young's modulus E, $10^{10} N/m^2$	Shear modulus G, $10^{10}\ N/m^2$	U_d (eV) per an inter-atomic interval
Aluminium	2.5	2.85	3.1
Copper	6.0	7.56	5.3
Silver	12.0	4.40	4.5
Diamond	95.0	43.0	29
Germanium	12.9	6.7	18
KCl	4.1	0.6	9.3
Silicon	16.7	7.9	19
Tungsten	50.0	15.1	13

For region at a distance less the one lattice parameter from the dislocation centre, the theory discussed is not valid. At a distance of two-three inter-atomic intervals, the discrete structure of the dislocation nucleus is of importance. Displacements in that region are sufficiently great, and non-linear addends appear in the deformation equation. Taking into account that the external (around the nucleus) is great, and the phenomena inside the nucleus can be neglected.

For example, the dislocation energy (9.71) is localised mainly in the deformed region (outside the nucleus) (the logarithms weakly depends on r_0. If that quantity is of order of one-two inter-atomic intervals, the ratio r_1 / r_0 is about $5 \cdot 10^3$.

The Burgers vector is about, $2.5A°$, the shear modulus $G \approx 10^{11} n/m^2$. Thus U_d is about $4 \cdot 10^{-9}$ joules per meter of a dislocation length or 6eV per an inter-atomic distance (2.5 $A°$). The range of screw dislocation energy is 3 – 10 eV per a unit distance along the dislocation line. The dislocation energy [see (9.71)] is listed in Table 9.1.

Displacement near an edge dislocation is more complicated then that one near a screw dislocation. The corresponding calculation is more tiresome but leads to the conclusions like the previous ones.

The number of dislocations does not depend on temperature and is rather small (opposite to vacancies). It is due to the great energy of its generation. When the elastic energy per an inter-atomic interval is about 8eV, the exponential factor is of no

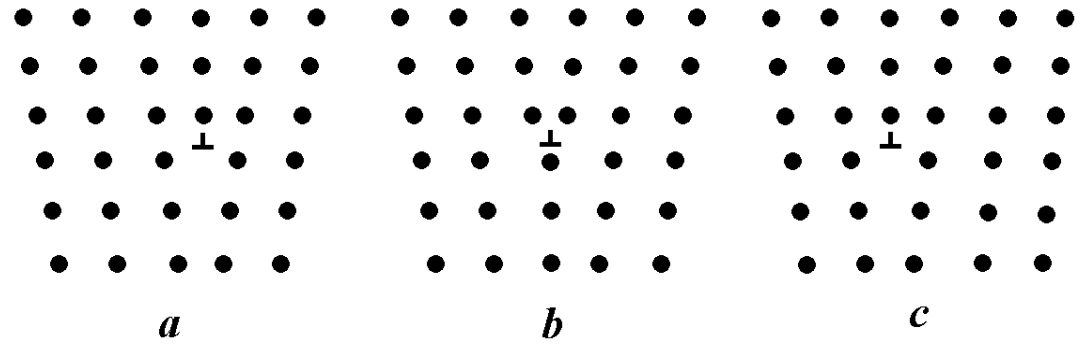


Fig.9.13. Sliding of dislocations. Coordinated motion of atoms leads to the sliding of a dislocation.

importance. That is why the density of dislocation depends on the previous mechanic and thermal treatment of a crystal, method of its manufacturing and others.

9.6.5 Crawling and Sliding

Dislocations like point defects can move through a crystalline lattice. There are two types of the motion: **crawling** and **sliding.**

When the edge of a dislocation plane moves in or out of the crystal, the process is called the **crawling.** The crawling corresponds to the motion of the dislocation upward or downward relative the sliding plane.

Sliding is the motion of dislocation in the along the plane, which is called naturally the **plane of sliding.** While moving of an edge dislocation from one node to another, atoms of the dislocation nucleus perform a little displacement. As a result the sliding mechanism is produced (Fig.9.13).

The motion of a dislocation is shown in Fig.9.14. When a dislocation appears at

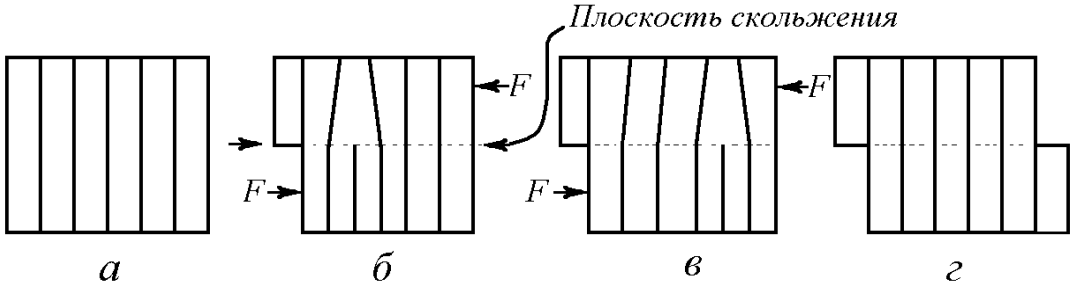


Fig.9.14. The motion of an edge dislocation through a crystal along the sliding plane When the dislocation passes through the crystal, the upper part would displace relative the down one at a distance of the Burgers vector length.

an edge of a crystal and begins to move to the other edge, the upper part of the crystal

displaces relative the down one at a distance equal to the lattice parameter. That is due to the shear strain.

The smooth motion is also possible for screw dislocations. As it was said before, all planes containing the screw dislocation, contain the Burgers vector. That is why the screw dislocation can slide in any direction. Hence, all the planes with a screw dislocation are the planes of smooth motion. All dislocation lines, which are not parallel to its Burgers vector, have only one plane of sliding.

After the screw dislocation has passed through a crystal, its form is changed in a way different then that one when an edge dislocation performs the throughout motion.

A glance at Fig.9.8 shows that the step on the crystal surface is not parallel to a screw dislocation (opposite to an edge dislocation). The step appears at the end points of a crystal, and follows the dislocation when it moves through the crystal.

9.6.6 Mobility and Reproducing of Dislocations

To move and reproduce dislocations, the strains are not to be great. That fact is

of very importance in the processes of plastic deformation.

The relative small resistance of crystals is due to dislocations. The elasticity of crystals is small, and at the great strains a crystal either plastically deforms or breaks. In an ideal crystal, the elastic deformation should be about ½ before the plastic deformation would start. Opposite to that statement, the experiments show that the plasticity process begins at deformations about $10^{-4} - 10^{-3}$.

To produce the residual deformation, the atoms are to displace from one place to another and can not return back. If the displacement is small, an atom can return back when the strain is released, and the deformation is elastic.

The critical situation would be reached when an atom is displaced at a distance greater then the half of the lattice period. The atom would be displaced in another equilibrium position. According to Gook's law to produce that, the strain must be the half of Yong's modulus ($10^{11} N/m^2$). More accurate consideration leads to the quantity by the factor 10 less: $10^{10} N/m^2$.

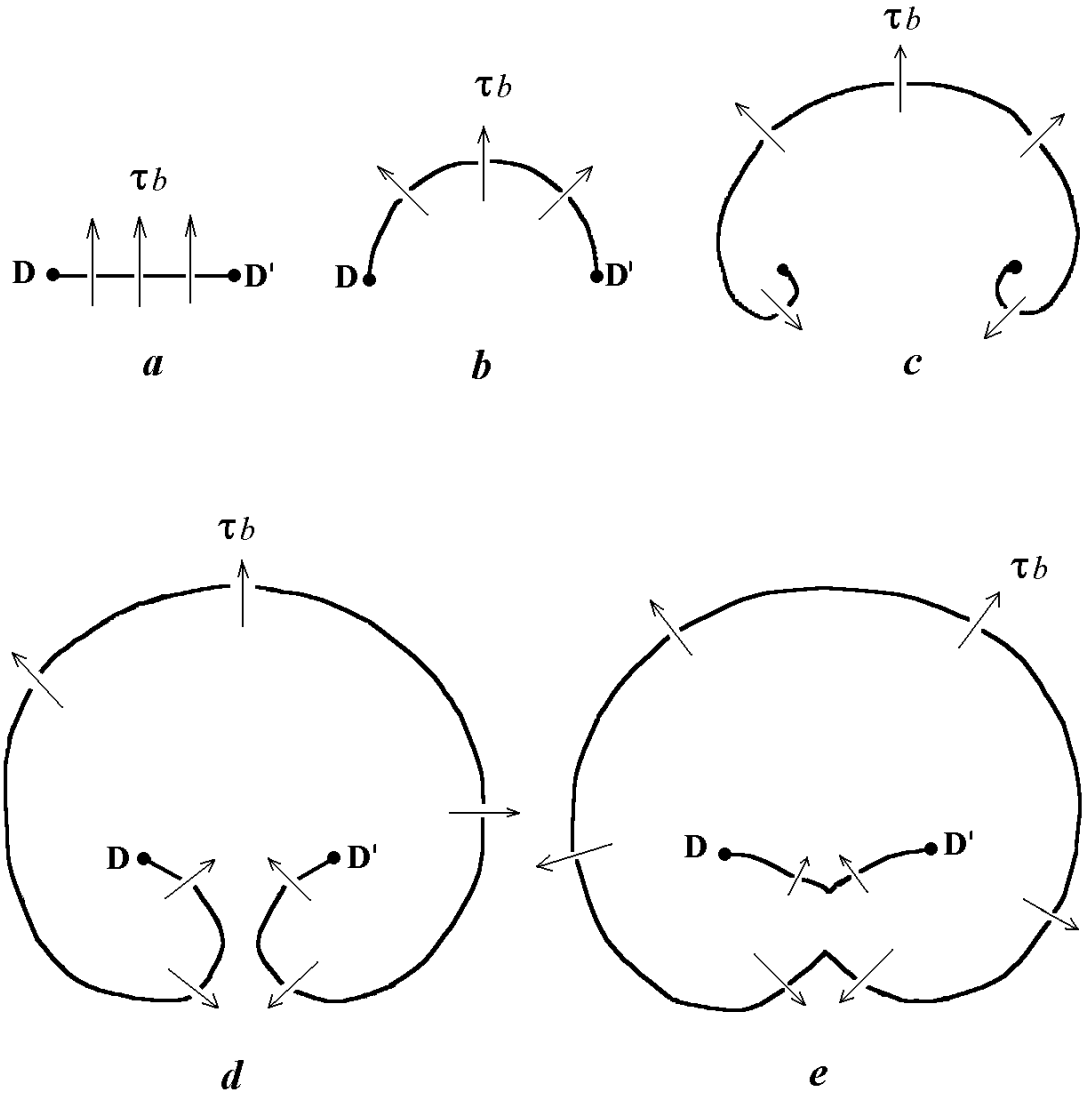
In accordance with experimental data, the plastic deformations begin at the strains $10^5 - 10^6 N/m^2$.

Dislocations begin to move at the strains much less then the shear modulus. To move a dislocation from one row of atoms to another, very small change in atomic disposition is needed (see Fig.9.13). Inside the dislocation center, displacements of some atoms are great and a small force is needed to move them further. If the dislocation nucleus is great in comparison with the lattice parameter, the strain needed to shift a dislocation is very small. If the size of a dislocation nucleus is like that one of the lattice parameter, the shear strains are the same as the shear modulus.

Many crystals with a small number of dislocations are soft and plastic (for example metals). The crystals like diamond, germanium, and silicon are not plastically deformed at room temperature; they just destroy. The fragility of those crystals is due to the fact that the process of destroying begins before then dislocations can produce great shearing. At high temperature, the germanium and silicon crystals (and many others) become plastic.

We assume that in the deformation process, the dislocation reproduce. Indeed the number of dislocations before the strain is applied is not sufficient to produce

great plastic deformations. An inspection of deformed monocrystals proves dislocations reproduce.



Fir.9.15. A Franck – Reed source. Plane or the figure is the plane of sliding of the dislocation segment DD'. The points D and D' are the points of fixation. τ is the strain applied to the lattice. τb is the force acting upon the segment DD'. (a) – The linear segment of the dislocation DD' is curved proportionally to the applied strain. (b) – A curvature reaches the maximum at a critical strain. The dislocation becomes unstable and expands. (c), (d) – The dislocation expands and transforms into a loop. (e) – Both sliding regions unite. A closed dislocation loop appears. The form of the segment DD' is restored. The repetition of the procedure described leads to formation of the following loop and so on.

Frank and Reed (Fig.9.15) proposed a mechanism of the dislocation reproducing.

When the strain increases the initial dislocation segment *b* is curved and transforms in series b – c – d – e. When the jog *e* constricts the segment restores its configuration building the expanding dislocation loop.

9.6.7 Interaction of Dislocations

The experiments prove that the critical strain of plastic deformation depends not only on intrinsic mobility of dislocations but also in great measure on forces needed for a dislocation to overcome the different defects in a crystal. Indeed metallic crystals manufactured without impurities, grain boundaries etc., are very plastic. Impurities can strongly diminish the local energy of dislocation.

In engineering attempts are made to produce alloys of very high stability. The following story is very typical. The iron monocrystals are very plastic. The plastic deformation begins at the strain about $5 \cdot 10^5 N/m^2$. From the other hand, a steel with a plastic deformation limit 100 times more can be produced. For that porpoise alloying by carbon, magnum, tungsten, molybdenum, vanadium is used. Those ingredients interact with dislocations and break its motion. The grains in steel are small. Thus the light sliding of a dislocation occurs at relative short distances till the border of a grain, which retards the motion of the dislocation.

Dislocations strongly interact with each other. At the first stage of the plastic flow, an almost ideal crystal deforms very easily. But the greater is the deformation the greater are the strains needed to deform the lattice. It is due to the great increment of dislocations. Sa a result, dislocations intersect with each other and their motion becomes slower. That phenomenon is called the **riveting** and is widely used to increase the mechanic stability of metals.