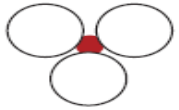
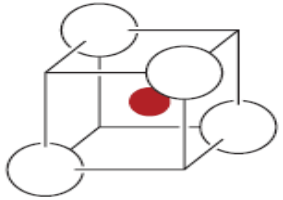
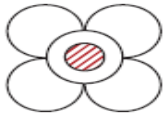
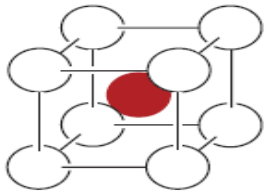
علم مواد

ادامه جلسات حضوری

جدول عدد همسایگی

Coordination Number	Location of Interstitial	Radius Ratio	Representation
2	Linear	0–0.155	
3	Center of triangle	0.155–0.225	
4	Center of tetrahedron	0.225–0.414	
6	Center of octahedron	0.414–0.732	
8	Center of cube	0.732–1.000	

مثال برای عدد همسایگی

Example 3-13 *Radius Ratio for KCl*

For potassium chloride (KCl), (a) verify that the compound has the cesium chloride structure and (b) calculate the packing factor for the compound.

SOLUTION

a. From Appendix B, $r_{K^+} = 0.113$ nm and $r_{Cl^-} = 0.181$ nm, so

$$\frac{r_{K^+}}{r_{Cl^-}} = \frac{0.133}{0.181} = 0.735$$

Since $0.732 < 0.735 < 1.000$, the coordination number for each type of ion is eight, and the CsCl structure is likely.

b. The ions touch along the body diagonal of the unit cell, so

$$\sqrt{3}a_0 = 2r_{K^+} + 2r_{Cl^-} = 2(0.133) + 2(0.181) = 0.628 \text{ nm}$$

$$a_0 = 0.363 \text{ nm}$$

$$\text{Packing factor} = \frac{\frac{4}{3}\pi r_{K^+}^3 (1 \text{ K ion}) + \frac{4}{3}\pi r_{Cl^-}^3 (1 \text{ Cl ion})}{a_0^3}$$

$$= \frac{\frac{4}{3}\pi(0.133)^3 + \frac{4}{3}\pi(0.181)^3}{(0.363)^3} = 0.73$$

انواع عیوب : ۱ـ نقطه ای ۲ـ خطی ۳ـ صفحه ای

عیوب نقطه ای:

الف: جای خالی ب: اتم بین نشین ج: اتم جانشین کوچک
د: اتم جانشین بزرگ ه: نقص فرنکل و: نقص شاتکی

عیوب خطی:

الف: نابجایی(دیسلوکاسیون) لبه ای (اسلاید ۶ و ۷ و ۱۳) Edge dislocation

ب: دیسلوکاسیون یا نابجایی پیچی (اسلاید ۶ و ۱۳) Screw dislocation

عیوب سطحی:

الف:مرز بین دانه ها

ب:نقص در چیده شدن اتمها

ج: مرز دو قلو ها

انواع عیوب نقطه ای :

الف: جای خالی ب: اتم بین نشین ج: اتم جانشین کوچک
د: اتم جانشین بزرگ ه: نقص فرنکل و: نقص شاتکی

Point Defects

Point defects are localized disruptions in otherwise perfect atomic or ionic arrangements in a crystal structure. Even though we call them point defects, the disruption affects a region involving several atoms or ions. These imperfections, shown in Figure 4–1, may be introduced by movement of the atoms or ions when they gain energy by heating, during processing of the material, or by the intentional or unintentional introduction of impurities.

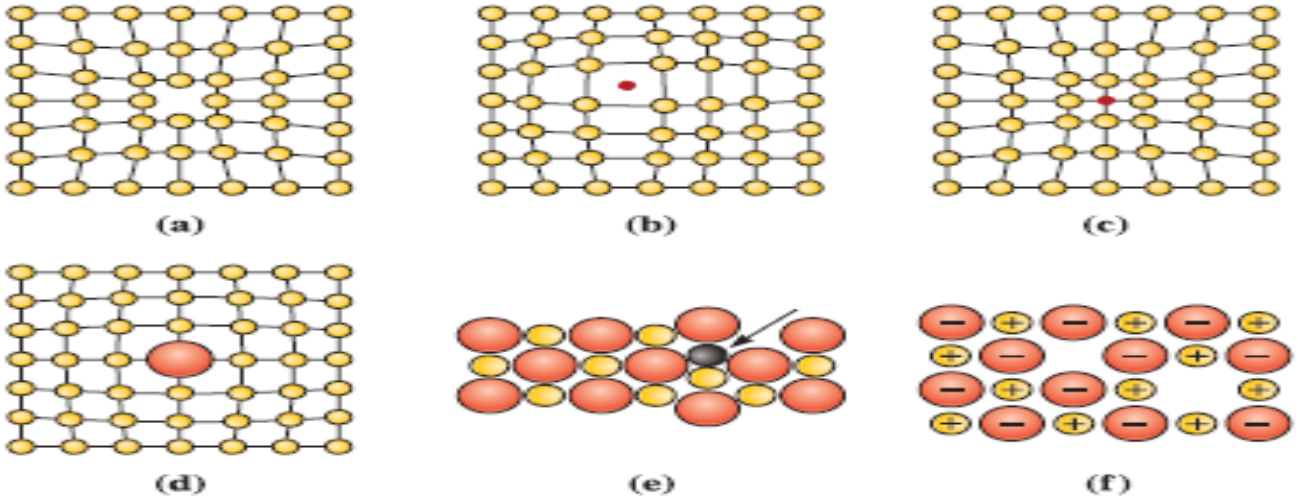


Figure 4–1 Point defects: (a) vacancy, (b) interstitial atom, (c) small substitutional atom, (d) large substitutional atom, (e) Frenkel defect, and (f) Schottky defect. All of these defects disrupt the perfect arrangement of the surrounding atoms.

نابجایی پیچی و لبه ای

Edge Dislocations

An **edge dislocation** (Figure 4-5) can be illustrated by slicing partway through a perfect crystal, spreading the crystal apart, and partly filling

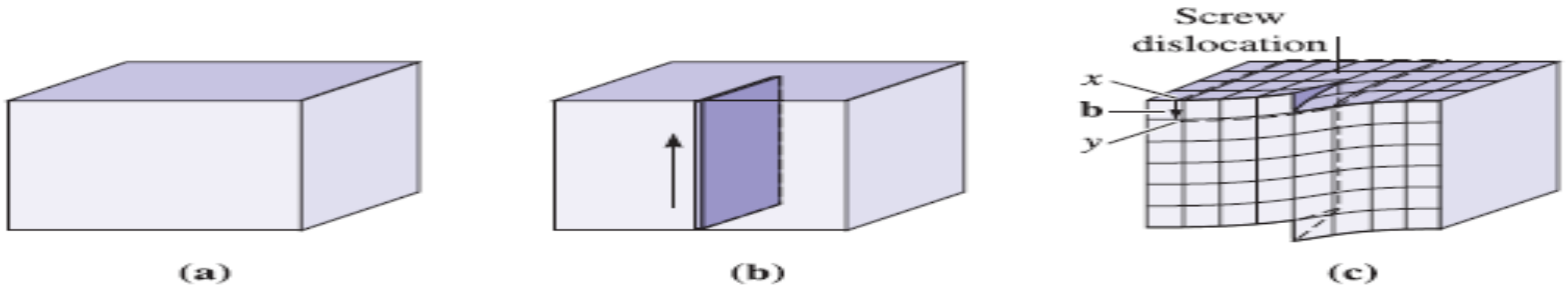


Figure 4-4 The perfect crystal (a) is cut and sheared one atom spacing, (b) and (c). The line along which shearing occurs is a screw dislocation. A Burgers vector **b** is required to close a loop of equal atom spacings around the screw dislocation.

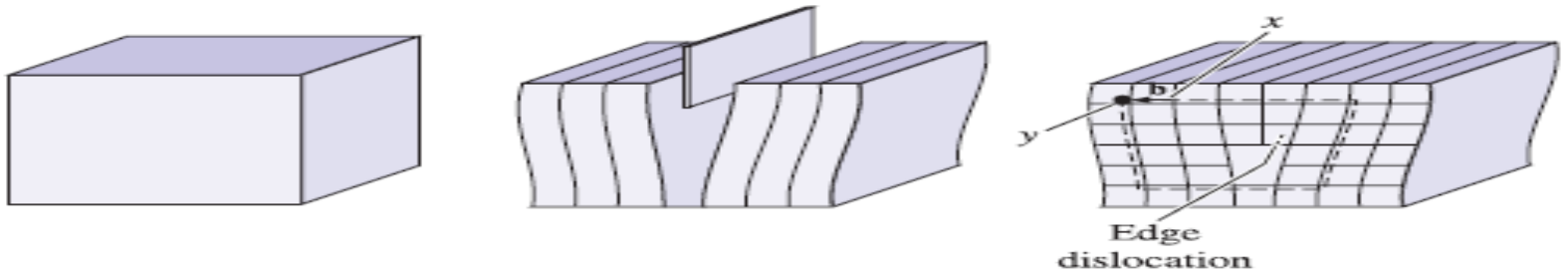


Figure 4-5 The perfect crystal in (a) is cut and an extra half plane of atoms is inserted (b). The bottom edge of the extra half plane is an edge dislocation (c). A Burgers vector **b** is required to close a loop of equal atom spacings around the edge dislocation. (*Adapted from J.D. Verhoeven, Fundamentals of Physical Metallurgy, Wiley, 1975.*)

عیوب خطی(لبه ای)

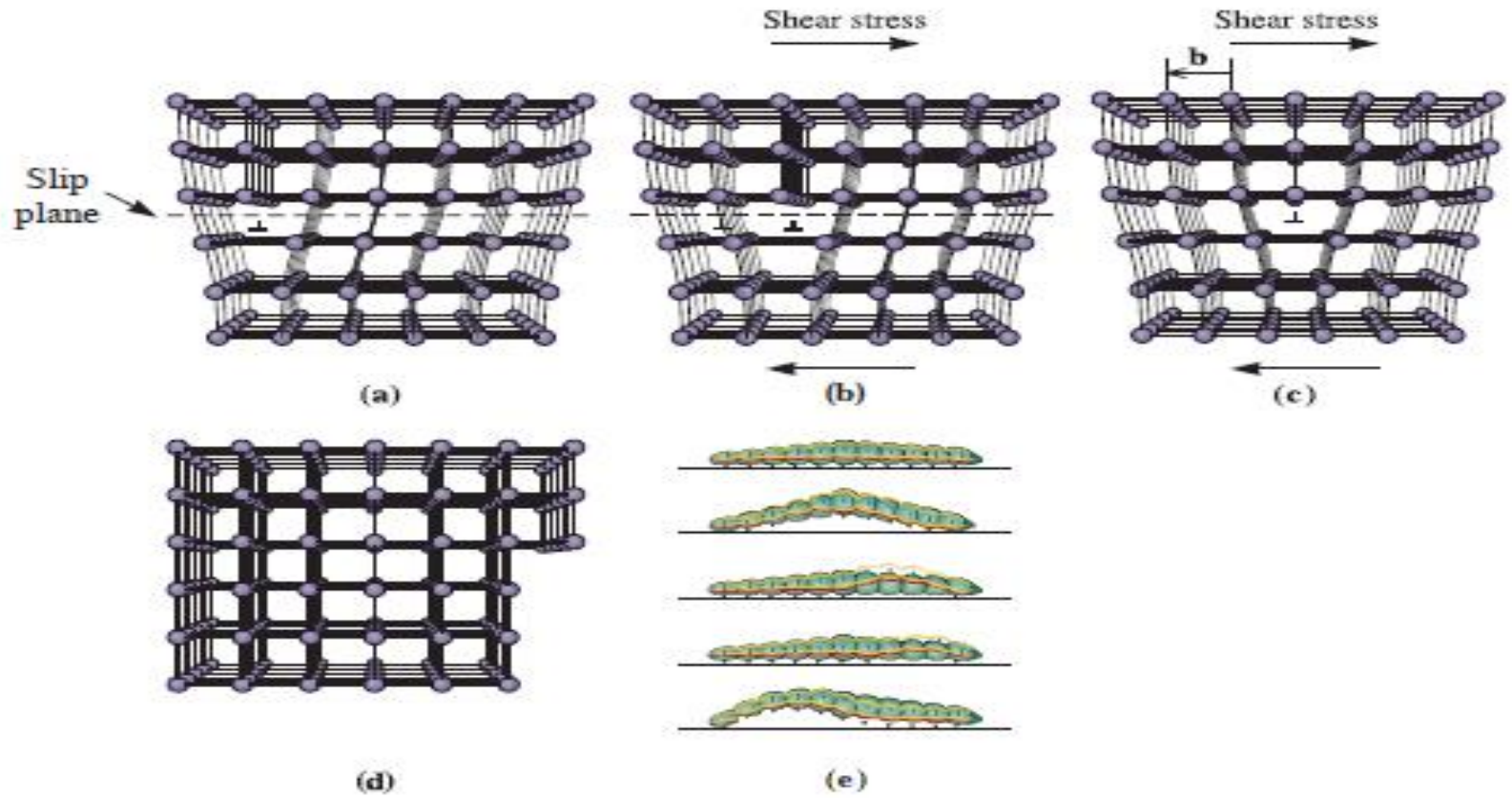


Figure 4-7 (a) When a shear stress is applied to the dislocation in (a), the atoms are displaced, (b) causing the dislocation to move one Burgers vector in the slip direction. (c) Continued movement of the dislocation eventually creates a step (d), and the crystal is deformed. (*Adapted from A.G. Guy, Essentials of Materials Science, McGraw-Hill, 1976.*) (e) The motion of a caterpillar is analogous to the motion of a dislocation.

schmids lawقانون اشـميد

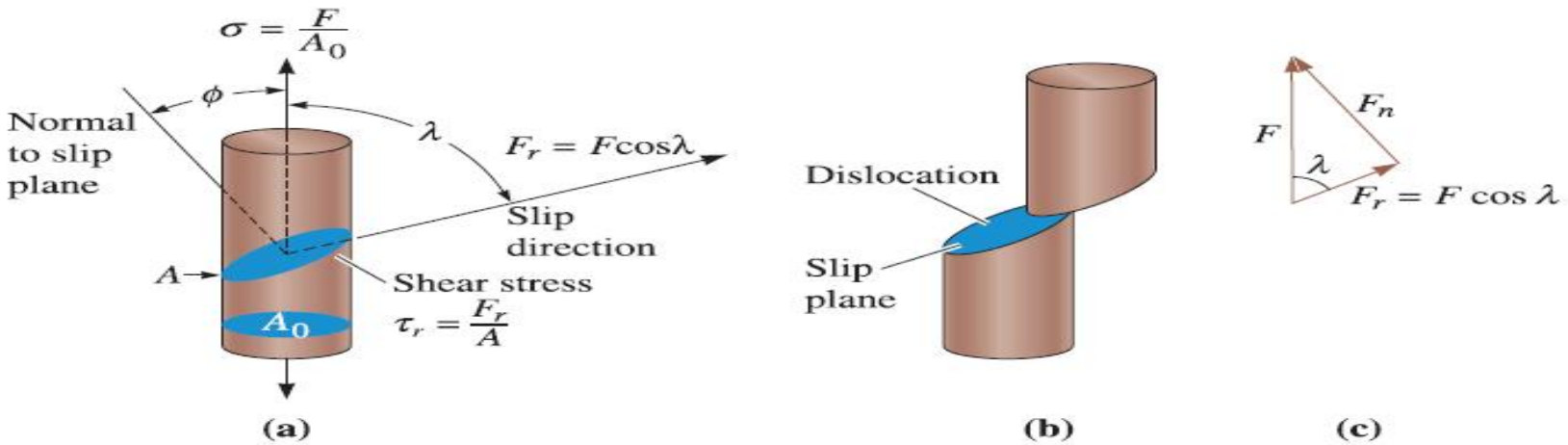


Figure 4-13 (a) A resolved shear stress τ is produced on a slip system. [Note: $(\phi + \lambda)$ does not have to equal 90°.] (b) Movement of dislocations on the slip system deforms the material. (c) Resolving the force.

In order for the dislocation to move in its slip system, a shear force acting in the slip direction must be produced by the applied force. This resolved shear force F_r is given by

$$F_r = F\cos\lambda$$

If we divide the equation by the area of the slip plane, $A = A_0/\cos\phi$, we obtain the following equation known as **Schmid's law**:

$$\tau_r = \sigma\cos\phi\cos\lambda \qquad (4\text{-}3)$$

where

$$\tau_r = \frac{F_r}{A} = \text{resolved shear } \textit{stress} \text{ in the slip direction}$$

and

$$\sigma = \frac{F}{A_0} = \text{normal } \textit{stress} \text{ applied to the cylinder}$$

مثال:مطلو بست تنش برشی روی سیستم لغزشی(۱۱۱) جهت ۱۰۱˚ اگر یک تنش ۷۰ مگا پاسگال در جهت ۰۰۱ واحد شبکه اعمال شود

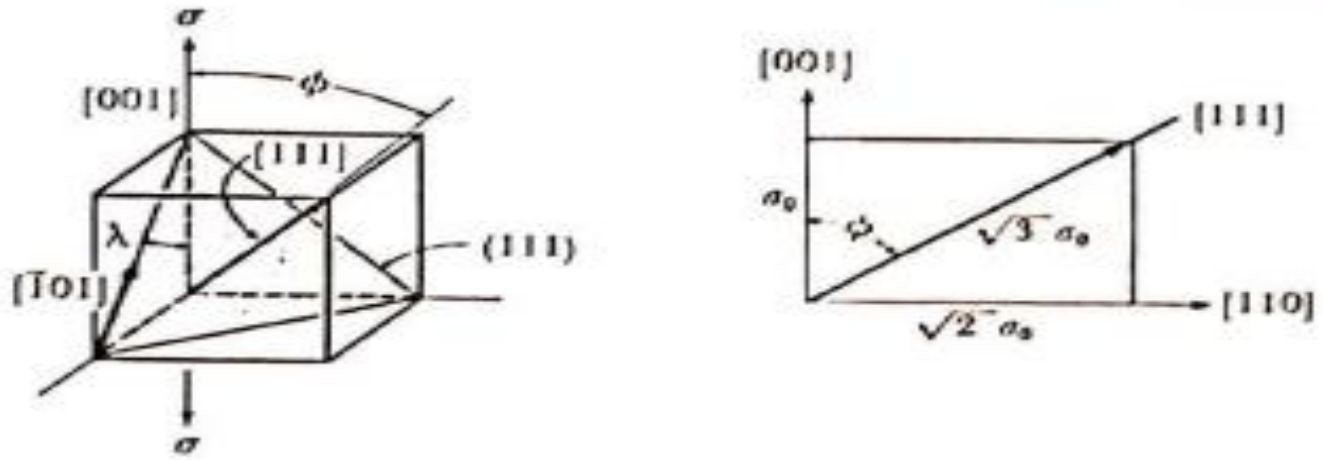


FIGURE 4-12 A normal stress σ is applied in the [001] direction of the unit cell. This produces an angle λ of 45° to the [101] slip direction and an angle ϕ of 54.76° to the normal to the (111) plane. (See Example 4-6.)

Answer:

By inspection, $\lambda = 45°$ and $\cos\lambda = 0.707$. The normal to the (111) plane must be the [111] direction. We can then calculate that

$$\cos\phi = \frac{1}{\sqrt{3}} = 0.577 \quad \text{or} \quad \phi = 54.76°$$

$$\tau_r = \sigma\cos\lambda\cos\phi = (70\ \text{MPa})(0.707)(0.577) = 28.56\ \text{MPa}$$

مرز دانه (اسلاید ۱۰ و ۱۳) grain boundary

Small Angle Grain Boundaries

A small angle grain boundary is an array of dislocations that produces a small misorientation between the adjoining crystals (Figure 4-18). Because the energy of the surface is less than that of a regular grain boundary, the small angle grain boundaries are not as effective in blocking slip. Small angle boundaries formed by edge dislocations are called **tilt boundaries**, and those caused by screw dislocations are called **twist boundaries**.

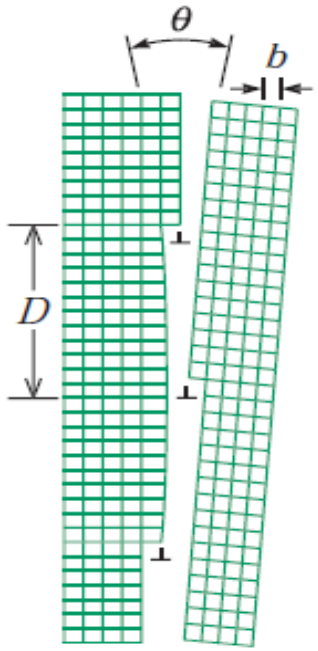


Figure 4-18
The small angle grain boundary is produced by an array of dislocations, causing an angular mismatch θ between the lattices on either side of the boundary.

نقص چیدن در شبکه های Fcc که موجب ایجاد یک شبکه HCP در بین شبکه های Fcc میشود

Stacking Faults

Stacking faults, which occur in FCC metals, represent an error in the stacking sequence of close-packed planes. Normally, a stacking sequence of *ABC ABC ABC* is produced in a perfect FCC crystal. Suppose instead the following sequence is produced:

$$ABC\ \underbrace{ABAB}\ CABC$$

In the portion of the sequence indicated, a type A plane replaces a type C plane. This small region, which has the HCP stacking sequence instead of the FCC stacking sequence, represents a stacking fault. Stacking faults interfere with the slip process.

محاسبه بردار برگرز

Example 4-7 *Burgers Vector Calculation*

Calculate the length of the Burgers vector in copper.

SOLUTION

Copper has an FCC crystal structure. The lattice parameter of copper (Cu) is 0.36151 nm. The close-packed directions, or the directions of the Burgers vector, are of the form ⟨110⟩. The repeat distance along the ⟨110⟩ directions is one-half the face diagonal, since lattice points are located at corners and centers of faces [Figure 4-10(a)].

$$\text{Face diagonal} = \sqrt{2}a_0 = (\sqrt{2})(0.36151) = 0.51125 \text{ nm}$$

The length of the Burgers vector, or the repeat distance, is

$$\mathbf{b} = \frac{1}{2}(0.51125)\text{nm} = 0.25563 \text{ nm}$$

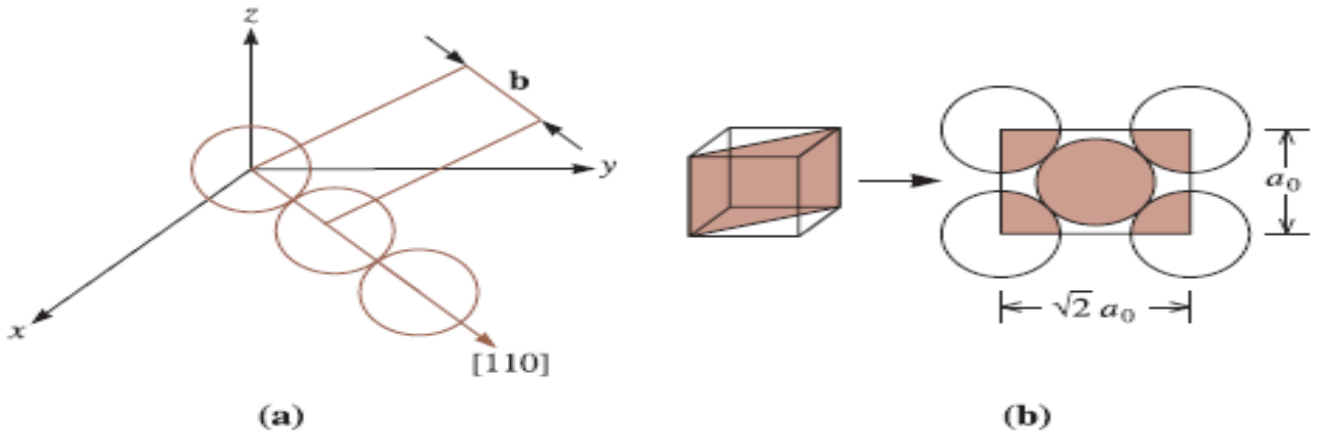


Figure 4-10 (a) Burgers vector for FCC copper. (b) The atom locations on a (110) plane in a BCC unit cell (for Examples 4-7 and 4-8, respectively).

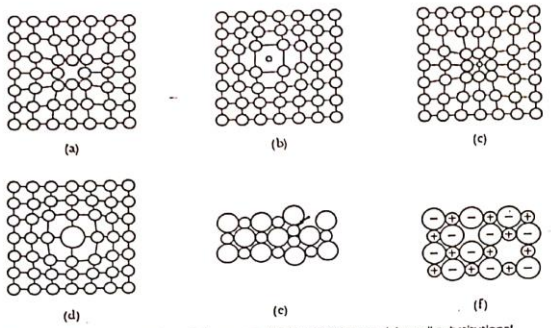


FIGURE 4-14 Point defects: (a) vacancy, (b) interstitial atom, (c) small substitutional atom, (d) large substitutional atom, (e) Frenkel defect, and (f) Schottky defect. All of these defects disrupt the perfect arrangement of the surrounding atoms.

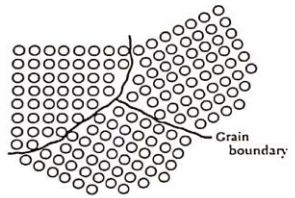


FIGURE 4-17 The atoms near the boundaries of the three grains do not have an equilibrium spacing or arrangement.

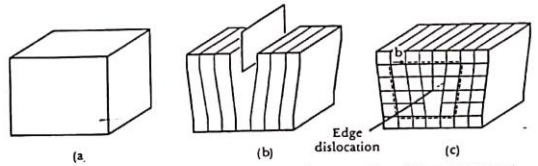


FIGURE 4-2 The perfect crystal in (a) is cut and an extra plane of atoms is inserted (b). The bottom edge of the extra plane is an edge dislocation (c). A Burgers vector **b** is required to close a loop of equal atom spacings around the edge dislocation.

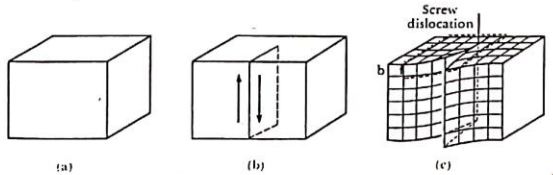


FIGURE 4-1 The perfect crystal (a) is cut and sheared one atom spacing, (b) and (c). The line along which shearing occurs is a screw dislocation. A Burgers vector **b** is required to close a loop of equal atom spacings around the screw dislocation.

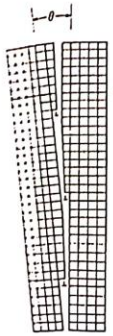


FIGURE 4-20 The small angle grain boundary is produced by an array of dislocations, causing an angular mismatch θ between the lattices on either side of the boundary.

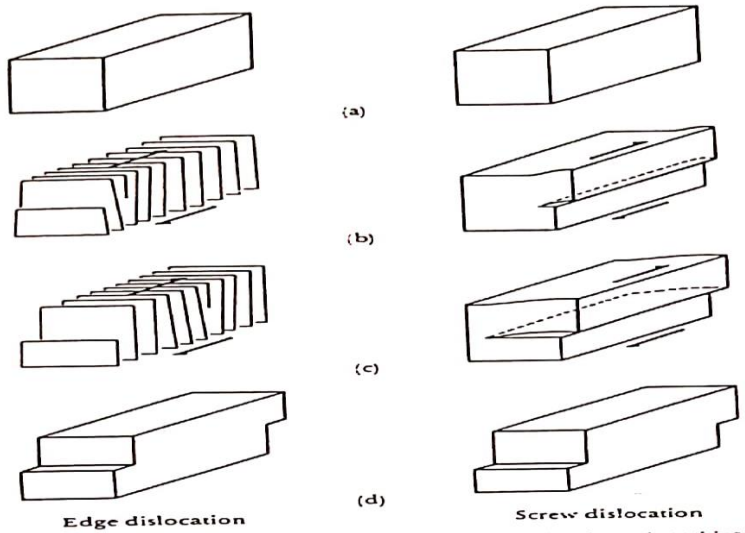


FIGURE 4-6 A shear force acting on a dislocation introduced into a perfect crystal (a) causes the dislocation to move through the crystal until a step is created (c). The crystal is now deformed.

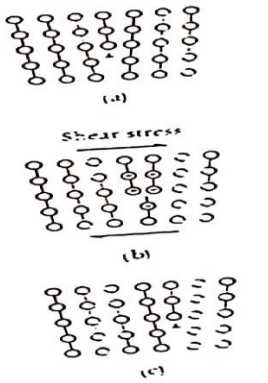


FIGURE 4-5
When a shear force is applied to the dislocation in (a), the atoms are displaced (b) until the dislocation moves one Burgers vector in the slip direction (c).

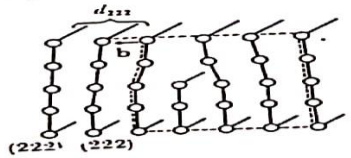


FIGURE 4-3 The Burgers vector for Example 4-1 is perpendicular to the (222) planes and has a length equal to the interplanar spacing between (222) planes.

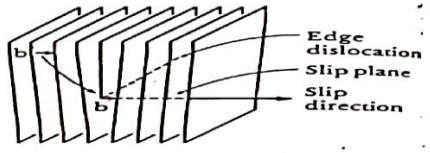


FIGURE 4-4 After the Burgers vector is translated from the loop to the dislocation line, a plane is defined.

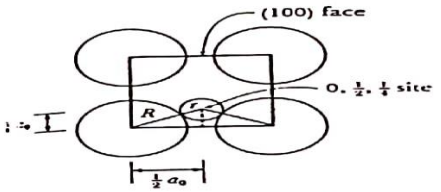


FIGURE 4-16 The location of the 0, ½, ¼ interstitial site in BCC metals, showing the arrangement of the normal atoms and the interstitial atom.

مکانیزم تغییر فرم پلاستیک ۱:لغزش(اسلاید ۱۸) ۲: تشکیل دو قلو ها

Twin Boundaries A **twin boundary** is a plane across which there is a special mirror image misorientation of the crystal structure (Figure 4-19). Twins can be produced when a shear force, acting along the twin boundary, causes the atoms to shift out of position. Twinning occurs during deformation or heat treatment of certain metals. The twin boundaries interfere with the slip process and increase the strength of the metal. Twinning also occurs in some ceramic materials such as monoclinic zirconia and dicalcium silicate.

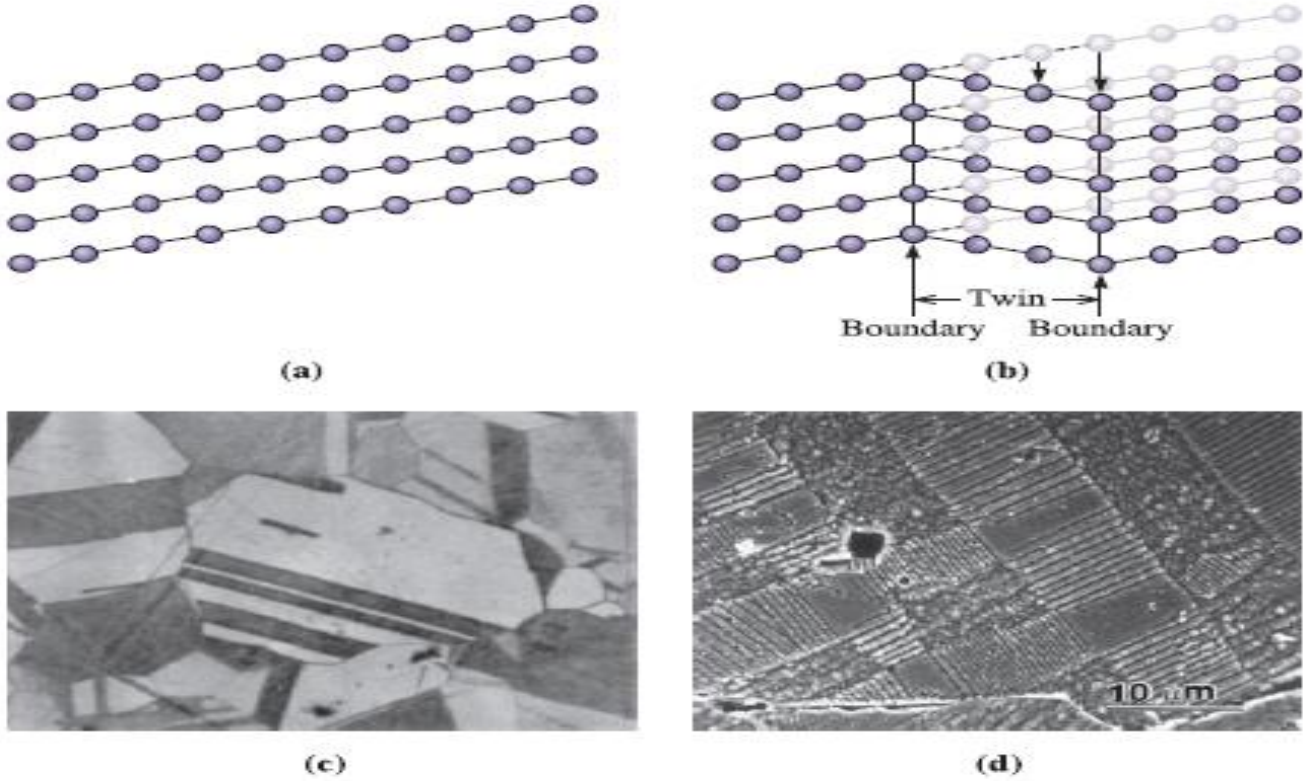


Figure 4–19 Application of stress to the (a) perfect crystal may cause a displacement of the atoms, (b) resulting in the formation of a twin. Note that the crystal has deformed as a result of twinning. (c) A micrograph of twins within a grain of brass (×250). (d) Domains in ferroelectric barium titanate. *(Courtesy of Dr. Rodney Roseman, University of Cincinnati.)* Similar domain structures occur in magnetic materials.

رابطه ترمودینامیکی برای محاسبه تعداد نابجایی

At room temperature (~298 K), the concentration of vacancies is small, but the concentration of vacancies increases exponentially as the temperature increases, as shown by the following Arrhenius type behavior:

$$n_v = n \exp\left(\frac{-Q_v}{RT}\right) \qquad (4\text{-}1)$$

where

n_v is the number of vacancies per cm^3;

n is the number of atoms per cm^3;

Q_v is the energy required to produce one mole of vacancies, in cal/mol or Joules/mol;

R is the gas constant, $1.987 \frac{\text{cal}}{\text{mol} \cdot \text{K}}$ or $8.314 \frac{\text{Joules}}{\text{mol} \cdot \text{K}}$; and

T is the temperature in degrees Kelvin.

اثر دما بر تعداد نابجایی

Example 4-1 *The Effect of Temperature on Vacancy Concentrations*

Calculate the concentration of vacancies in copper at room temperature (25°C). What temperature will be needed to heat treat copper such that the concentration of vacancies produced will be 1000 times more than the equilibrium concentration of vacancies at room temperature? Assume that 20,000 cal are required to produce a mole of vacancies in copper.

SOLUTION

The lattice parameter of FCC copper is 0.36151 nm. There are four atoms per unit cell; therefore, the number of copper atoms per cm^3 is

$$n = \frac{4 \text{ atoms/cell}}{(3.6151 \times 10^{-8} \text{ cm})^3} = 8.466 \times 10^{22} \text{ copper atoms/cm}^3$$

At room temperature, $T = 25 + 273 = 298$ K:

$$n_v = n \exp\left(\frac{-Q_v}{RT}\right)$$

$$= \left(8.466 \times 10^{22} \frac{\text{atoms}}{\text{cm}^3}\right) \exp\left[\frac{-20{,}000 \frac{\text{cal}}{\text{mol}}}{\left(1.987 \frac{\text{cal}}{\text{mol} \cdot \text{K}}\right)(298 \text{ K})}\right]$$

$$= 1.814 \times 10^8 \text{ vacancies/cm}^3$$

We wish to find a heat treatment temperature that will lead to a concentration of vacancies that is 1000 times higher than this number, or $n_v = 1.814 \times 10^{11}$ vacancies/cm^3.

We could do this by heating the copper to a temperature at which this number of vacancies forms:

$$n_v = 1.814 \times 10^{11} = n \exp\left(\frac{-Q_v}{RT}\right)$$

$$= (8.466 \times 10^{22}) \exp(-20{,}000)/(1.987T)$$

$$\exp\left(\frac{-20{,}000}{1.987T}\right) = \frac{1.814 \times 10^{11}}{8.466 \times 10^{22}} = 0.214 \times 10^{-11}$$

$$\frac{-20{,}000}{1.987T} = \ln(0.214 \times 10^{-11}) = -26.87$$

$$T = \frac{20{,}000}{(1.987)(26.87)} = 375 \text{ K} = 102°\text{C}$$

(الغزش)slip

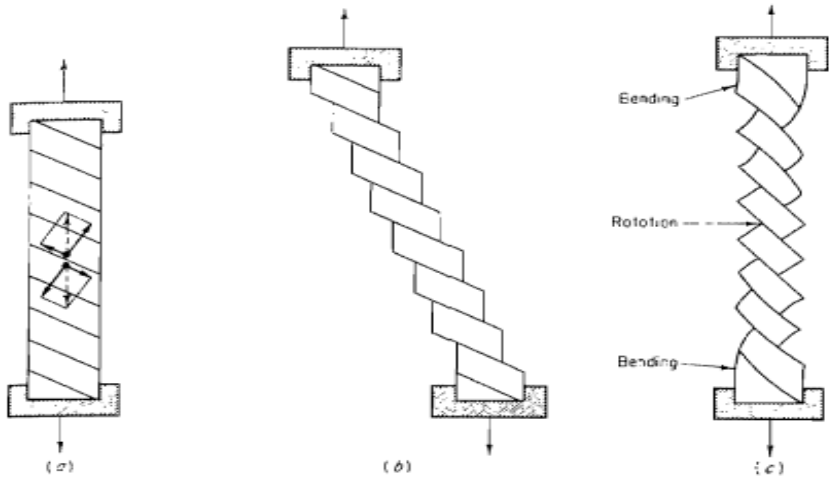


Fig. 3·4 Schematic representation of slip in tension. (a) Before straining; (b) with ends not constrained; (c) ends constrained. (From B. D. Cullity, "Elements of X-ray Diffraction," Addison-Wesley Publishing Company, Inc., Reading, Mass., 1956.)

packed [$\bar{1}10$] direction, a distance of one lattice dimension or multiple of that dimension. The series of steps formed will generally appear under the microscope as a group of approximately parallel lines (Figs. 3·7 and 3·8). In Fig. 3·7, a single vertical line was scribed on the surface before

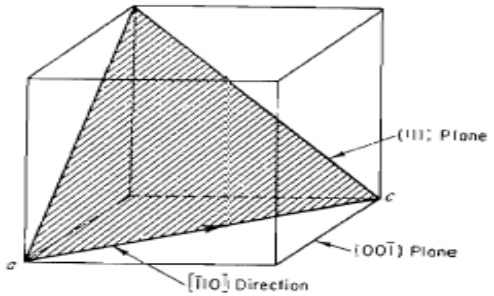


Fig. 3·5 Slip plane and slip direction in an f.c.c. lattice.