

University of Anbar
College of Science
Department of Physics



فيزياء المواد Physics of Materials

المرحلة الثالثة
الكورس الاول

اعداد
م.د. قيس عبدالله عباس

4. Imperfections in solid materials العيوب في المادة الصلبة

4.1 Point defects العيوب النقطية

Point defects are localized disruptions **خلال موضعي** in otherwise perfect atomic or ionic arrangements **الترتيب** in a crystal structure. Even though we call them point defects, the disruption affects **يؤثر** a region **الحيز** involving **المتضمن** several **عدد** atoms or ions. These imperfections, shown **المبينة** in Figure 4.1, may be introduced **تمثل** by movement **انتقال** of the atoms or ions when they gain **تكتسب** energy **طاقة** by heating **بالحرارة**, during **خلال** processing **تصنيع** of the material, or by the intentional or unintentional introduction of impurities. **الإدخال المتعمد أو غير المتعمد للشوائب**.

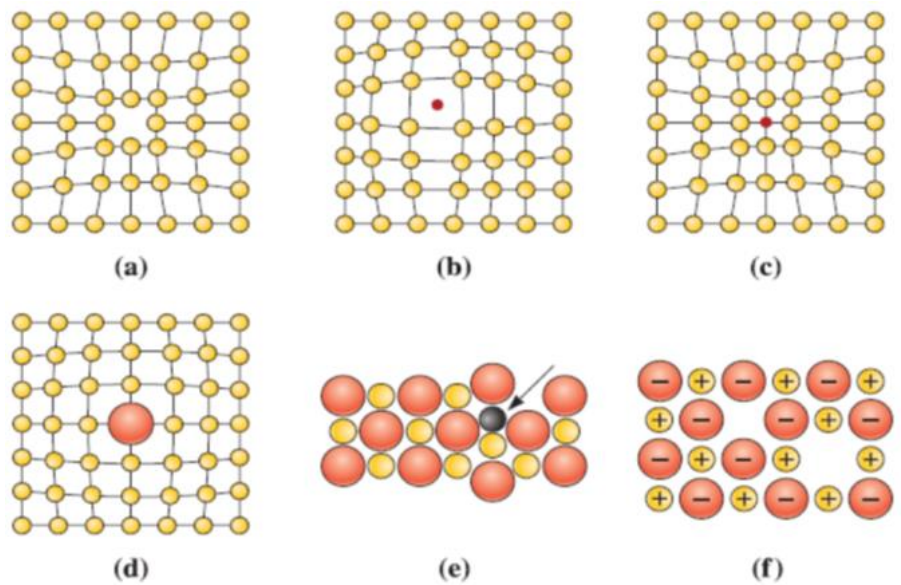


Figure 4.1 Point defects: (a) vacancy, (b) interstitial atom, (c) small substitutional atom, (d) large substitutional atom, (e) Frenkel defect, and (f) Schottky defect.

4.1.1 A vacancy: مكان شاغر

A vacancy is produced **يتكون** when an atom or an ion is missing **ينفقد** from its normal site **مكانه الاعتيادي** in the crystal structure as in Figure 4.1(a). When atoms or ions are missing **تنفقد**, the overall randomness **العشوائية العامة** or entropy of the material increases **يزداد**, which affects **تؤثر** the thermodynamic stability **الاستقرار الترموداينميكي** of a crystalline material. All crystalline materials have **تمتلك** vacancy defects. Vacancies are introduced **موجوده** into metals and alloys **السبائك** during **خلال** solidification **عملية التصلب**, at high temperatures, or as a consequence **نتيجة** of radiation damage **ضرر الاشعاع**. Vacancies play **تلعب** an

important role **دورا مهما** in determining **لتحديد** the rate **معدل** at which atoms or ions move **تتحرك** around **حول** or diffuse **تنتشر** in a solid material, especially **المعادن النقية** in pure metals **خصوصا**.

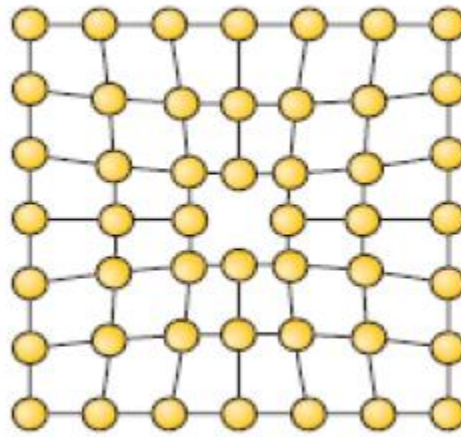


Fig. 4.1.a

At room temperature **عند حرارة الغرفة** (~298 K), the concentration **تركيز** of vacancies is small, but the concentration of vacancies increases **يزداد** exponentially **اوسيا** as **كلما** the temperature increases **تزداد الحرارة**, as shown **كما** **بالتالي** by the following **موضح**:

$$n_v = n \exp\left(\frac{-Q_v}{RT}\right) \quad \dots \dots \dots (1)$$

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, $1.987 \frac{\text{Cal}}{\text{mol.K}}$ or $8.314 \frac{\text{Joules}}{\text{mol.K}}$ and;

T is the temperature in degrees Kelvin.

Example (4.1): The Effect of Temperature on Vacancy Concentrations.

Calculate **احسب** the concentration **تركيز** of vacancies **الفراغات** in FCC copper **النحاس** at room temperature **حرارة الغرفة** (25°C). What temperature **ما** **الحرارة** is needed **للمعالجة النحاس حراريا** to heat treat copper **التي نحتاجها** such that the concentration of vacancies produced is 1000 times **من المرات** more

than **اكثر من** the equilibrium **توازن** concentration of vacancies at room temperature? Assume that **افتراض ان** 20,000 cal are required **تحتاجها** to produce **لانتاج** a mole of vacancies in copper.

Solution:

The lattice parameter **معامل الشبكة** of FCC copper is 0.36151 nm. There are **يوجد** four atoms **اربعة ذرات** per unit cell **لوحة الخلية**; therefore **لذلك**, the number of copper atoms per cm³ 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, $T = 25 + 273 = 298 \text{ K}$:

$$\begin{aligned} n_v &= n \exp\left(\frac{-Q_v}{RT}\right) \\ &= \left(8.466 \times 10^{22} \frac{\text{atoms}}{\text{cm}^3}\right) \exp\left[\frac{-20,000 \frac{\text{cal}}{\text{mol}}}{\left(1.987 \frac{\text{cal}}{\text{mol} \cdot \text{K}}\right)(298 \text{ K})}\right] \\ &= 1.814 \times 10^8 \text{ vacancies/cm}^3 \end{aligned}$$

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/cm³.

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

$$\begin{aligned} n_v &= 1.814 \times 10^{11} = n \exp\left(\frac{-Q_v}{RT}\right) \\ &= (8.466 \times 10^{22}) \exp(-20,000)/(1.987T) \\ \exp\left(\frac{-20,000}{1.987T}\right) &= \frac{1.814 \times 10^{11}}{8.466 \times 10^{22}} = 0.214 \times 10^{-11} \\ \frac{-20,000}{1.987T} &= \ln(0.214 \times 10^{-11}) = -26.87 \\ T &= \frac{20,000}{(1.987)(26.87)} = 375 \text{ K} = 102^\circ\text{C} \end{aligned}$$

Example 4.2

Calculate the equilibrium number of vacancies per cubic meter for copper at 1000°C. The energy for vacancy formation is 0.9 eV/atom; the atomic weight and density (at 1000°C) for copper are 63.5 g/mol and 8.4 g/cm³, respectively.

Solution

This problem may be solved by using Equation 4.1; it is first necessary, however, to determine the value of N , the number of atomic sites per cubic meter for copper, from its atomic weight A_{Cu} , its density ρ , and Avogadro's number N_A , according to

$$\begin{aligned} N &= \frac{N_A \rho}{A_{\text{Cu}}} \\ &= \frac{(6.022 \times 10^{23} \text{ atoms/mol})(8.4 \text{ g/cm}^3)(10^6 \text{ cm}^3/\text{m}^3)}{63.5 \text{ g/mol}} \\ &= 8.0 \times 10^{28} \text{ atoms/m}^3 \end{aligned}$$

Thus, the number of vacancies at 1000°C (1273 K) is equal to

$$\begin{aligned} N_v &= N \exp \left(-\frac{Q_v}{kT} \right) \\ &= (8.0 \times 10^{28} \text{ atoms/m}^3) \exp \left[-\frac{(0.9 \text{ eV})}{(8.62 \times 10^{-5} \text{ eV/K})(1273 \text{ K})} \right] \\ &= 2.2 \times 10^{25} \text{ vacancies/m}^3 \end{aligned}$$

4.1.2 Interstitial Defects العيوب الخلالية

An **interstitial defect** is formed when an extra atom or ion is inserted into the crystal structure at a normally unoccupied position, as in Figure 4.1 b

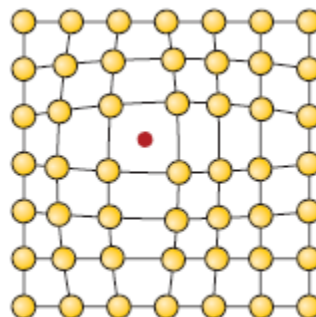


Fig. 4.1. b

Interstitial atoms or ions **على الرغم من انها** much smaller than **من اصغر بكثير** the atoms or ions located **الموجودة** at the lattice points **في نقاط الشبكة**, are still larger than **من الا انها لاتزال اكبر** the interstitial sites **المواقع البينية** that they occupy **التي تحتلها**; consequently **وبالتالي**, the surrounding **وبتشوه** crystal region **الحيز البلوري** is compressed **ينضغط** and distorted

Example 4.3: Sites **مواقع** for Carbon in Iron

In FCC iron, carbon atoms are located **تقع** at octahedral **ثمانى السطوح** sites, which **والتى** occur **توجد** at the center **في مركز** of each edge **كل حافة** of the unit cell at sites **مواقع** such as **مثلا** (0, 0, 1/2) and at the center **مركز** of the unit cell (1/2, 1/2, 1/2). In BCC iron, carbon atoms enter tetrahedral sites **مواقع رباعية السطوح**, such as (0, 1/2, 1/4). The lattice parameter is 0.3571 nm for FCC iron and 0.2866 nm for BCC iron. Assume that **افترض ان** carbon atoms have **تمتلك** a radius **نصف قطر** of 0.071 nm. Would we expect **نتوقع** a greater distortion **تشويها كبيرا** of the crystal by **بواسطة** an interstitial carbon atom **ذرة الكربون الخلالية** in FCC or BCC iron?

Solution:

We can calculate the size of the interstitial site in BCC iron at the (0, 1/2, 1/4) location with the help of Figure 4.2(a). The radius R_{BCC} of the iron atom is:

$$R_{\text{BCC}} = \frac{\sqrt{3}a_0}{4} = \frac{(\sqrt{3})(0.2866)}{4} = 0.1241 \text{ nm}$$

From Figure 4-2(a), we find that

$$\left(\frac{1}{2}a_0\right)^2 + \left(\frac{1}{4}a_0\right)^2 = (r_{\text{interstitial}} + R_{\text{BCC}})^2$$

$$(r_{\text{interstitial}} + R_{\text{BCC}})^2 = 0.3125a_0^2 = (0.3125)(0.2866 \text{ nm})^2 = 0.02567$$

$$r_{\text{interstitial}} = \sqrt{0.02567} - 0.1241 = 0.0361 \text{ nm}$$

For FCC iron, the interstitial site such as the (0, 0, 1/2) lies along $\langle 001 \rangle$ directions. Thus, the radius of the iron atom and the radius of the interstitial site are [Figure 4.2(b)]:

$$R_{\text{FCC}} = \frac{\sqrt{2}a_0}{4} = \frac{(\sqrt{2})(0.3571)}{4} = 0.1263 \text{ nm}$$

$$2r_{\text{interstitial}} + 2R_{\text{FCC}} = a_0$$

$$r_{\text{interstitial}} = \frac{0.3571 - (2)(0.1263)}{2} = 0.0523 \text{ nm}$$

The interstitial site in BCC iron is smaller than the interstitial site in FCC iron. Although both are smaller than the carbon atom, carbon distorts **تشوه** the BCC crystal structure more than **اكثر من** the FCC structure. As a result, fewer carbon atoms are expected to enter interstitial positions in BCC iron than in FCC iron.

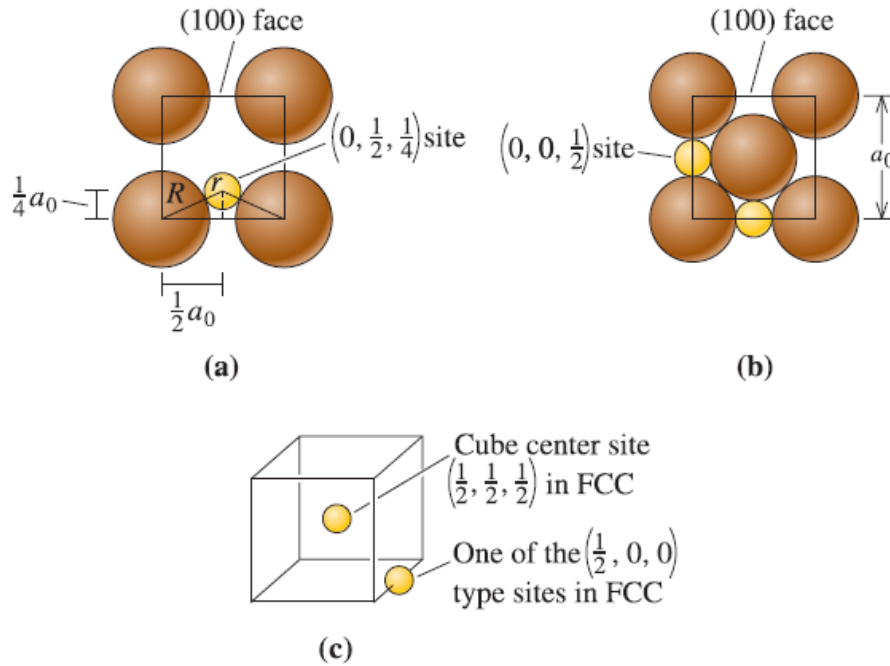
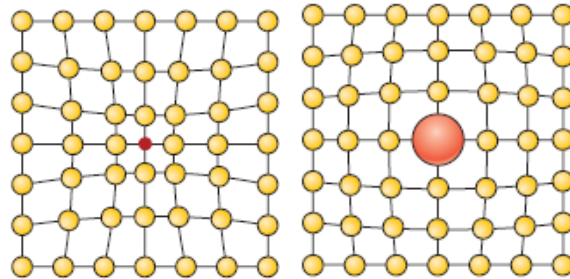


Figure 4.2 (a) The location of the $(0, \frac{1}{2}, \frac{1}{4})$ interstitial site in BCC metals. (b) $(0, 0, \frac{1}{2})$ site in FCC metals. (c) Edge centers and cube centers are some of the interstitial sites in the FCC structure.

4.1.3 Substitutional Defects عيوب الاستبدال

A substitutional defect is created **ينشاء او يتكون** when one atom or ion is replaced **تتبدل** by a different type **مختلف بنوع** of atom or ion as in Figure 4.1 c, d



Figs. 4.1. c and d

The substitutional atoms or ions **الذرات او الايونات الابدالية** occupy **تحتل** the normal lattice site **موقع الشبكة الاعتيادي**. And they may either be larger **اكثر** than the normal atoms or ions **الذرة او الايون الاعتيادي** in the crystal structure, in which case **المسافات البينية** the surrounding **المحيطة** interatomic spacings **في حالة** are

reduced **تقل**, or smaller **اصغر** causing **مسببة** the surrounding atoms **الذرات المحيطة** to have **مساافات بينية اكبر** larger interatomic spacings **تمتلك**.

4.1.4 A Frenkel defect **عييب فرانكل**

A **Frenkel defect** is a vacancy-interstitial pair **يتشكل** formed **هو زوج فارغ - خلافي** when an ion jumps **يقفز** from **من** a normal lattice point **نقطة شبكية اعتيادي** to an interstitial site **الى موقع خلافي**, as in Figure 4.1e leaving **تاركا** behind a vacancy **فراغ**. Although **بالرغم من**, this is usually associated **يرافق** with ionic materials **المواد الايونية**, a Frenkel defect can occur **ان يوجد** in metals **عييب فرانكل يمكن ان يوجد** and covalently bonded materials **المواد المرتبطة تساهميا** **في المعادن**.

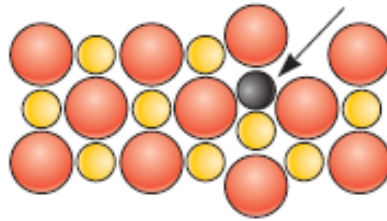


Fig. 4.1.e

4.1.5 A Schottky defect **عييب شوتكي**

A **Schottky defect** is unique **مميز** to ionic materials **المواد الايونية** and is commonly **وشائع** found **موجود** in many ceramic materials **في اغلب المواد السيراميكية**. When vacancies occur **توجد فراغات** in an ionically bonded material **في مواد مترابطة ايونيا**, as shown in figure 4.1. f.

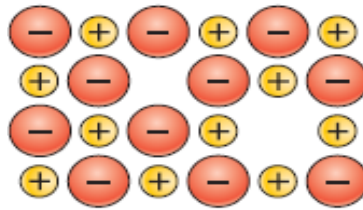


Fig. 4.1.f

4.2 Dislocations **الانخلاعات**

Dislocations **الانخلاعات** are line imperfections **هي عيوب خطية** in an otherwise perfect **مثالية** crystal. They typically **تتشاء** are created **في** a crystal during **التصلب البلوري** solidification **خلال** of the material or when **او عندما** the material is deformed **مشوهة** permanently **بشكل دائم**. Although **من ان** dislocations **الانخلاعات** are present **توجد** in all materials **في جميع المواد**, including **بضمنها** ceramics **السيراميك** and polymers **البوليمر** they are particularly **انها** useful **مفيدة** in explaining **شرح** deformation **التشوه** and

strengthening التقوية in metallic materials في المواد المعدنية. We can identify ان يمكن three types ثلاث انواع of dislocations

4.2.1 Screw Dislocations الانخلاعات البرمية

The screw dislocation (Figure 4.3) can be illustrated توضيحها by cutting قطع partway جزئياً through خلال a perfect crystal البلورة المثالية and then skewing انحراف the crystal by one atom spacing بمسافة ذرة واحدة. If we follow نتتبع a crystallographic plane المستوى البلوري one revolution دوران around حول the axis المحور on which the crystal is skewed تتحرك, starting at point x and traveling تنتقل equal atom spacings مسافات ذرية متساوية in each direction في كل اتجاه, it is finished تنتهي at point y one atom spacing below our starting point. If a screw dislocation are not present غير موجود, the loop would close مسار مغلق. The vector required المتجه الذي to complete لاكمال the loop المسار is the Burgers vector b هو متجه براغ. If it is continued استمر the rotation الدوران, it would trace out تتبع a spiral path مسار حلزوني. The axis المحور or line الخط around حول which it trace out تتبع this path هذا, is the screw dislocation. The Burgers vector is parallel موازي to the screw dislocation.

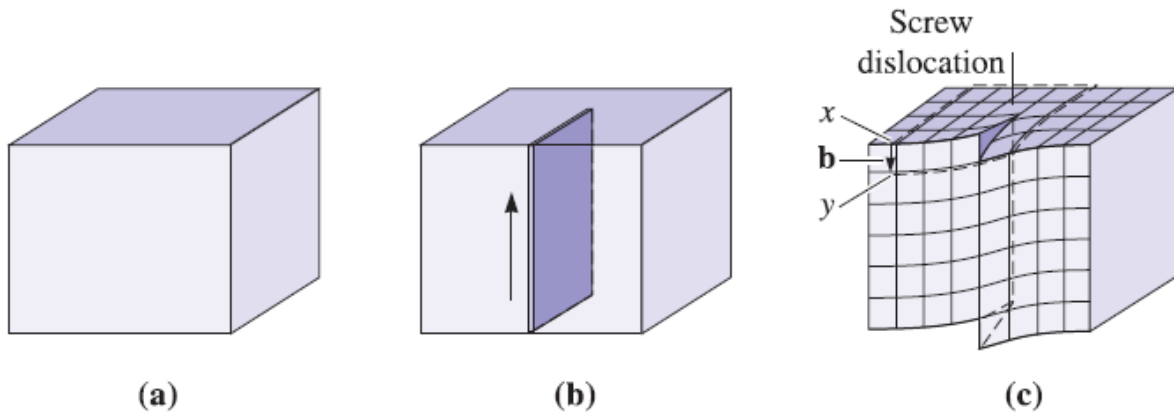


Figure 4.3 (a) The perfect crystal (b) is cut and sheared one atom spacing, and (c). The line along which shearing occurs is a screw dislocation. A Burgers vector b is required to close a loop of equal atom spacings around the screw dislocation.

4.2.2 Edge Dislocations الانخلاعات الحافي

An edge dislocation (Figure 4.4) can be illustrated يتوضح by slicing تقطيع partway جزئياً through a perfect crystal, spreading ينتشر the crystal apart جزء, and partly filling جزئياً the cut قطع with an extra half plane اضافي of atoms. The bottom edge الحافة السفلى of this inserted plane المستوي represents يمثل the edge dislocation انخلاع حافي. If we describe اذا وصفناه a clockwise عقارب الساعة loop وتتتبع around حول the edge dislocation, starting بدايتاً at point x and traveling تنتقل an equal number بعدد متساوي of atomic spacings المسافات الذرية in each direction في كل اتجاه, it is finished تنتهي at point y one atom spacing مسافة ذرية واحدة

from the starting point من نقطة البداية. The Burgers vector is perpendicular to the dislocation. A “ \perp ” symbol is often used غالبا يستخدم to denote ليُمثل an edge dislocation.

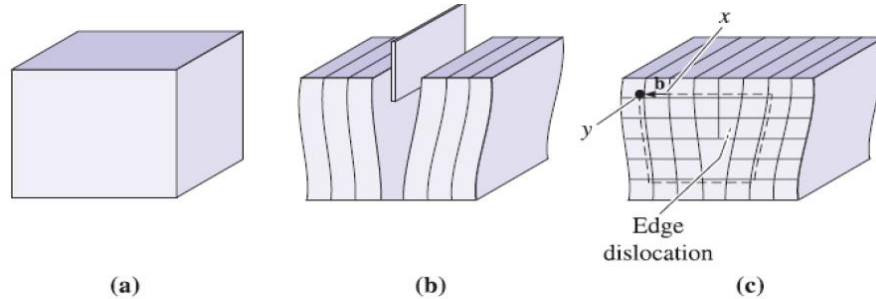


Figure 4-4 (a) The perfect crystal (b) in is cut and an extra half plane of atoms is inserted. (c) The bottom edge of the extra half plane is an edge dislocation. A Burgers vector b is required to close a loop of equal atom spacings around the edge dislocation.

4.2.3 Mixed Dislocations انخلاعات مختلطة

Mixed dislocations have both edge and screw components, with a transition region between them. The Burgers vector, however, remains the same for all portions of the mixed dislocation.

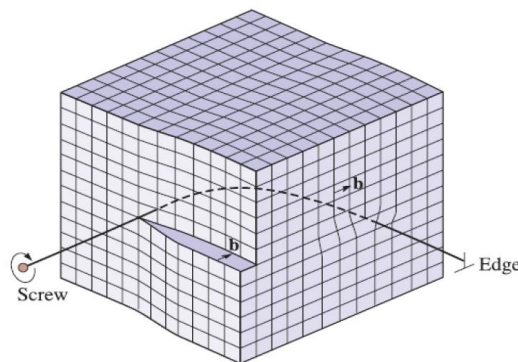


Figure 4.5 A mixed dislocation. The screw dislocation at the front face of the crystal gradually changes to an edge dislocation at the side of the crystal.

References

- 1- Fundamentals of Materials Science and Engineering, William D. Callister, Jr. David G. Rethwisch
- 2- Materials _Science_ and _Engineering_9th . William D. Callister, Jr. David G. Rethwisch