**Republic of Iraq**

**Ministry of Higher Education**

**and Scientific Research**

**Al-Mustaqbal University College**

**Chemical Engineering and Petroleum Industries Department**

# Subject: Materials Science and Engineering

## 2nd Class

## Lecture six

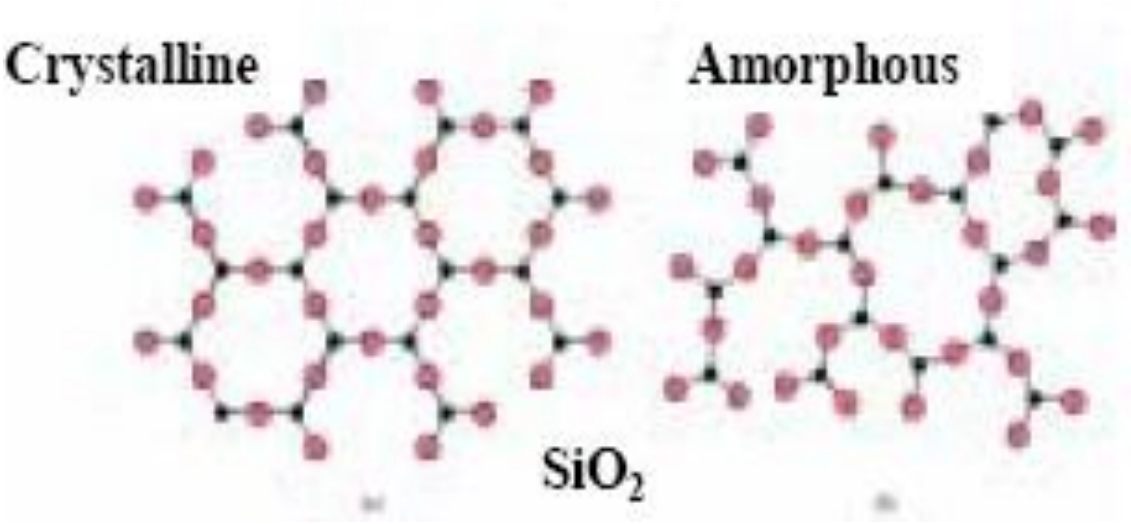
# The structure of crystalline solids

Solid materials may be classified according to the regularity with which atoms or ions are arranged with respect to one another. A **crystalline** material is one in which the atoms are situated in a repeating or periodic array over large atomic distances; that is, **long-range order** exists.

All metals, many ceramic materials, and certain polymers form crystalline structures under normal solidification conditions.

For those that do not crystallize, this long-range atomic order is absent; these are called ***noncrystalline*** or ***amorphous*** materials

المواد الصلبة تصنف حسب انتظام الذرات أوعلى ترتيب الايونات مع بعضها البعض . المواد البلورية هي المواد التي تكون فيها الذرات في صفيف متكرر أو دوري على مسافات ذرية كبيرة ؛ وهذا هو ، وجود ترتيب بعيد المدى.
جميع المعادن والعديد من المواد الخزفية وبعض البوليمرات تشكل هياكل بلورية تحت ظروف التصلب العادية.
بالنسبة لأولئك الذين لا يتبلورون ، فإن هذا النظام الذري البعيد المدى غائب ؛ وتسمى هذه المواد غير البلورية أو غير المتبلور

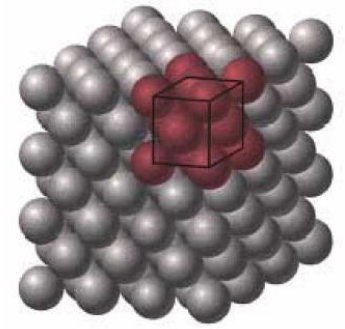



## Crystal structure:

Some of the properties of crystalline solids depend on the **crystal structure**. There is an extremely large number of different crystal structures all having long-range atomic order; these vary from relatively simple structures for metals, to exceedingly complex ones, as displayed by some of the ceramic and

polymeric .We can consider crystalline structure as a lattice of points at atom/sphere centers.

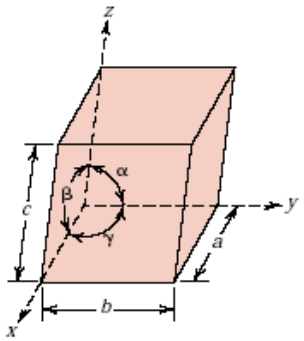
تعتمد بعض خواص المواد الصلبة البلورية على التركيب البلوري هناك عدد كبير للغاية من الهياكل البلورية المختلفة ، وكلها ذات ترتيب ذري بعيد .المدى ؛ هذه تختلف من هياكل بسيطة نسبيًا للمعادن ، إلى هياكل معقدة للغاية ، كما هو موضح في بعض السيراميك والبوليمرية. يمكننا اعتبار التركيب البلوري بمثابة شبكة من النقاط في مراكز الذرة / المجال.

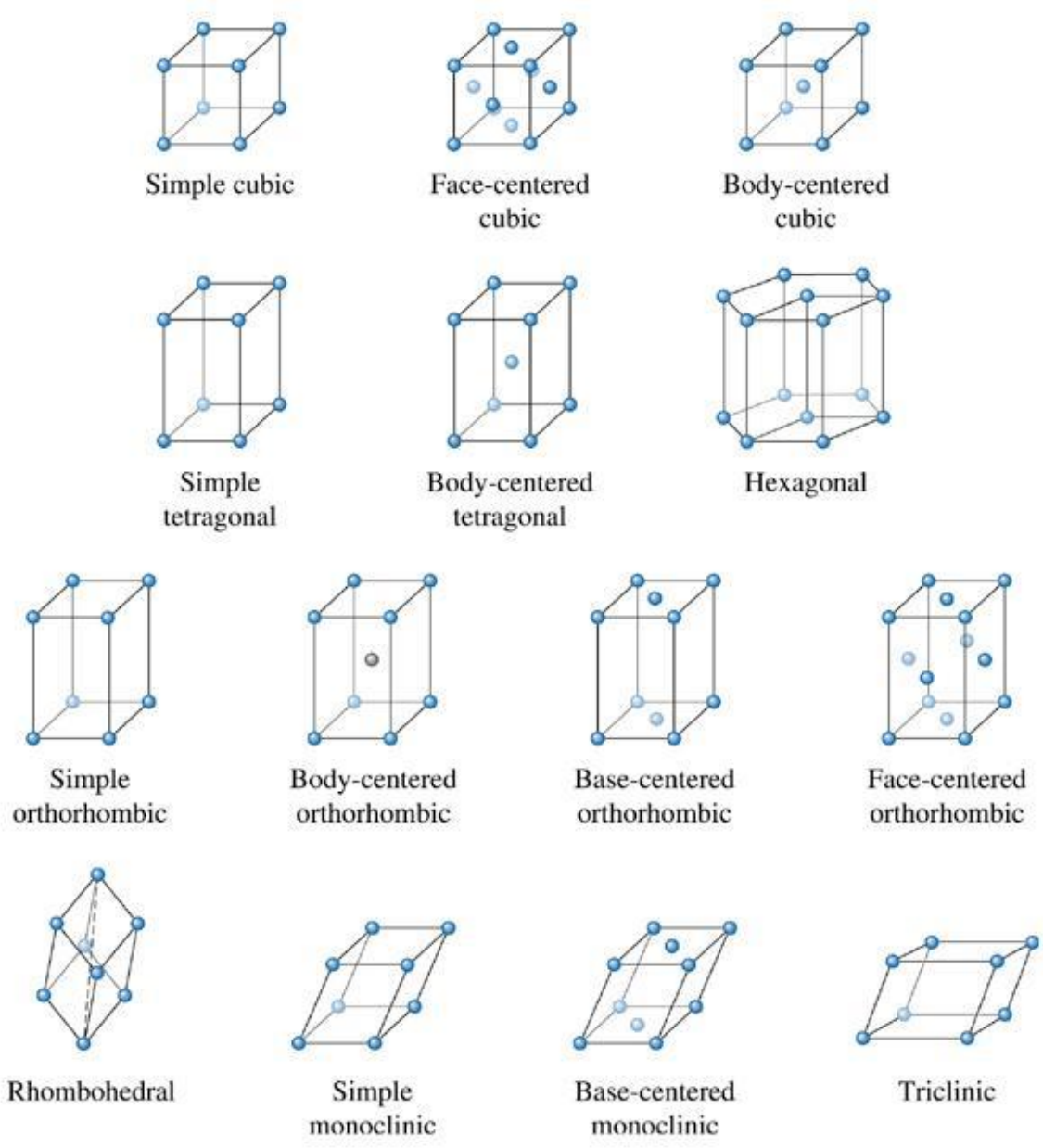


## Unit Cell :

The unit cell is the smallest structural unit or building block that can describe the crystal structure. Repetition of the unit cell generates the entire crystal. The shape of the unit cell is defined by lattice parameters :The **edge lengths** ( a, b, c ), **Angles** ( α, β, γ ). There are **fourteen** types of **Bravais lattices** grouped in **seven** crystal systems:

خلية الوحدة هي أصغر وحدة هيكلية أو كتلة بناء يمكنها وصف التركيب البلوري يتم تعريف شكل خلية .تكرار خلية الوحدة يولد البلورة بأكملها .الوحدة بواسطة معلمات شعرية: أطوال الحافة (أ ، ب ، ج) ، الزوايا (α ، β، γ). هناك أربعة عشر نوعًا من شبكات Bravais المجمعة في سبعة أنظمة بلورية :






The Fourteen Bravias Lattice

**TABLE 3-1 ■ *Characteristics of the seven crystal systems***

| Structure | Axes | Angles between Axes | Volume of the Unit Cell |
|---|---|---|---|
| Cubic | $a = b = c$ | All angles equal 90° | $a^3$ |
| Tetragonal | $a = b \neq c$ | All angles equal 90° | $a^2c$ |
| Orthorhombic | $a \neq b \neq c$ | All angles equal 90° | abc |
| Hexagonal | $a = b \neq c$ | Two angles equal 90°. One angle equals 120°. | $0.866a^2c$ |
| Rhombohedral or trigonal | $a = b = c$ | All angles are equal and none equals 90° | $a^3\sqrt{1 - 3\cos^2\alpha + 2\cos^3\alpha}$ |
| Monoclinic | $a \neq b \neq c$ | Two angles equal 90°. One angle ($\beta$) is not equal to 90° | $abc \sin\beta$ |
| Triclinic | $a \neq b \neq c$ | All angles are different and none equals 90° | $abc\sqrt{1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma}$ |

## Metallic Crystal Structures :

Metals are usually (poly)crystalline; although formation of amorphous metals is possible by rapid cooling. Since the atomic bonding in metals is non-directional ; no restriction on numbers or positions of nearest-neighbor atoms ; large number of nearest neighbors and dense atomic packingThe most common types of unit cells are the faced centered cubic (FCC), the body-centered cubic (FCC) and the hexagonal close-packed (HCP).In the studying of the crystalline structures , we interest with four parameters :

1- a/R relationship .

2- No. of atoms per unit cell.

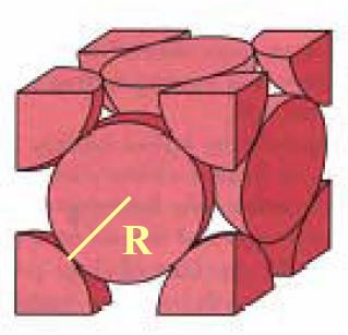
3-Coordination number(CN): the number of nearest-neighbor or touching atoms that surround specific atom.

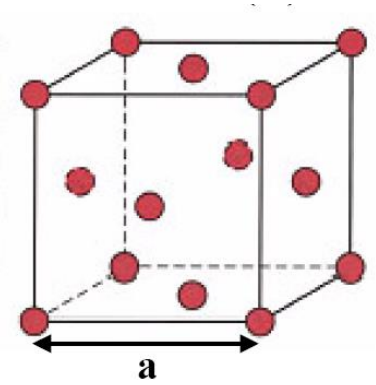
4-Atomic packing factor (APF): it is also called packing efficiency, and represents the fraction of atoms volume in a unit cell.

$$APF = \frac{volume of\ atoms\ in unit cell}{total unit cell volume}$$

## Face-Centered Cubic (FCC) Crystal Structure :

Atoms are located at each of the corners and on the centers of all the faces of cubic unit cell.




**Number of atoms per unit cell, n = 4**.

6 face atoms shared by two cells: 6 x 1/2 = 3

8 corner atoms shared by eight cells: 8 x 1/8 = 1

## Body-Centered Cubic (BCC) Crystal Structure:

Atom at each corner and at center of cubic unit cell

**Number of atoms per unit cell, n = 2**

Center atom (1) shared by no other cells: 1 x 1 = 1

8 corner atoms shared by eight cells: 8 x 1/8 = 1

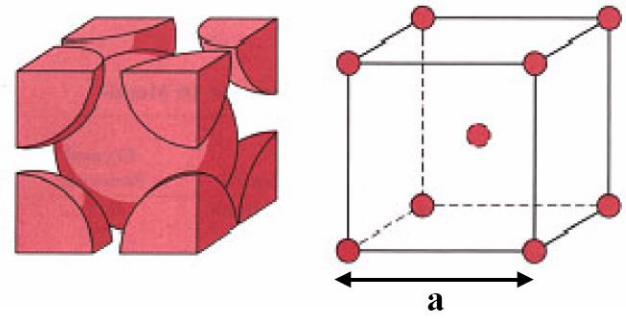


**TABLE 3-2 ■ *Crystal structure characteristics of some metals***

| Structure | $a_0$ versus $r$ | Atoms per Cell | Coordination Number | Packing Factor | Examples |
|---|---|---|---|---|---|
| Simple cubic (SC) | $a_0 = 2r$ | 1 | 6 | 0.52 | Polonium (Po), α-Mn |
| Body-centered cubic | $a_0 = 4r/\sqrt{3}$ | 2 | 8 | 0.68 | Fe, Ti, W, Mo, Nb, Ta, K, Na, V, Zr, Cr |
| Face-centered cubic | $a_0 = 4r/\sqrt{2}$ | 4 | 12 | 0.74 | Fe, Cu, Au, Pt, Ag, Pb, Ni |
| Hexagonal close-packed | $a_0 = 2r$<br>$c_0 \approx 1.633a_0$ | 2 | 12 | 0.74 | Ti, Mg, Zn, Be, Co, Zr, Cd |

## Example 3.2
## Determining the Relationship between Atomic Radius and Lattice Parameters

Determine the relationship between the atomic radius and the lattice parameter in SC, BCC, and FCC structures when one atom is located at each lattice point.

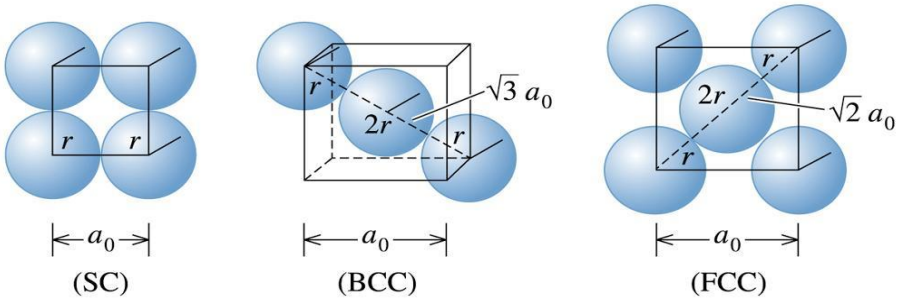





**Figure 3.14 The relationships between the atomic radius and the Lattice parameter in cubic systems (for Example 3.2).**

Example 3.2 SOLUTION

Referring to Figure 3.14, we find that atoms touch along the edge of the cube in SC structures.

$$a_0 = 2r$$

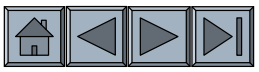
In BCC structures, atoms touch along the body diagonal. There are two atomic radii from the center atom and one atomic radius from each of the corner atoms on the body diagonal, so

$$a_0 = \frac{4r}{\sqrt{3}}$$

In FCC structures, atoms touch along the face diagonal of the cube. There are four atomic radii along this length—two radii from the face-centered atom and one radius from each corner, so:

$$a_0 = \frac{4r}{\sqrt{2}}$$





## Example 3.3
## Calculating the Packing Factor

Calculate the packing factor for the FCC cell.

Example 3.3 SOLUTION

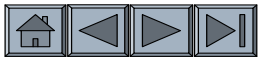
In a FCC cell, there are four lattice points per cell; if there is one atom per lattice point, there are also four atoms per cell. The volume of one atom is $4\pi r^3/3$ and the volume of the unit cell is $a_0^3$

$$\text{Packing Factor} = \frac{(4\,\text{atoms/cell})(\frac{4}{3}\pi r^3)}{a_0^3}$$

$$\text{Since, for FCC unit cells, } a_0 = 4r/\sqrt{2}$$

$$\text{Packing Factor} = \frac{(4)(\frac{4}{3}\pi r^3)}{(4r/\sqrt{2})^3} = \frac{\pi}{\sqrt{18}} \cong 0.74$$





**Note:**

As a general rule to determine the number of atoms per unit cell for cubic crystalline system:

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

**Where:**

**$N_i$: No. of atoms in the center of cube.**

**$N_f$: No. of atoms in the faces of cube.**

**$N_c$: No. of atoms in the corners of cube.**