Fundamentals of Materials Science Homework 7

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Homework Problems:

1. **Please describe in your own understanding what the crystal structure is. You are expected to describe in both Chinese and English. Your description should be from two directions as I discussed in class. One is from Space Lattice to Crystal Structure, while the other way is to extract the concept of Space Lattice from Crystal Structure. Please show me that you really understand the concept.**

Solution:

From Space Lattice to Crystal Structure:

in English:

A space lattice is an infinite,periodic array of mathematical points,in which each point has identical surroundings to all others.

The motif is the group of atoms repeated an each lattice point.

So A Crystal structure=Lattice+Motif (Atom decoration;Basis)

中文：

空间点阵是数学点的无限周期阵列，其中每个点具有与所有其他点相同的周围环境。（即在任取一点，空间点阵就是与该点相同的所有点构成集合。这些点是相同的且具有相同的相对位置。）

结构基元是每个点阵点重复的原子组。

晶体结构=空间点阵+结构基元

From Crystal Structure to Space Lattice :

in English:

To the atomic center through some of the illusion of the atom in the three-dimensional space in the form of geometric arrangement drawn, the intersection point called the node. Each node is the center of the atom. Such an abstract model representing the arrangement of atoms in the crystal is called "spatial lattice" or "lattice".

中文：

以通过原子中心的一些假想连线把原子在三维空间的几何排列形式描绘出来，连线交点称之为结点。每个结点都是原子的中心所在位置。这样的表示晶体中原子排列的抽象模型叫做“空间点阵”或“晶格”。

2. **Show for the body-centered cubic crystal structure that the unit cell edge length *a* and the atomic radius *R* are related through** $a = 4R/\sqrt{3}$ **.**

Solution:

The coordination number=8

$$(4R)^2 = a^2 + \left(\sqrt{2}a\right)^2 \quad \therefore a = \frac{4R}{\sqrt{3}}$$

3. Calculate the atomic radius in cm for the following: (a) BCC metal with a = 0.3294 nm; and (b) FCC metal with a = 4.0862 Å.

Solution:

For BCC metal: $\because a = \frac{4R}{\sqrt{3}} \quad \therefore R = \frac{\sqrt{3}a}{4} = \frac{\sqrt{3}}{4} \times 0.3294nm = 1.4263 \times 10^{-8} cm$

For FCC metal: $\because a = 2R\sqrt{2} \quad \therefore R = \frac{a}{2\sqrt{2}} = \frac{1}{2\sqrt{2}} \times 4.0862 \overset{0}{\text{A}} = 1.4449 \times 10^{-8} cm$

4. Calculate the lattice parameter of each of the following elements using their atomic radii: (a) iron, (b) aluminum, (c) copper, and (d) magnesium.

Solution:

(a) ∵ iron is the BCC metal , atomic radii=0.1241nm

$$\therefore a = \frac{4R}{\sqrt{3}} = \frac{4}{\sqrt{3}} \times 0.1241nm = 0.2866nm$$

(b) ∵ aluminum is the FCC metal , atomic radii=0.1431nm

$$\therefore a = 2R\sqrt{2} = 2\sqrt{2} \times 0.1431nm = 0.4047nm$$

(c) ∵ copper is the FCC metal , atomic radii=0.1278nm

$$\therefore a = 2R\sqrt{2} = 2\sqrt{2} \times 0.1278nm = 0.3614nm$$

(d) ∵ magnesium is the HCP metal , atomic radii=0.16nm

$$\therefore a = 2R = 2 \times 0.16nm = 0.32nm$$

5. Determine the crystal structure for the following: (a) a metal with a = 4.9489 Å, r = 1.75 Å, and one atom per lattice point; and (b) a metal with a = 0.42906 nm, r = 0.1858 nm and one atom per lattice point.

Solution:

$$BCC: a = \frac{4R}{\sqrt{3}} \qquad FCC: a = 2R\sqrt{2}$$

(a) $\because \dfrac{a}{r} = \dfrac{4.9489\,\overset{0}{\text{A}}}{1.75\,\overset{0}{\text{A}}} = 2.828 = 2\sqrt{2} \quad \therefore \text{FCC}$

(b) $\because \dfrac{a}{r} = \dfrac{0.42906nm}{0.1858nm} = 2.309 = \dfrac{4}{\sqrt{3}} \quad \therefore \text{BCC}$

6. If the atomic radius of aluminum is 0.143 nm, calculate the volume of its unit cell in cubic meters. What is its coordination number and atomic packing factor? Please show your calculations.

Solution:

$\because$ Aluminum is the FCC metal $\quad \therefore a = 2R\sqrt{2}$

$$a^3 = \left(2R\sqrt{2}\right)^3 = \left(2\sqrt{2} \times 0.143nm\right)^3 = 6.62 \times 10^{-29} m^3$$

the coordination number：12

$$APF = \frac{\left(8 \times \frac{1}{8} + 6 \times \frac{1}{2}\right) \times \frac{4}{3}\pi R^3}{16\sqrt{2}R^3} = 74\%$$

7. Assume that a metal exists having a simple cubic crystal structure, that is, atoms located only at the corners of a cube and touching one another along the cube edge (shown below). (a) What is the coordination number for this crystal structure? (b) Calculate the atomic packing factor.

Solution:

(a) Coordination number: 6

(b) $\because a = 2R \quad \therefore APF = \dfrac{\left(8 \times \frac{1}{8}\right) \times \frac{4}{3}\pi R^3}{2R^3} = 52\%$