FSK324 Solid State Physics
Test 1 - memo

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1. i.) Amorphous materials: are those in which there exists ordering only at the short distance range and not at long range.

   Poly-crystalline materials: consist of small, single-crystal grains characterized by grain boundaries.

   Single-crystals: are materials in which there is a periodic ordering of atoms, or groups of atoms, over a longer distance range.

   ii.) A vacancy is the *permanent* absence of an atom or groups of atoms from the expected "normal" position in a lattice due to temperature effects above zero kelvin.

   A Schottky defect is a vacancy in which the atom or group of atoms leaves its position and sits on the surface. (Contrast this with a Frenkel pair, where the atom or group of atoms form a vacancy but sits in the interstitial spaces of the lattice. An analogy is a thermally generated "hole-electron" pair in the bulk of an intrinsic semiconductor. The hole is the vacancy).

2. i.) For the Wigner-Seitz unit cell and construction, refer to your class notes.

   ii.) A Brillouin zone is the result of constructing a Wigner-Seitz cell in reciprocal lattice space.

3. Given that $\bar{A} = (\bar{a}_1, \bar{a}_2, \bar{a}_3)$ and $\bar{B} = (\bar{b}_1, \bar{b}_2, \bar{b}_3)$, let V_c define the volume of the unit cell in the form of a parallel-piped, whose sides in normal lattice space are $\bar{A}$. The volume of such a parallel-piped is the scalar:

$$V_c = \bar{a}_p \cdot (\bar{a}_q \wedge \bar{a}_r), \qquad \text{for all} \qquad p, q, r \in \{1, 2, 3\}, \qquad \text{where} \qquad p \neq q \neq r.$$

   By definition,

$$b_1 = \frac{2\pi}{V_c} a_2 \wedge a_3, \quad b_2 = \frac{2\pi}{V_c} a_3 \wedge a_1, \quad b_3 = \frac{2\pi}{V_c} a_1 \wedge a_2.$$

   As a consequence of these cross (vector) products, $b_1 \perp (a_2,\ a_3)$, $b_2 \perp (a_1,\ a_3)$ and $b_3 \perp (a_1,\ a_2)$. Now consider the scalar product

$$\bar{b}_p \cdot \bar{a}_q = \begin{cases} \text{if } p = q \ \text{ then } \ \bar{b}_p \cdot \bar{a}_q = \bar{b}_p \cdot \bar{a}_p = \frac{2\pi}{V_c}(\bar{a}_q \wedge \bar{a}_r) \cdot \bar{a}_p = \frac{2\pi}{V_c} \times V_c = 2\pi \\ \text{if } p \neq q \ \text{ then } \ \bar{b}_p \cdot \bar{a}_q = \frac{2\pi}{V_c}(\bar{a}_q \wedge \bar{a}_r) \cdot \bar{a}_q = \frac{2\pi}{V_c}|\bar{a}_q \wedge \bar{a}_r||\bar{a}_q| \cos 90^o = 0. \end{cases}$$

   The definition of the Kronecker delta (see also Wikipedia) is

$$\delta_{ij} = \begin{cases} 1, & \text{if } i = j \\ 0, & \text{if } i \neq j \end{cases}$$

   which leads immediately to $\bar{b}_i \cdot \bar{a}_j = 2\pi\delta_{ij}$ for all combinations of $i, j \in \{1, 2, 3\}$. (QED)

4. i.) In class it was shown that the distance between the *hkl* planes is d_{hkl}, where

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

   and where a is the lattice parameter. In FCC the number of atoms n is given by:

$$n = 8 \text{ corners} \times \frac{1}{8} \text{ atoms per corner} + 6 \text{ faces} \times \frac{1}{2} \text{ atoms per face} = 4 \text{ atoms.}$$

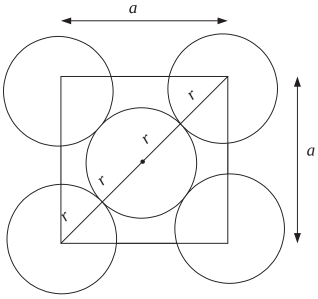


Figure 1: FCC showing the face diagonal.

Each mol weighs M grams and contains N_A atoms, where $N_A = 6.022 \times 10^{23}$ atoms per mol. Each atom must weigh M/N_A grams. The unit cell having n atoms therefore weighs nM/N_A grams. Since the unit cell is still gold, it has the same density ρ such that

$$\rho = \frac{\text{total mass of unit cell}}{\text{volume of unit cell}} = \frac{nM/N_A}{a^3}.$$

Hence

$$a = \sqrt[3]{\frac{nM}{\rho N_A}} = \sqrt[3]{\frac{4 \times 197g}{19.3\text{g cm}^{-3} \times 6.022 \times 10^{23}}} = 4.078 \times 10^{-8}\text{cm}.$$

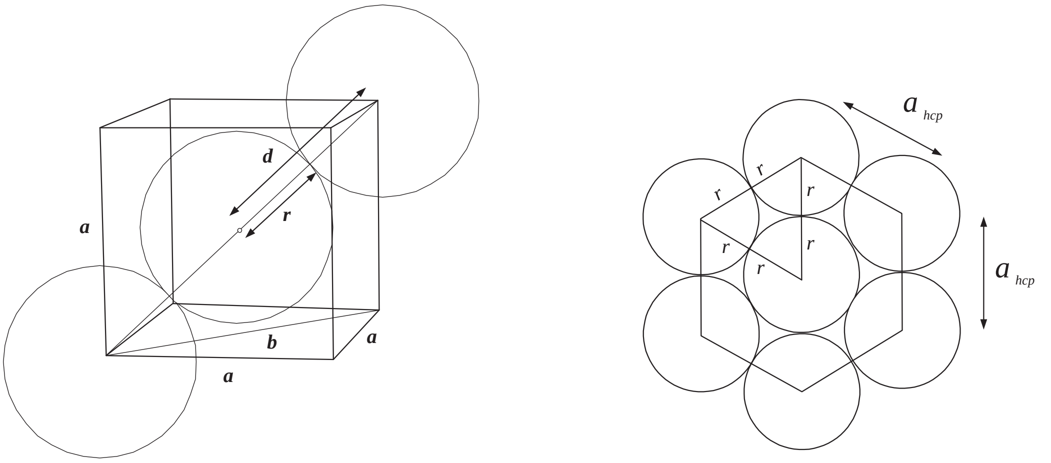
Therefore $a = 4.078$Å or 0.4078nm. Hence

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{4.078}{\sqrt{1^2 + 1^2 + 1^2}} = \frac{4.078}{\sqrt{3}} = 0.235\text{nm}.$$

ii.) To find the atomic radius consider only one face, as shown in Fig. 1. Evidently the length of the diagonal is $4r$, where r is the radius of each hard sphere. Then

$$(4r)^2 = a^2 + a^2 \quad \Rightarrow \quad r = \frac{a}{\sqrt{8}} = \frac{0.4078}{\sqrt{8}} \approx 0.1442\text{nm}.$$

5. See your notes for the proof that in HCP $c/a = \sqrt{8/3}$. It was done in class.
6. Computing the lattice parameter under the Martensitic transformation at first appears difficult, but inspection of the geometry shows that once the constant sodium atomic radius is known from BCC, the lattice parameter



(a) BCC diagonal showing bond length $d = 2r$.

(b) Base or top hexagon showing equilateral triangles.

Figure 2: Martensitic transformation of sodium from BCC to HCP phase.

a_{hcp} in HCP phase is easy to find. Consider the nearest neighbour distance or bond length, for BCC shown in Fig. 2(a).

Clearly

$$d^2 = \left(\frac{b}{2}\right)^2 + \left(\frac{a}{2}\right)^2 \quad \text{where} \quad b^2 = a^2 + a^2 \quad \Rightarrow d = 2r = \frac{a\sqrt{3}}{2} \quad \Rightarrow r = \frac{a\sqrt{3}}{4}.$$

From Fig. 2(b),

$$a_{hcp} = 2r = d = a\frac{\sqrt{3}}{2}$$

This implies that $a_{hcp} = 0.423 \times \sqrt{3}/2 \approx 0.366$nm. Finding c_{hcp} is then trivial, i.e.

$$\frac{c_{hcp}}{a_{hcp}} = \sqrt{\frac{8}{3}} \quad \Rightarrow \quad c_{hcp} = a_{hcp}\sqrt{\frac{8}{3}} \quad \Rightarrow \quad c_{hcp} = a\sqrt{2}.$$

or $c_{hcp} = 0.423 \times \sqrt{2} \approx 0.598$nm. From this point one might need to know how many full (sodium) atoms occupy the HCP structure. Since the density is known from BCC, the volume can be found from HCP using a_{hcp} and c_{hcp}, determining n is trivial. I leave this as an exercise for you.

7. Refer to your class notes for the solution to this problem.

8. Define $\bar{G} = h\bar{b}_1 + k\bar{b}_2 + l\bar{b}_3$ and $\bar{r}_j = x_j\bar{a}_1 + y_j\bar{a}_2 + z_j\bar{a}_3$. Then $\bar{G} \cdot \bar{r}_j = hx_j + ky_j + lz_j$. This is because $\bar{b}_i \cdot \bar{a}_j = 2\pi\delta_{ij}$ (see problem 3). Consequently replacing the continuum integral with N discrete points summed over j gives

$$S_{\overline{G}}(hkl) = \sum_{j}^{N} f_j e^{-2\pi i(hx_j + ky_j + lz_j)}$$

provided that the atomic form factor can be defined such that

$$f_j = \int n_j(\bar{\rho}) e^{-i\bar{G}\cdot\bar{\rho}} dV.$$

For the next items please refer to the earlier memos given to you.

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