Solid State Physics Hw 4

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Problems Chapter 12

12.1

Consider the NaCl crystal structure shown in Fig. 12.21. If the lattice constant is $a = 0.563nm$, what is the distance from a sodium atom to the nearest chlorine? What is the distance from a sodium atom to the nearest other sodium atom?

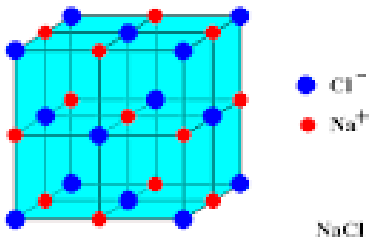


Figure 1: Crystal structure fro NaCl

Now if we consider the crystal structure shown in 1 it is clear that the distance between sodium atom and chlorine has to be half the distance of the unit cell

$$d = \frac{a}{2} = .2185nm$$

If so then for the distance between sodium - sodium can be calculated by applying Pythagoras theorem :

$$d = a \cdot \sqrt{\frac{1}{2}^2 + \frac{1}{2}^2} = \frac{a}{\sqrt{2}} = .398nm$$

12.3

The diagram of Fig. 12.22 shows a plan view of a structure of cubic ZnS (zincblende) looking down the z axis. The numbers attached to some atoms represent the heights of the atoms above the z = 0 plane expressed as a fraction of the cube edge a. Unlabeled atoms are at z = 0 and z = a. (a) What is the Bravais lattice type? (b) Describe the basis. (c) Given that a = 0.541 nm, calculate the nearestneighbor Zn–Zn, Zn–S, and S–S distances.

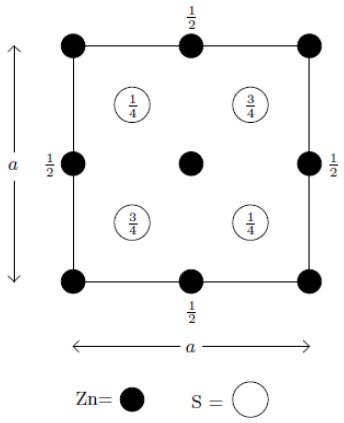


Figure 2: Crystal structure fro ZnS

It is clear from 2 that the lattices type has to be FCC or Face centred since we have an atom of Zn in the center of one of the sides of the structure. Form the structure we can also tell that Zn $[0,0,0]$ and the nearest S which is the one in the first quadrant nearest to Zn is $\left[\frac{1}{4},\frac{1}{4},\frac{3}{4}\right]$.
Now just as we shown in the first problem we can apply the same approach to calculate the distances S-S Zn-S Zn-Zn , we must be careful with two thing in 2 we can see that instead of all Zn being in the same plane , the ones between opposing corners are in a plain coming out of the page by a/2 so just as in the last problem $d_{Zn-Zn} = a/\sqrt{2} = 0.383nm$, For Zn-S it is clear that the closest S in in bad notation $\left[\frac{1}{4},\frac{1}{4},-\frac{1}{4}\right]$ and applying Pythagoras $d_{Zn-S} = a \cdot \sqrt{1/16+1/16+1/16} = 0.234nm$ an just as before $d_{S-S} = a/\sqrt{2} = 0.383nm$

Problems Chapter 13

13.1

Show that the reciprocal lattice of a fcc (face-centered cubic) lattice is a bcc (body-centered cubic) lattice. Correspondingly, show that the reciprocal lattice of a bcc lattice is an fcc lattice. If an fcc lattice has conventional unit cell with lattice constant a, what is the lattice constant for the conventional unit cell of the reciprocal bcc lattice? Consider now an orthorhombic face-centered lattice with conventional lattice constants a1, a2, a3. What it the reciprocal lattice now?

Lets recall that by definition

$$b_i = \frac{2\pi \cdot (a_j \times a_k)}{a_1 \cdot (a_2 \times a_3)} \tag{1}$$

for any cyclical combination of 1,2,3 so we can apply this to the primitive lattice vectors and transform to the reciprocal basis so for simplicity lest show BCC→FCC, lets remember that that standard basis

$$BCC \rightarrow [1,0,0], [0,1,0], \left[\frac{1}{2},\frac{1}{2},\frac{1}{2}\right]$$

this basis is in units of a so lets focus in the denominator of eq. 1

$$a_1 \cdot (a_2 \times a_3) \rightarrow a_2 \times a_3 = a^2 \cdot \left(\frac{1}{2}, 0, -\frac{1}{2}\right) \rightarrow a_1 \cdot (a_2 \times a_3) = \frac{a^3}{2}$$

Now lets see what the numerator for b_1, b_2, b_3 as in eq. 1

$$\begin{aligned} b_1 \rightarrow a_2 \times a_3 =& a^2 \cdot \left(\frac{1}{2}, 0, -\frac{1}{2}\right) \rightarrow b_1 = \frac{4\pi}{a}\left(\frac{1}{2}, 0, -\frac{1}{2}\right) \\ b_2 \rightarrow a_3 \times a_1 =& a^2 \cdot \left(0, \frac{1}{2}, -\frac{1}{2}\right) \rightarrow b_2 = \frac{4\pi}{a}\left(0, \frac{1}{2}, -\frac{1}{2}\right) \\ b_3 \rightarrow a_1 \times a_2 =& a^2 \cdot (0, 0, 1) \rightarrow b_3 = \frac{4\pi}{a}(0, 0, 1) \end{aligned}$$

Now this is not the basis for FCC but we now that any liner combination of a basis is also a basis so lets look for combinations to generate the basis of FCC. First lets notice that b_1, b_2 are very close to what we want but with out the minus sing in in z so we can add to both of them b_3 and we would have the right expression now for lets remember that the basis for FCC is a cyclical rotation of a zero in a vector that has $1/2$ in the non zero position.

$$b_1' = b_1 + b_3 = \frac{4\pi}{a}\left(\frac{1}{2}, 0, \frac{1}{2}\right) \rightarrow b_2' = b_2 + b_3 = \frac{4\pi}{a}\left(0, \frac{1}{2}, \frac{1}{2}\right)$$

$$b_3' = b_1 + b_2 + b_3 \rightarrow \frac{4\pi}{a}\left(\frac{1}{2}, \frac{1}{2}, 0\right)$$

$$FCC \rightarrow \left[\frac{1}{2}, \frac{1}{2}, 0\right], \left[\frac{1}{2}, 0, \frac{1}{2}\right], \left[0, \frac{1}{2}, \frac{1}{2}\right]$$

Now for FCC→BCC its easy to see that :

$$a_2 \times a_3 = \left(-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}\right) \rightarrow a_1 \cdot (a_2 \times a_3) = -\frac{a^3}{4}$$

$$b_1 = \frac{4\pi}{a}\left(-\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\right), b_2 = \frac{4\pi}{a}\left(-\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\right), b_3 = \frac{4\pi}{a}\left(\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}\right)$$

$$b_1' = b_1 + b_2 = \frac{4\pi}{a}(1, 0, 0), \; b_2' = b_1 + b_3 = \frac{4\pi}{a}(0, 1, 0)$$

$$b_3' = b_1 + b_2 + b_3 = \frac{4\pi}{a}\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$$

Witch its clear its BCC so its we can see how one basis transforms to an other in the reciprocal space. If each side of the cube has a different length we can adapt the calculations don before as follows

$$BCC \rightarrow [a_1, 0, 0], [0, a_2, 0], \left[\frac{a_1}{2}, \frac{a_2}{2}, \frac{a_3}{2}\right]$$

$$a_1 \cdot (a_2 \times a_3) \rightarrow a_2 \times a_3 = \frac{a_1 a_2 a_3}{2}$$

$$b_1 \rightarrow a_2 \times a_3 = \left(\frac{a_1}{2}, 0, -\frac{a_2}{2}\right) \rightarrow b_1 = 4\pi\left(\frac{1}{2a_1}, 0, -\frac{1}{2a_3}\right)$$

such that we can infer that the only difference in the calculation done previously is that each entrey of the respective $a_1\ a_2\ a_3$ has a value of $\frac{2\pi}{a_i}$.

13.3

- ‡Explain briefly what is meant by the terms "crystal planes" and "Miller indices".
- Show that the general direction [hkl] in a cubic crystal is normal to the planes with Miller indices (hkl).
- Is the same true in general for an orthorhombic crystal?
- Show that the spacing d of the (hkl) set of planes in a cubic crystal with lattice parameter a is $d = \frac{a}{\sqrt{h2+k2+l2}}$
- What is the generalization of this formula for an orthorhombic crystal

A crystal plane is one such that it intersects at least three non-co-linear points of the unit cell or the lattice, and the miller indices is a set of integers witch represent a plane that can construct a vector in the reciprocal space as

$$\mathbf{G}_{(hkl)} = h \cdot \vec{b}_1 + k \cdot \vec{b}_2 + l \cdot \vec{b}_3$$

which can be constructed by finding the intersection of the unit cell with the plane. Now lets suppose a orthorhombic lattice such with lengths $\vec{a}_1,\ \vec{a}_2,\ \vec{a}_3$ a plane (hkl) is defined by being on such that $\vec{a}_1/h,\ \vec{a}_2/k,\ \vec{a}_3/l$ are connected so to make a vector normal to this on we know from linear algebra that we can take the cross product between to non co-linear vectors in the plane $P_{(hkl)}$.

$$\vec{p}_1,\ \vec{p}_2\ \epsilon\ P_{(hkl)} \rightarrow \vec{p}_1 = \frac{\vec{a}_1}{h} - \frac{\vec{a}_2}{k},\ \vec{p}_2 = \frac{\vec{a}_1}{h} - \frac{\vec{a}_3}{l}$$

$$\vec{p}_1 \times \vec{p}_2 = \left(\frac{\vec{a}_1}{h} - \frac{\vec{a}_2}{k}\right) \times \left(\frac{\vec{a}_1}{h} - \frac{\vec{a}_3}{l}\right) = -\frac{\vec{a}_1 \times \vec{a}_3}{hl} + \frac{\vec{a}_2 \times \vec{a}_3}{kl} - \frac{\vec{a}_2 \times \vec{a}_1}{hk}$$

$$= \frac{\vec{a}_1}{lk} + \frac{\vec{a}_2}{hl} - \frac{\vec{a}_3}{hk} = \frac{1}{lhk}\left(h\vec{a}_1 + k\vec{a}_2 - l\vec{a}_3\right) \rightarrow \mathbf{G} \cdot (\vec{p}_1 \times \vec{p}_2) = \pm 1$$

its clear that the vectors are co-linear such that the plan and the unit vector are orthogonal.Noe by definition in [1] we can find the spacing between adjacent planes in a family specified by the indices (hkl) as follows

$$d_{(hkl)} = \frac{2\pi}{|\mathbf{G}|} \rightarrow |\vec{b}_1|^2 = 1 \rightarrow |\mathbf{G}| = \sqrt{h^2|\vec{b}_1|^2 + k^2|\vec{b}_2|^2 + l^2|\vec{b}_3|^2}$$

$$d_{(hkl)} = \frac{2\pi}{\sqrt{h^2|\vec{b}_1|^2 + k^2|\vec{b}_2|^2 + l^2|\vec{b}_3|^2}}$$

Problems Chapter 14

14.1

Consider the lattice described in Exercise 13.5 (a two-dimensional rectangular crystal having a unit cell with sides a 1 =0.468 nm and a =0.342 nm).A collimated beam of monochromatic X-rays with wavelength 0.166 nm is used to examine the crystal. (a) Draw to scale a diagram of the reciprocal lattice. (b) Calculate the magnitude of the wave vectors k and k' of the incident and reflected X-ray beams, and hence construct on your drawing the "scattering triangle" corresponding to the Laue condition $\Delta k = \mathbf{G}$ for diffraction from the (210) planes (the scattering triangle includes k, k and Δk).

14.2

BaTiO has a primitive cubic lattice and a basis with atoms having fractional coordinates Ba [0,0,0] Ti [1/2,1/2,1/2] O[1/2,1/2,0],[1/2,0,1/2], [0,1/2,1/2].

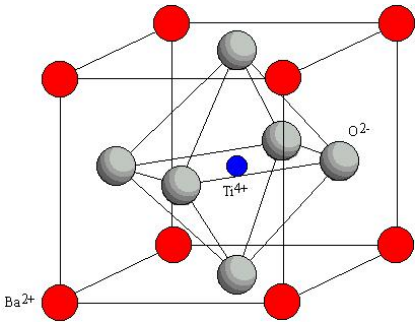


Figure 3: Crystal structure fro $BaTiO_3$

By definition we know the structure factor

$$S_{(hkl)} = \sum_d f_d \; e^{i\mathbf{k}_{(hkl)}\mathbf{R}_d} \qquad (2)$$

where $\mathbf{R}$ is the position of an atom d in the unit such that $\mathbf{R} = (x_d, y_d, z_d)$ now $\mathbf{k} = (h, k, l)$ and remember that $b_i \cdot a_i = 2\pi\delta_{ij}$ applying this to the structure factor.

$$S_{(hkl)} = \sum_d f_d e^{2\pi i(hx_d + ky_d + lz_d)}$$

Now since we are going to take the the form factor y proportional to Z_d, since we are interested in the plane (00l)→ h=k=0, now if we apply the sum to the different atoms we can see the individual structure factor

$$S_{(hkl)} = f_{Ba}e^{2\pi il0} + f_{Ti}e^{2\pi il\frac{1}{2}} + f_O\left(e^{2\pi il0} + e^{2\pi il\frac{1}{2}} + e^{2\pi il\frac{1}{2}}\right)$$

$$S_{(hkl)} = Z_{Ba} + (-1)^l Z_{Ti} + Z_O(1 + 2(-1)^l)$$

Now if we know that the intensity it proportional to the square of the form factor, then if we calculate the ratio we get ($Z_{Ba} = 56,\ Z_{Ti} = 22, Z_o = 8$)

$$\frac{I_{(002)}}{I_{(001)}} = \frac{(Z_{Ba} + Z_{Ti} + 3Z_O)^2}{(Z_{Ba} - Z_{Ti} - Z_O)^2} \approx 15.4$$

References

[1] Steven H. Simon (2013) The Oxford Solid State Basics. *Oxford*. 76-160.