1 Chapter 6

6.2 - The FCC lattice as a simple cubic with a basis

a) The FCC lattice can be represented as a simple cubic lattice with the basis

\[ d_1 = 0, \quad d_2 = \frac{a}{2} (\hat{x} + \hat{y}), \quad d_3 = \frac{a}{2} (\hat{y} + \hat{z}), \quad d_4 = \frac{a}{2} (\hat{x} + \hat{z}). \]  

Furthermore, the reciprocal lattice vectors are of the form

\[ K = \frac{2\pi}{a} (n_1, n_2, n_3), \]  

where \( n_i \) are integers. We now calculate the structure factor

\[ S_K = \sum_{j=1}^{4} e^{i K d_j} = 1 + e^{\pi i n_1} + e^{\pi i n_2} + e^{\pi i n_3}. \]  

However, \( e^{\pi i} = -1 \) so we get

\[ S_K = 1 + (-1)^{n_1} + (-1)^{n_2} + (-1)^{n_3}. \]  

By testing out a few different values for \( n_i \) we may find that if \( \sum n_i \) is even then \( S_K = 4 \) and if it odd then \( S_K = 0 \)

\[ S_K = \begin{cases} 4 & \sum_{i=1}^{3} n_i = \text{even} \\ 0 & \sum_{i=1}^{3} n_i = \text{odd} \end{cases} \]  

b) We hence see that treating an FCC lattice as a simple cubic lattice with a basis shows us that we get constructive interference \( K = k - k' \), where \( k \) and \( k' \) are the wave vectors of the incoming and outgoing light, when \( K \) is in the form

\[ K = \frac{2\pi}{a} (n_1, n_2, n_3), \]  

where \( \sum_i n_i \) is even. However, from (4.2) we know that such vectors form a BCC lattice. Since the reciprocal lattice of the FCC lattice is a BCC lattice this is what we expect.

6.5 - Sodium chloride and zincblende structures

a) The sodium chlorid (NaCl) structure can be thought of as an FCC lattice with cube side \( a \) where at each point of the lattice you put a positively charge ion and then an negatively charged ion at the point \((a/2)\hat{x}\). We hence have the following basis

\[ d_+ = 0 \quad \text{positive ion}, \]  

\[ d_- = \frac{a}{2} \hat{x} \quad \text{negative ion}. \]
The reciprocal lattice has a BCC structure which can be written in the form

\[ \mathbf{K} = \frac{4\pi}{a} (\nu_1 \hat{x} + \nu_2 \hat{y} + \nu_3 \hat{z}), \]

where all \( \eta_i \) are either integers or all integers +1/2. Try to draw this and see that this is indeed a way to represent a BCC structure. For example if all \( \nu_i = 0 \) we get one of the corners of a cubic cell and if we then take all \( \nu_i = 1/2 \) we get the center point.

In this case we have we have two different types of ions sitting at the different points in the basis and we must take into account the different form factors (the different ions will scatter light differently in different directions). Let \( f_+ \) and \( f_- \) be the form factors in the different directions. We then get the following structure factor

\[ S_\mathbf{K} = \sum_i f_i e^{i \mathbf{K} \cdot \mathbf{d}_i} = f_+ e^{i \mathbf{K} \cdot \mathbf{d}_+} + f_- e^{i \mathbf{K} \cdot \mathbf{d}_-}. \]

Now we use Eqs. (8), (8) and (9) and we get

\[ S_\mathbf{K} = f_+ + f_- e^{2\pi i \nu_1}. \]

Warning: At this point you might be tempted to use that \( e^{2\pi i} = 1 \) so that \( e^{2\pi i \nu} = 1^{\nu} \) and you might want to say that this is always 1. However, if we take \( \nu_1 = 1/2 \) we actually have \( 1^{1/2} = \sqrt{1} = \pm 1 \) and you may ask which one is the correct value! This apparent ambiguity is related the fact that the square root is a multivalued function in the complex plane. One needs do define something called branch cut to solve this properly. If we just keep the form (11) and only do the simplifications after we have chosen \( \nu_1 \) we will obtain the correct results.

Now, if all the \( \nu_i \) are integers the last term in (11) is 1 and we get \( S_\mathbf{K} = f_+ + f_- \) and if we have that all \( \nu_i \) are integers +1/2 we get the \( S_\mathbf{K} = f_+ - f_- \). In the latter case, the structure factor is zero if \( f_+ = f_- \) and this means that the light coming from the positive ions and the negative ions exactly cancels out by destructive interference.

b) The zincblende structure is an FCC with

\[ \mathbf{d}_1 = \mathbf{0} \quad \text{positive ion}, \]
\[ \mathbf{d}_2 = \frac{a}{4} (\hat{x} + \hat{y} + \hat{z}) \quad \text{negative ion}. \]

Now, using the same notation as above we have

\[ S_\mathbf{K} = f_+ + f_- e^{i \pi (\nu_1 + \nu_2 + \nu_3)}, \]

where, as before, \( \nu_i \) are all integers or all integers +1/2. In the latter case we have \( \sum_i \nu_i = n + 1/2 \), where \( n \) is an integer and the structure factor is

\[ S_\mathbf{K} = f_+ + f_- e^{i \pi (n + 1/2)} = f_+ + f_- e^{i \pi n} e^{i \pi/2} = f_+ \pm if_- \].

(15)

If all \( \nu_i \) are integers we get

\[ S_\mathbf{K} = f_+ + f_- (-1)^{\nu_1 + \nu_2 + \nu_3} \]

and we see that \( S_\mathbf{K} = f_+ + f_- \) if the sum of \( \nu_i \) is even and \( S_\mathbf{K} = f_+ - f_- \) if the sum is odd.

c) If we know that we have closed-shell ions then the form factors only depend on the magnitude of \( \mathbf{K} \), i.e. \( f_\pm(\mathbf{K}) = f_\pm(\mathbf{K}) \) (this can be seen by studying atomic physics). When we make an x-ray experiment we may be able to determine that the position of the peaks corresponds to an FCC lattice. Now, how can we determine if we are dealing with a sodium chloride or a zincblende structure? Remember that the intensity of the light scattered in the direction \( \mathbf{K} \) is proportional \( |S_\mathbf{K}| \). By looking at the relative strength of the peaks in the x-ray image we may be able to determine which structure we are dealing with. For example, if we are considering \( \mathbf{K} \)-vectors where all \( \nu_i \) are integers then for the sodium chloride the peaks will all have the form factor \( f_+ + f_- \) and the peaks should be approximately equally strong. For zincblende, on the other hand, we have that the structure factor is either \( f_+ + f_- \) or \( f_+ - f_- \) and the peaks for integer \( \nu_i \) varies in strength.