1. Honeycomb lattice

Let the atomic spacing be $a$.

(It is not a Bravais lattice because, for example, starting at $A$, there is a vector $\vec{e}_2$, say, to $B$, but the vector $-\vec{e}_2$, starting at $A$, does not go to a lattice point.)

The Bravais lattice is the lattice formed by, say, all the $A$ sites, this is a triangular lattice.

2. (a) This is a bcc lattice with a the side of the conventional cubic cell equal to 2.

2. (b) This is an Fcc lattice with $a$, the side of the conventional cubic cell equal to 2.

3. 

O is at $(0,0,0)$.

A is at $(2,2,0)$.

B is at $(1,1,1)$.

\[
\cos(\vec{OB} \cdot \vec{BA}) = \frac{\vec{OB} \cdot \vec{BA}}{|\vec{OB}| \cdot |\vec{BA}|} = \frac{-1}{\sqrt{3} \cdot \sqrt{3}} = \frac{-1}{3} = -0.333
\]

\[\theta \approx 109.47^\circ \]

\[
\vec{OB} = \cos\left(-\frac{1}{3}\right) = 109.47^\circ
\]
Reciprocal lattice basis vectors \( \vec{b}_i = \frac{\vec{a}_i^* \times \vec{a}_j^*}{\vec{a}_i^* \cdot \vec{a}_j^*} \) etc.

For bcc, \( \vec{a}_1 = \frac{a}{2} (-1, 1, 1) \) \( \vec{a}_2 = \frac{a}{2} (1, -1, 1) \) \( \vec{a}_3 = \frac{a}{2} (1, 1, -1) \)

\( \vec{a}_2 \times \vec{a}_3 = \left( \frac{a}{2} \right)^2 \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix} \)

and \( \vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3 = \left( \frac{a}{2} \right)^3 \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix} \)

Hence \( \vec{b}_1 = \frac{2\pi}{a^3} \begin{bmatrix} \frac{a}{2} \\ 0 \\ 0 \end{bmatrix} = \frac{\pi}{a} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} \)

This is a basis vector of the fcc lattice.

A similar calculation shows \( \vec{b}_2 \) and \( \vec{b}_3 \) are basis vectors of the fcc lattice.

Hence reciprocal lattice of the bcc is fcc.

Similarly for fcc, \( \vec{a}_1 = \frac{a}{2} (0, 1, 1) \) \( \vec{a}_2 = \frac{a}{2} (1, 0, 1) \) \( \vec{a}_3 = \frac{a}{2} (1, 1, 0) \)

Hence \( \vec{b}_1 = \frac{2\pi}{a^3} \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix} \frac{a}{4} \\ \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix} = \frac{\pi}{a} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \)

which is a reciprocal lattice of the fcc lattice.

Similarly \( \vec{b}_2 \) and \( \vec{b}_3 \) are basis vectors of the fcc lattice.

Hence reciprocal lattice of fcc is bcc.

\( \Sigma \vec{V} = \vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3 \)

\( \Sigma V_{br} = \vec{b}_1 \cdot \vec{b}_2 \times \vec{b}_3 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} (\vec{b}_2 \times \vec{b}_3) \)

Now \( (\vec{a} \times \vec{b}) \cdot (\vec{c} \times \vec{d}) = (\vec{a} \cdot \vec{c})(\vec{b} \cdot \vec{d}) - (\vec{a} \cdot \vec{d})(\vec{b} \cdot \vec{c}) \)

\( \Sigma V_{br} = \frac{2\pi}{a^3} \left( \vec{a}_2 \cdot \vec{b}_2 \right) \left( \vec{a}_3 \cdot \vec{b}_3 \right) - \left( \vec{b}_2 \cdot \vec{b}_3 \right) \frac{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}{\vec{a}_2 \cdot \vec{a}_3} \)

But \( \delta_{ij} b_j = 2\pi \delta_{ij} \) \( \Rightarrow V_{br} = \frac{(2\pi)^2}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} = \frac{4\pi^2}{V} \)
See Ashcroft & Mermin, p. 90
See Ashcroft & Mermin, p. 99-100

NaCl: Bravais lattice is Fcc, basis vectors
\( \mathbf{a}_1 = \frac{a}{2} (1, 0, 0) \), \( \mathbf{a}_2 = \frac{a}{2} (0, 1, 0) \), \( \mathbf{a}_3 = \frac{a}{2} (0, 0, 1) \)

Basis of 1 atom at \( \mathbf{0} \) and the other at \( \frac{a}{2} (1, 1, 1) \)

As shown in problem 4, the reciprocal lattice is bcc with reciprocal lattice basis vectors
\( \frac{2\pi}{a} (1, 1, 1) \), \( \frac{2\pi}{a} (1, -1, -1) \), \( \frac{2\pi}{a} (1, -1, 1) \)

Since the bcc is 2 interpenetrating simple cubic lattices, a reciprocal lattice vector is \( \frac{2\pi}{a} (m_1, m_2, m_3) \) where the \( m_i \) are either all even, or all odd, see Eq. 2(b).

Equivalently we can say
\[ \mathbf{g} = \frac{2\pi}{a} (v_1, v_2, v_3) \]

where either all \( v_i \) are integer

Form factor of the unit cell is
\[ \sum_{i} \mathbf{f}_i \cdot e^{i\mathbf{g} \cdot \mathbf{r}_i} = \mathbf{f}_1 \cdot \mathbf{f}_2 \cdot e^{i\mathbf{g} \cdot \mathbf{r}_1} \]

\[ \mathbf{r} = \frac{a}{2} (1, 1, 1) \]

\[ \mathbf{e}^2 = e \]

Now \( e^{i\mathbf{g} \cdot \mathbf{r}_i} = 1 \)

\[ \mathbf{r} = \frac{a}{4} (1, 1, 1) \] if \( v_i \) is integer

\[ \mathbf{r} = \frac{a}{4} (1, 1, 1) \] if \( v_i \) is integer + \( \frac{1}{2} \)

Hence form factor of cell is
\[ \mathbf{f}_1 \cdot \mathbf{f}_2 \] if \( v_i \) is integer
\[ \mathbf{f}_1 \cdot \mathbf{f}_2 \] if \( v_i \) is integer + \( \frac{1}{2} \)

If \( f_1 = f_2 \) there is no difference between the atoms (as far as the scattering experiment is concerned). We (effectively) have a sc lattice with lattice spacing \( a/2 \) so the reciprocal lattice is also sc with reciprocal lattice vectors
\[ \frac{4\pi}{a} (m_1, m_2, m_3) \] where the \( m_i \) are integer.

Thus the spots with \( v_i \) = integer + \( \frac{1}{2} \) must vanish.
Scattering amplitude from a chain of atoms

\[ F = \frac{\hbar}{\pi} e^{-\alpha(\Delta k)N} = \frac{1 - e^{-i\alpha(\Delta k)N}}{1 - e^{-i\alpha(\Delta k)}} \]

Scattering intensity \( \propto |F|^2 \)

\[ = \frac{2 - 2\cos(\alpha N \Delta k)}{2 - 2\cos \alpha \Delta k} \]
\[ = \frac{\sin^2 \left( \frac{1}{2} \alpha N \Delta k \right)}{\sin^2 \left( \frac{1}{2} \alpha \Delta k \right)} \]

\[ \Delta k \to 0 \quad |F|^2 = N^2 \quad \text{i.e., very large if } N \text{ is large.} \]

Intensity zero at \( \Delta k = \frac{2\pi}{Na} \), so width of peak \( \propto \frac{1}{N} \).

\[ \text{i.e., very sharp if } N \text{ is large.} \]
Bragg diffraction from a chain: \( N=10, \ x=\Delta k / 2\pi \)
Bragg diffraction from a chain: N=10, x=Delta k/2π