8.511 Problem Set 1

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1 Constructive Interference and Bravais Lattice

1.1 Part (a)

Since $e^{i\vec{Q}\cdot\vec{R}_j} = e^{i\alpha}$, $\vec{Q}\cdot\vec{R}_j$ only differs from α by an integer multiple of 2π. The same is true if we replace $\vec{R}_j$ with $2\vec{R}_j$, for $2\vec{R}_j$ is also a lattice point. Therefore, we have

$$\begin{aligned}\vec{Q}\cdot\vec{R}_j &= \alpha + 2k\pi \\ \vec{Q}\cdot 2\vec{R}_j &= \alpha + 2k'\pi\end{aligned}$$

where $k, k' \in \mathbb{Z}$. Subtracting from the second equation twice the first one, we get

$$\alpha = 2(k' - 2k)\pi$$

Therefore, α is an integer multiple of 2π. Since α is a phase and can be restricted to the interval $[0, 2\pi)$, it is clear that constructive interference requires $\alpha = 0$.

1.2 Part (b)

Let $\vec{Q} = \vec{Q}_0$ be an arbitrary solution to the original equation. Since $\vec{b}_1, \vec{b}_2, \vec{b}_3$ span the reciprocal space, there are $x_1, x_2, x_3 \in \mathbb{R}$ such that

$$\vec{Q}_0 = x_1\vec{b}_1 + x_2\vec{b}_2 + x_3\vec{b}_3$$

To prove the uniqueness of the general solution $\vec{Q} \in \{\vec{G}|\vec{G} = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3, m_1, m_2, m_3 \in \mathbb{Z}\}$, it suffices to show that $x_1, x_2, x_3 \in \mathbb{Z}$.

Since $e^{i\vec{Q}_0\cdot\vec{a}_1} = e^{i2\pi x_1} = 1$, $x_1 \in \mathbb{Z}$. Similarly taking $\vec{R}_j = \vec{a}_2, \vec{a}_3$, we have $x_2, x_3 \in \mathbb{Z}$. This proves the uniqueness of the solution.

2 Problem 2

2.1 Part (a)

Proof: The volume of the Bravais lattice is $V = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$. The volume of the first Brillouin zone is

$$\begin{aligned}V_k &= \vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3) \\ &= (2\pi)^3 \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_2 \cdot (\vec{a}_3 \times \vec{a}_1)} \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_3 \cdot (\vec{a}_1 \times \vec{a}_2)} \\ &= \frac{(2\pi)^3}{V^3}(\vec{a}_2 \times \vec{a}_3) \cdot (((\vec{a}_3 \times \vec{a}_1) \cdot \vec{a}_2)\vec{a}_1 - ((\vec{a}_3 \times \vec{a}_1) \cdot \vec{a}_1)\vec{a}_2) \\ &= \frac{(2\pi)^3}{V^3}(\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3))(\vec{a}_2 \cdot (\vec{a}_3 \times \vec{a}_1)) \\ &= \frac{(2\pi)^3}{V}\end{aligned}$$

Therefore, $V_k V = (2\pi)^3$.

2.2 Part (b)

A conventional unit cell of the fcc lattice contains 4 atoms, so $4V^{fcc} = a^3$. On the other hand, a conventional unit cell of the bcc lattice contains 2 atoms, so $2V^{bcc} = a^3$.

The reciprocal lattice of fcc is bcc. Let its linear dimension be b. Then the first Brillouin zone has volume $V_k^{fcc} = b^3/2$. From the previous part, we have

$$\left(\frac{1}{2}b^3\right)\left(\frac{1}{4}a^3\right) = (2\pi)^3$$

whose solution gives $b = \frac{4\pi}{a}$.

3 Problem 3

3.1 Part (a)

The Bravais lattice and the corresponding unit cell is sketched below. The unit cell has a squared base whose linear scale is a. The primitive vectors are $\vec{a}_1 = (a, 0, 0), \vec{a}_2 = (0, a, 0), \vec{a}_3 = (0, 0, c)$. The basis contains three vectors: $\vec{d}_1^{Cu} = (0, 0, 0), \vec{d}_1^O = (a/2, 0, 0), \vec{d}_2^O = (0, a/2, 0)$.

3.2 Part (b)

The primitive cell of the up-and-down CuO_2 layer is sketched below. Its area is $2a^2$. So the lattice spacing on the CuO_2 plane is $\sqrt{2}a$. The primitive vectors are (since I am only talking about one layer, the third dimension is left out) $\vec{a}_1 = (a, -a)$ and $\vec{a}_2 = (a, a)$.

The reciprocal lattice is also a square lattice. $\vec{b}_1 = (\pi/a, -\pi/a)$ and $\vec{b}_2 = (\pi/a, \pi/a)$.

Notice that the flat CuO_2 plane has a reciprocal lattice that is twice as large. This means, when the distortion vanishes, half of the G points are "lost", so that half of the diffraction peaks vanish. This can be understood as a gradual decrease of the structure factor at these k points.