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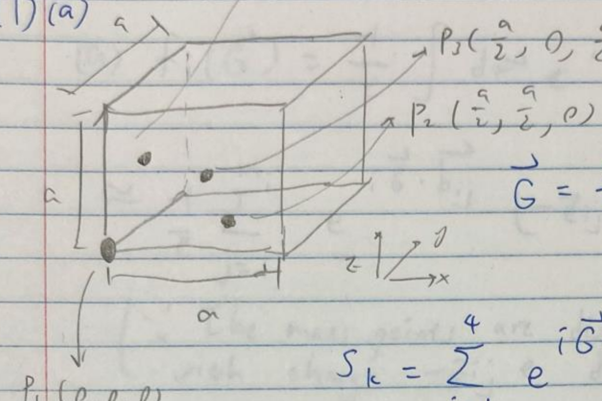
A&M 6.2 $P_4(0, \frac{a}{2}, \frac{a}{2})$

(1) (a)



$$\vec{G} = \frac{2\pi}{a}(n_1, n_2, n_3)$$

$$S_k = \sum_{i=1}^{4} e^{i\vec{G}\cdot\vec{P}_i}$$

$$= 1 + e^{i\pi(n_1+n_2)} + e^{i\pi(n_2+n_3)} + e^{i\pi(n_1+n_3)}$$

We now divide into 4 cases of $\{n_1, n_2, n_3\}$

① 3 odds ; all $n_i + n_j$ = even $\Rightarrow S_k = 4$

② 2 odds, 1 even ; $S_k = 1+1-1-1 = 0$

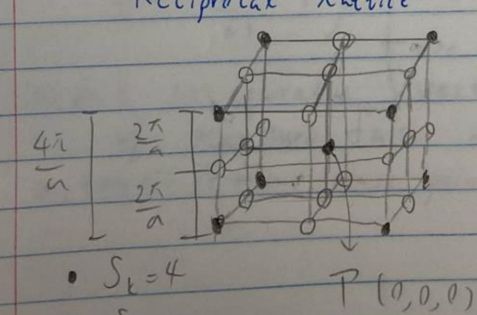
③ 1 odd , 2 evens ; $S_k = 1+1-1-1 = 0$

④ 3 evens ; $S_k = 4$

∴ No bragg diffraction if not all are even or odd.

(b)

Reciprocal lattice



∴ Body-centered in reciprocal space

(∴ Reciprocal lattice of FCC is BCC)

(2) A&M 6.4

(a) $$f_i(\vec{G}) = \frac{-1}{e}\int d\vec{r}\, e^{i\vec{G}\cdot\vec{r}} \rho_i(\vec{r})$$

(A&M 6.22)

$$\approx \frac{-1}{e}\sum_{j=1}^{m_i} e^{i\vec{G}\cdot\vec{b}_{ij}} (-Z_{ij} e)$$

(∵ The mass points are distributed at $\vec{b}_{ij}$ with charge $-Z_{ij} e$ discretely.)

$$= \sum_{j=1}^{m_i} e^{i\vec{G}\cdot\vec{b}_{ij}} Z_{ij}$$

(b) $$S_{\vec{G}} = \sum_{i=1}^{n} f_i(\vec{G})\, e^{i\vec{G}\cdot\vec{d}_i}$$

$$= \sum_{i=1}^{n}\sum_{j=1}^{m_i} e^{i\vec{G}\cdot(\vec{d}_i+\vec{b}_{ij})} Z_{ij}$$

$$= \sum_{k=1}^{N} e^{i\vec{G}\,\vec{r}_k} Z_k$$

$\left(N = \sum_{i=1}^{n} m_i\right)$ ($Z_k := Z_{ij}$, $\vec{r}_k = \vec{d}_i + \vec{b}_{ij}$ are the charges and the position vectors of the k-th mass points)

Which is equivalent to the structure factor of a basis consisting of $m_1 + m_2 + \dots + m_n$ mass points.