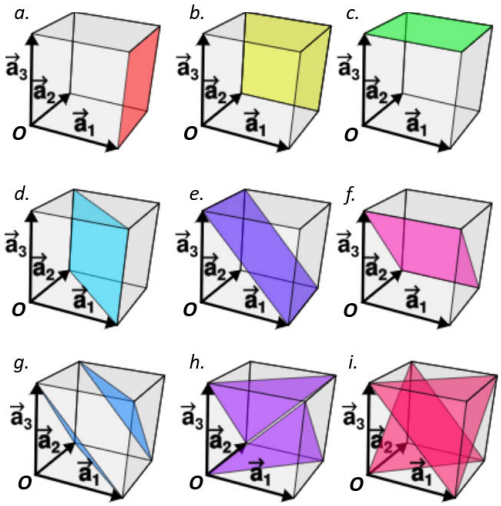
C3-1 Assignment Answer

1. (1) Write down the indices of the following 9 crystal planes in the cubic lattice system.



a. (1, 0, 0); *b*. (0, 1, 0); *c*. (0, 0, 1);
d. (1, 1, 0); *e*. (1, 0, 1); *f*. (0, 1, 1);
g. (1, 1, 1); *h*. $(\bar{1}, 1, 1)$; *i*. $(1, \bar{1}, 1)$.

以上每个写对给 2 分

(2) Write down the indices of the shortest lattice vector which starts from the point *O* and ends at the crystal planes with colors in the above figure.

a. (1, 0, 0); *b*. (0, 1, 0); *c*. (0, 0, 1);
d. (1, 1, 0); *e*. (1, 0, 1); *f*. (0, 1, 1);
g. $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$; $(\frac{2}{3}, \frac{2}{3}, \frac{2}{3})$; *h*. $(-\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$; (0, 0, 0); *i*. $(\frac{1}{3}, -\frac{1}{3}, \frac{1}{3})$; (0, 0, 0).

以上每个写对给 2 分
如果写成下面这样也算对

g. (1, 1, 1); *h*. $(\bar{1}, 1, 1)$; *i*. $(1, \bar{1}, 1)$.

2. (1) Write down the reciprocal vector $\vec{G}$ of the 1D and 2D lattice of

$$\vec{R} = u\vec{a}$$
$$\vec{R} = u\vec{a}_1 + v\vec{a}_2$$

在一维情况下，令$\vec{\boldsymbol{a}}_1 = a\vec{\boldsymbol{\imath}}$，$\vec{\boldsymbol{a}}_2 = \vec{\boldsymbol{\jmath}}$，$\vec{\boldsymbol{a}}_3 = \vec{\boldsymbol{k}}$

$$\vec{b} = \frac{2\pi}{a}\vec{\imath}, \qquad \vec{G} = u\vec{b}$$

以上写对给 10 分

在二维情况下，令$\vec{\boldsymbol{a}}_1 = a_1\vec{\boldsymbol{\imath}}$，$\vec{\boldsymbol{a}}_2 = a_2\vec{\boldsymbol{\jmath}}$，$\vec{\boldsymbol{a}}_3 = \vec{\boldsymbol{k}}$

$$\vec{b}_1 = \frac{2\pi}{a_1}\vec{\boldsymbol{\imath}}$$

$$\vec{b}_2 = \frac{2\pi}{a_2}\vec{\boldsymbol{j}}$$

$$\vec{G} = u\vec{b}_1 + v\vec{b}_2$$

以上写对给 10 分

(2) Prove that in the Bloch's theorem, where $\vec{G}$ is the 1D reciprocal vector.

$$u_k(x) = \sum_h A_h e^{iGx}$$

$$G = \frac{2\pi}{a}h,\ h = 0,\ \pm 1,\ \pm 2,\ \ldots$$

Comparing to,

$$\vec{G} = u\frac{2\pi}{a}\vec{\boldsymbol{i}}$$

QED.

以上写对给 10 分

3. (Text book* Problem 6.5)

Show that Equation 6.12 follows from Equation 6.11. Hint: First write $\psi(x) = e^{iqx}u(x)$, which is certainly true for some $u(x)$, and then show that $u(x)$ is necessarily a periodic function of *x*.

从 6.11 式出发

$$\psi_q(x-a) = e^{-iqa}\psi_q(x)$$

我们发现波矢为$\vec{q}$的平面波$\varphi_q(x) = e^{iqx}$ 满足布洛赫定理:

$$\varphi_q(x-a) = e^{iq(x-a)} = e^{iqx}e^{-iqa} = e^{-iqa}\varphi_q(x)$$

写出平面波满足布洛赫定理给 7 分

我们还发现波矢为$\vec{q}+\vec{G}$的平面波满足布洛赫定理，其中$\vec{G} = \frac{2\pi}{a}h$, 是一维周期性晶格的倒格矢

$$\varphi_{q+G}(x-a) = e^{i(q+G)(x-a)} = e^{-i(q+G)a}\varphi_{q+G}(x) = e^{-iqa}\varphi_{q+G}(x)$$

写出倒格矢周期性叠加的平面波满足布洛赫定理给 10 分

令布洛赫波$\varphi_q(x)$ 为平面波$\varphi_{q+G}(x) = e^{i(q+G)x}$的线性叠加

$$\psi_q(x) = e^{iqx}u_q(x) = e^{iqx}\sum_h A_h e^{iGx} = \sum_h A_h e^{i(q+G)x}$$

写出关于 u(x)的布洛赫定理给 10 分

其中

$$u_q(x) = \sum_h A_h e^{iGx}$$

写出关于 u(x)的表达式给 7 分

* David J. Griffiths, and Darrell F. Schroeter, Introduction to Quantum Mechanics (3rd Edition),

Cambridge University Press (2018).