Crystal Date: Page:

Real space unit vector $\vec{a_1}, \vec{a_2}, \vec{a_3}$.
Unit vector reciprocal lattice are given as

$$\vec{b_1} = \frac{2\pi\, \vec{a_2} \times \vec{a_3}}{\vec{a_1} \cdot (\vec{a_2} \times \vec{a_3})} \qquad \vec{b_2} = \frac{2\pi (\vec{a_3} \times \vec{a_1})}{\vec{a_1} \cdot (\vec{a_2} \times \vec{a_3})}.$$

$$\vec{b_3} = 2\pi \frac{\vec{a_1} \times \vec{a_2}}{\vec{a_1} \cdot (\vec{a_2} \times \vec{a_3})}$$

Unit vectors given of fcc lattice, with cubic lattice constant a_0.

$$\vec{a_1} = \frac{a_0}{2} (\hat{x} + \hat{y}).$$

$$\vec{a_2} = \frac{a_0}{2} (\hat{y} + \hat{z})$$

$$\vec{a_3} = \frac{a_0}{2} (\hat{z} + \hat{x}).$$

For sc lattice $\vec{a_1} = a\hat{x}, \vec{a_2} = a\hat{y}, \vec{a_3} = a\hat{z}$
determining reciprocal lattice vector $\vec{b_1}, \vec{b_2}, \vec{b_3}$

$$\vec{b_1} = 2\pi \frac{(\vec{a_2} \times \vec{a_3})}{a^3} = \frac{2\pi}{a} \hat{x}.$$

similarly $\vec{b_2} = \frac{2\pi}{a} \hat{y}$ $\vec{b_3} = \frac{2\pi}{a} \hat{z}$.

reciprocal of reciprocal is real lattice

$$\left.\begin{aligned} \vec{a_1} &= \tfrac{1}{2} a_0 (-\hat{x} + \hat{y} + \hat{z}). \\ \vec{a_2} &= \tfrac{1}{2} a_0 (\hat{x} - \hat{y} + \hat{z}). \\ \vec{a_3} &= \frac{a_0}{2} (\hat{x} + \hat{y} - \hat{z}) \end{aligned}\right\} \text{bcc lattice.}$$

Date :
Page:

So $\vec{a_1} \cdot (\vec{a_2} \times \vec{a_3}) = \frac{1}{4} a^3$

$$\vec{b_1} = \frac{a^2/4}{a^3/4} (\hat{x} - \hat{y} + \hat{z}) \times (\hat{x} + \hat{y} - \hat{z}) \times 2\pi$$

$$\vec{b_1} = \frac{2\pi}{a} (\hat{y} + \hat{z})$$

using cyclic symmetry

$$\vec{b_2} = \frac{2\pi}{a} (\hat{x} + \hat{z})$$

$$\vec{b_3} = \frac{2\pi}{a} (\hat{x} + \hat{y}).$$

reciprocal lattice of fcc is bcc.