Assignment 2 (Addendum): SOLID STATE PHYSICS – RECIPROCAL LATTICE

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Problem 6

Reciprocal Lattice to fcc Lattice (a) Solve for the primitive translation vectors of the lattice reciprocal to fcc lattice. (b) Determine the planes that are perpendicular bisectors of six other reciprocal lattice vectors that formed the octahedron boundaries of the first Brillouin zone.

Answer 1: a.) The primitive translation vectors of the fcc lattice are expressed by

$$a_1 = \frac{1}{2}a(0,1,1),\ a_2 = \frac{1}{2}a(1,0,1),\ a_3 = \frac{1}{2}a(1,1,0) \tag{1}$$

Using the above expressions, we can produce all the points of the fcc lattice described by

$$I = l_1 a_1 + l_2 a_2 + l_3 a_3 \tag{2}$$

with l_1, l_2, and l_3 integers. The volume of the primitive cell is

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

The reciprocal lattice vectors are defined as follows

$$b_1 = \frac{2\pi(a_2 \times a_3)}{a_1 \cdot (a_2 \times a_3)} = \frac{2\pi}{a}(-1,1,1) \tag{4}$$

$$b_2 = \frac{2\pi(a_3 \times a_1)}{a_1 \cdot (a_2 \times a_3)} = \frac{2\pi}{a}(1,-1,1) \tag{5}$$

$$b_3 = \frac{2\pi(a_1 \times a_2)}{a_1 \cdot (a_2 \times a_3)} = \frac{2\pi}{a}(1,1,-1) \tag{6}$$

The reciprocal lattice vectors can be defined as

$$G = g_1 b_1 + g_2 b_2 + g_3 b_3 = \frac{2\pi}{a}(-g_1 + g_2 + g_3, g_1 - g_2 + g_3, g_1 + g_2 - g_3) \tag{7}$$

Meanwhile, the translation vectors of the conventional unit cell can be defined as

$$a_x = a(1,0,0);\ a_y = a(0,1,0);\ a_z = a(0,0,1) \tag{8}$$

The volume of the said cubic sell can be defined as

$$a_x \cdot (a_y \times a_z) = \frac{a^3}{4} \tag{9}$$

The reciprocal lattice vectors for the conventional unit cell are as follows:

$$b_x = \frac{2\pi(a_y \times a_z)}{a_x \cdot (a_y \times a_z)} = \frac{2\pi}{a}(1,0,0) \tag{10}$$

$$b_y = \frac{2\pi(a_z \times a_x)}{a_x \cdot (a_y \times a_z)} = \frac{2\pi}{a}(0,1,0) \tag{11}$$

$$b_z = \frac{2\pi(a_x \times a_y)}{a_x \cdot (a_y \times a_z)} = \frac{2\pi}{a}(0,0,1) \tag{12}$$

From the above expressions, the reciprocal lattice vector can be expressed as

$$G = g_x b_x + g_y b_y + g_z b_x = \frac{2\pi}{a}(g_x, g_y, g_z) \tag{13}$$

where

$$g_x = -g_1 + g_2 + g_3 \tag{14}$$

$$g_y = g_1 - g_2 + g_3 \tag{15}$$

$$g_x = g_1 + g_2 - g_3 \tag{16}$$

b.) The central cell's boundaries in the reciprocal lattice are mostly defined by the eight planes normal to these vectors at their center points. However, the corners of the resulting octahedron are split by planes that are orthogonal bisectors of six other reciprocal lattice vectors:

$$\frac{2\pi}{a}(\pm 2,0,0),\ \frac{2\pi}{a}(0,\pm 2,0),\ \frac{2\pi}{a}(0,0,\pm 2) \tag{17}$$

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