NORTHERN ILLINOIS UNIVERSITY

PHYSICS DEPARTMENT

Physics 580 – Solid State Physics Fall 2024

Problem Set #5

Problem Set Due: Thurs., Oct. 17, 2024
Read Kittel: Chapter 1 & 2, notes on *Brillouin Zones* posted on Blackboard

1. Indium crystallized in a body centered tetragonal lattice. For the conventional unit cell, the lattice parameters are $a = 3.244\,\text{Å}$ $c = 4.938\,\text{Å}$, and the basis is (000) and $\left(\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}\right)$. The primitive translation vectors are

$$\vec{\mathbf{a}} = (a/2)(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}}) + (c/2)\hat{\boldsymbol{z}}$$
$$\vec{\mathbf{b}} = (a/2)(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}}) - (c/2)\hat{\boldsymbol{z}}$$
$$\vec{\mathbf{c}} = (a/2)(\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}}) - (c/2)\hat{\boldsymbol{z}}$$

   (a) Make a careful sketch of the primitive unit cell defined by the above vectors (use Vesta).

   (b) What is the volume of the primitive unit cell? How much smaller is the volume compared to the conventional unit cell?

   (c) What are the angles (α, β, γ) of the primitive unit cell, and what lattice type is it?

Table 1 The 14 lattice types in three dimensions

System	Number of lattices	Restrictions on conventional cell axes and angles
Triclinic	1	$a_1 \neq a_2 \neq a_3$ $\alpha \neq \beta \neq \gamma$
Monoclinic	2	$a_1 \neq a_2 \neq a_3$ $\alpha = \gamma = 90° \neq \beta$
Orthorhombic	4	$a_1 \neq a_2 \neq a_3$ $\alpha = \beta = \gamma = 90°$
Tetragonal	2	$a_1 = a_2 \neq a_3$ $\alpha = \beta = \gamma = 90°$
Cubic	3	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90°$
Trigonal	1	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma < 120°, \neq 90°$
Hexagonal	1	$a_1 = a_2 \neq a_3$ $\alpha = \beta = 90°$ $\gamma = 120°$

(d) Make a careful sketch of the Wigner-Seitz cell in real space, and find the intercepts of the cell with the x, y, z axes. Note that $c > a\sqrt{2}$.

(e) Find the primitive translation vectors of the reciprocal lattice. What lattice type is the reciprocal lattice? What is the lattice type of the conventional unit cell and what are its non-primitive translation vectors?

(f) Make a careful sketch of the first Brillouin zone, and find where it intercept the x, y, z axes.

(g) Find an expression for the structure factor for this lattice in terms of the indices of the various points of the reciprocal lattice (h, k, l). Evaluate this expression for the points (100), (200), (300), (110), (111), (112), and (221). What is the condition h, k, and l must satisfy for allowed and forbidden reflections?