Solid State Physics Spring 2022

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Homework 1: Due March 4th

1. Draw the Wigner-Seitz unit cell of a 3D hexagonal lattice.

2. A&M page 94 Chapter 5 exercise #2

(a) Using the primitive vectors given in Eq (4.9) and the construction (5.3) (or by any other method) show that the reciprocal of the simple hexagonal Bravais lattice is also simple hexagonal, with lattice constants $2\pi/c$ and $4\pi/\sqrt{3}a$, rotated through $30°$ about the c-axis with respect to the direct lattice.

(b) For what value of c/a does the ratio have the same value in both direct and reciprocal lattices? If c/a is ideal in the direct lattice, what is its value in the reciprocal lattice?

(c) The Bravais lattice generated by three primitive vectors of equal length a, making equal angles θ with one another, is known as the trigonal Bravais lattice (see Chapter 7, note: trigonal lattice belongs to the "Crystal system" instead of the "lattice system". So far we have learnt only about lattice system, crystal system will be discussed later in the class). Show that the reciprocal of a trigonal Bravais lattice is also trigonal, with an angle θ^* given by $-\cos\theta^* = cos\theta/[1 + cos\theta]$, and a primitive vector length a^*, given by $a^* = (2\pi/a)\left(1 + 2\cos\theta\cos\theta^*\right)^{-1/2}$.

Eq (4.9): $\mathbf{a_1} = a\hat{\boldsymbol{x}}, \boldsymbol{a_2} = \frac{a}{2}\hat{\boldsymbol{x}} + \frac{\sqrt{3}a}{2}\hat{\boldsymbol{y}}, \boldsymbol{a_3} = c\hat{\boldsymbol{z}}$

Construction (5.3): $\mathbf{b_1} = 2\pi\frac{\boldsymbol{a_2}\times\boldsymbol{a_3}}{\boldsymbol{a_1}\cdot(\boldsymbol{a_2}\times\boldsymbol{a_3})}, \boldsymbol{b_2} = 2\pi\frac{\boldsymbol{a_3}\times\boldsymbol{a_1}}{\boldsymbol{a_1}\cdot(\boldsymbol{a_2}\times\boldsymbol{a_3})}, \boldsymbol{b_3} = 2\pi\frac{\boldsymbol{a_1}\times\boldsymbol{a_2}}{\boldsymbol{a_1}\cdot(\boldsymbol{a_2}\times\boldsymbol{a_3})}$.

3. Show that the reciprocal lattice of a fcc lattice is the bcc structure; show that the reciprocal lattice of a bcc lattice is the fcc structure; explain why there is no face-centered tetragonal structure.

Homework 2
Due date: 2022-3-11 before class

1. Find the selection rule for simple cubic, BCC and FCC structure with a basis of two atoms: Atom A (0,0,0) and Atom B (1/4, 1/2, 1/4).
2. Which of the possible crystal structure of MoTe2 has an inversion center (1T' or Td)?
   What Bravais lattices do 1T' and Td phases belong to, respectively?
   Why a lattice has to have an inversion center?
   Why some crystals like MoTe2 are without inversion center?
   Examples of such class of broken inversion symmetry crystals are $TaIrTe_4$, (one phase of) WTe_2, they all have a special name, what was this name?
3. Show that $e^{-1}=e$; $a^{-1}*a=e$; and $e*a=a$
4. A&M C7 problem 6