

## Homework 2

Due 1/26/2012

- [10 pts] Consider the planes with Miller indices (100) and (110): the lattice is bcc, and the indices refer to the conventional cubic cell with lattice constant  $a$ . What are the Miller indices of these planes when referred to the primitive axes defined by the three primitive vectors  $\vec{a} = \frac{1}{2}a(\hat{x} + \hat{y} - \hat{z})$ ,  $\vec{b} = \frac{1}{2}a(-\hat{x} + \hat{y} + \hat{z})$ ,  $\vec{c} = \frac{1}{2}a(\hat{x} - \hat{y} + \hat{z})$  ?
- [20 points] Consider a Bravais lattice with  
 $a = b = c$ , and  $\alpha = \beta = \gamma$   
where  $a \equiv |\vec{a}|$ ,  $b \equiv |\vec{b}|$ ,  $c \equiv |\vec{c}|$  and  $\alpha = \angle(\vec{b}, \vec{c})$ ,  $\beta = \angle(\vec{c}, \vec{a})$ ,  $\gamma = \angle(\vec{a}, \vec{b})$ . So, this lattice is characterized, in this case, with just two numbers,  $a$  and  $\alpha$ . This lattice can be thought of as a simple cube Bravais lattice stretched, or compressed, along a diagonal direction of the cube.
  - Find the value of  $\alpha$ , for which this Bravais lattice becomes an fcc lattice.
  - Find the value of  $\alpha$ , for which this Bravais lattice becomes a bcc lattice.
  - For a general value of  $\alpha$ , this lattice is called the *trigonal* lattice. Show that it is always possible to take a hexagonal lattice as the conventional lattice for any given trigonal lattice and find the ratio of the volume of the conventional cell and the volume of the primitive cell.
- [10 points] Prove that the reciprocal of a bcc lattice is an fcc lattice, and vice versa.
- [20 pts] In this problem, you can do 1) or 2). Note that if you do 2) first then the answers to 1) follow very easily, as 2) gives very general results. However, 1) can be done geometrically for the given specific examples, without relying on the general results of 2). Using the end results of 2) for 1) without proving them will result in very low points.
  - Consider two dimensional lattices.
    - For a square lattice with lattice constant  $a$ , show that the distance  $d$  between the  $(h k)$  set of lattice lines is given by
$$d = \frac{a}{\sqrt{h^2 + k^2}}$$
    - For a rectangular lattice with lattice constants  $a$  and  $b$ , which are different from each other, find a similar expression for  $d$  between the  $(h k)$  set of lattice lines in terms of  $a, b, h, k$ .
  - Consider a  $D$ -dimensional Bravais lattice, where the dimension  $D$  can be any positive integer, spanned by  $D$  linearly independent vectors  $\vec{a}_1, \vec{a}_2, \dots, \vec{a}_D$ , as

$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + \dots + n_D \vec{a}_D$  with  $n_1, \dots, n_D \in \mathbb{Z}$  (the set of integers).  
 The corresponding reciprocal lattice is spanned by  $\vec{a}_1^*, \vec{a}_2^*, \dots, \vec{a}_D^*$  (cf. Problem 5). Consider Miller indices  $(h_1 h_2 \dots h_D)$  and the corresponding set of lattice (hyper-)planes. Prove that (i) the reciprocal lattice vector  $\vec{G}_0 = \sum_{i=1}^D h_i \vec{a}_i^*$  is perpendicular to this set of planes, that (ii)  $\vec{G}_0$  is the smallest non-zero reciprocal lattice vector perpendicular to this set of planes, and that (iii) the spacing between any two adjacent lattice planes is given by  $d = \frac{2\pi}{|\vec{G}_0|}$ .

5. [20 points] Consider a  $D$ -dimensional Bravais lattice, where the dimension  $D$  can be any positive integer, generated by  $D$  linearly independent vectors  $\vec{a}_1, \vec{a}_2, \dots, \vec{a}_D$ , as  $\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + \dots + n_D \vec{a}_D$  with  $n_1, \dots, n_D \in \mathbb{Z}$  (the set of integers). Then, the definition of its reciprocal lattice  $\{\vec{G}\}$  can be generalized (following what we did in class) as follows. First, find  $D$   $\vec{a}_i^*$  vectors that satisfy

$$\vec{a}_i^* \cdot \vec{a}_j = 2\pi \delta_{ij} \quad i, j = 1, \dots, D$$

And span the reciprocal lattice using

$$\vec{G} = m_1 \vec{a}_1^* + m_2 \vec{a}_2^* + \dots + m_D \vec{a}_D^*, \quad m_i \in \mathbb{Z}$$

Let  $V$  be the volume of the unit cell of the original Bravais lattice and  $V^*$  be the volume of the unit cell of the reciprocal Bravais lattice. Show that

$$VV^* = (2\pi)^D$$

Hint: With  $\vec{a}_i$  vectors, form a  $D \times D$  matrix. Similarly for  $\vec{a}_i^*$  vectors. Use matrix algebra (determinant, the geometrical meaning of the determinant, transpose, multiplication).