

Eðlisfræði þéttfnis I

Dæmablað 3

Skilafrestur 15. September 2015 kl. 15:00

1. Hexagonal reciprocal lattice (10)

(a) For a hexagonal lattice with primitive lattice vectors $\mathbf{a}_1 = a(1, 0, 0)$, $\mathbf{a}_2 = a(1/2, \sqrt{3}/2, 0)$, $\mathbf{a}_3 = c(0, 0, 1)$ calculate the primitive vectors of the reciprocal lattice using the standard construction shown in class. What type of lattice is the reciprocal lattice? What is its angle of rotation with respect to the original lattice?

(b) Using the reciprocal lattice vectors, calculate the volume of the first Brillouin zone. Draw a careful diagram of the first Brillouin zone in reciprocal space.

2. HCP structure (10)

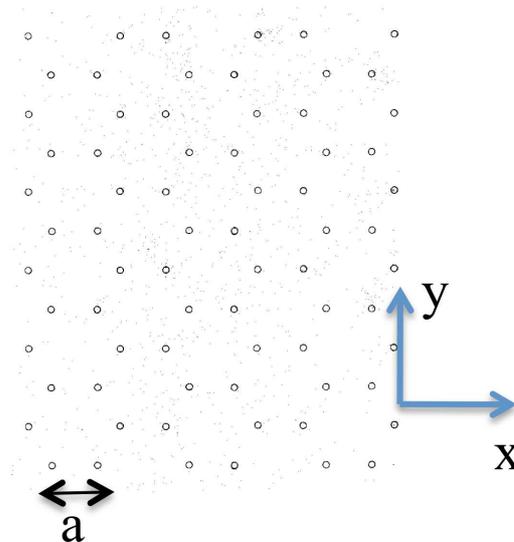
(a) Show that the c/a ratio for an ideal hexagonal close-packed structure is $(8/3)^{1/2} = 1.633$. (c is the distance between hexagonally packed planes; a is the distance b/w nearest neighbors in-plane.) If c/a is significantly larger than this value, the crystal structure may be thought of as composed of planes of closely packed atoms, the planes being loosely stacked.

(b) Calculate the packing fraction for the ideal close-packed HCP structure.

3. **Graphene (honeycomb)** (10)

(a) Indicate whether graphene structure (below) is a Bravais lattice. If it is, give two primitive vectors; if it is not, describe it as a Bravais lattice with as small as possible a basis.

(b) Using the following grid, draw primitive vectors and a primitive cell for the Bravais lattice. Calculate the area of the primitive cell.



4. **Density of atoms in silicon** (10)

Consider the diamond structure of a Si crystal, for which the cubic lattice constant is $a = 5.431 \text{ \AA}$.

(a) Compute the distance, in \AA , between nearest-neighbor Si atoms in the crystal.

(b) Compute the distance, in \AA , between nearest-neighbor Si atoms in the (100), (110), and (111) planes of the Si crystal.

(c) Compute the density of atoms (atoms/cm³) in the Si crystal.

5. **Miller indices** (10)

Find the Miller indices for the following planes:

(a) A plane parallel to both \mathbf{a}_1 and \mathbf{a}_3 ,

(b) The plane containing the points $3 \mathbf{a}_1$, $2 \mathbf{a}_2$, and $1/2(\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3)$,

(c) A plane that contains a cube edge and cuts two other cube edges of the same cube at their midpoints, in a simple cubic lattice.