MSN 501- Homework 1

Atomic Structure, Mechanical and Thermal Properties of Materials

Spring 2018

1.In each of the following cases indicate whether the structure is a Bravais lattice. If it is, give three primitive vectors; if it is not, describe it as a Bravais lattice with as small as possible a basis.

(a) Base-centered cubic (simple cubic with additional points in the centers of the horizontal faces of the cubic cell).

(b) Side-centered cubic (simple cubic with additional points in the centers of the vertical faces of the cubic cell).

(c) Edge-centered cubic (simple cubic with additional points at the midpoints of the lines joining nearest neighbors).

2.Show that the angle between any two of the lines (bonds) joining a site of the diamond lattice to its four nearest neighbors is $\cos^{-1}(-1/3) = 109^{o}28'$.

3. (a) Prove that the ideal c/a ratio for the hexagonal close-packed structure is $\sqrt{\frac{8}{3}} = 1.633$

(b) Sodium transforms from bee to hcp at about 23K (the martensitic transformation). Assuming that the density remains fixed through this transition, find the lattice constant a of the hexagonal phase, given that a = 4.23 A in the cubic phase and that the c/a ratio is indistinguishable from its ideal value.

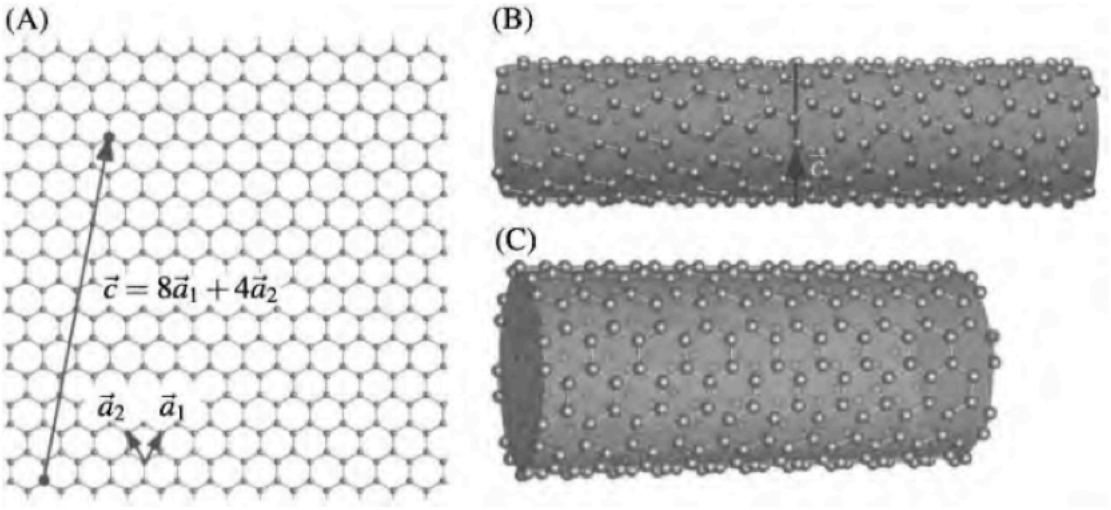
4. Calculate the packing fraction (assume close-packed spheres) for bcc, fcc, and diamond structure

5. Nanotube structures: To form a single-walled nanotube, one rolls up a single atomic layer of graphite, graphene, as shown in Figure below. Referring to (A) and (B), all nanotubes can be indexed with two integers m and n where $\mathbf{c} = m\mathbf{a}_1 + n\mathbf{a}_2$ and $\mathbf{a}_1$ and $\mathbf{a}_2$ are primitive vectors; one created in this way is an (m,n)-nanotube.

(a) Are all structures labeled by distinct pairs of integers m, n $(-\infty,\infty)$ different from each other?

(b) What are the indices for the nanotube appearing in (C)?

(c) Suppose that the atoms of a two-dimensional crystal lie at locations **R**, and that the crystal is rolled into a cylinder by pulling together two atoms separated by vector **c** as shown in Figure (A). Write down an explicit expression for locations of atoms after the sheet has been rolled into a tube.


(A)
$\vec{c} = 8\vec{a}_1 + 4\vec{a}_2$
$\vec{a}_2$
$\vec{a}_1$
(B)
$\vec{c}$
(C)