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Physics 731 **HOMEWORK ASSIGNMENT #1** **Fall 2006**

Read: A&M, Chap. 4 (by Tues., 9/5), chap. 7 (study pp. 112-3, skimming the rest); D&G 0-1.3

Due date: Tuesday, Sept. 12 **Deadline:** Thursday, Sept. 14

1. What is the Bravais lattice formed by all points with Cartesian coordinates (n_x, n_y, n_z) if:

a) the n_i are all even or all odd? (Consider the union of both possibilities: so a lattice of points, all of whose indices are even integers or odd; it is not simple cubic since, e.g., (2 2 1) is not occupied.)

b) the *sum* of the n_i is even?

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

Do NOT turn in this formerly-assigned problem, but its solution will be posted along with the assigned problems: **3**. Show that only 1-, 2-, 3-, 4-, and 6-fold rotation axes are permitted in the case of a Bravais lattice. (Hint: Use the following argument of Buergers: Consider points A and A' of a Bravais lattice a repeat distance *a* apart. If an n-fold axis passes through A and A', the points B and B' are obtained by rotating through $\phi = 2\pi/n$ clockwise and counterclock-wise, respectively. If B and B' are Bravais lattice points, what do you know about *b/a*? Now express *b* in terms of *a* and ϕ, derive the allowed values of ϕ.) (Answer is given in DG, also more amply in Weinreich.)

4. a) How many atoms are there in the primitive cell of diamond?

b) What is the length in angstroms of a primitive translation vector?

c) Show that the angle between the tetrahedral bonds of diamond is $\cos^{-1}(-1/3) = 109° 28'$.

d) How many atoms are there in the conventional cubic unit cell?

5. Show that the packing fraction (the fraction of volume filled by hard spheres that just touch) have the following values for the common lattice structures: simple cubic, 0.52; body-centered cubic, 0.68; face-centered cubic, 0.74; diamond, 0.34. Without doing any calculation, give the packing fraction of a hexagonal close-packed crystal. (Explain.)

6. It is remarkable that by squeezing on a small number of layers of atoms one changes the symmetry that yields optimal packing. Specifically, the hexagonal structure of fcc crystals turns into square symmetry! The classic reference is Pawel Pieranski, L. Strzelecki, and B. Pansu, "Thin Colloidal Crystals," Phys. Rev. Lett. 50, 900–903 (1983). The following problem provides a simple illustration.

a) Show that the areal packing fraction of spheres in a single layer is $\pi/(2\sqrt{3}) = 0.907$ for a hexagonal net and □/4 = 0.786 for a square lattice. Thus, the number of spheres contained by 2 layers between a pair of parallel large plates of area A is 2A divided by the area per unit (2D) cell, so $[2A/(\pi R^2)]$ times this packing fraction.

b) The smallest the distance between the 2 plates that permits the bilayer of hexagonal nets is $2R + d_0$, where d_0 is the interlayer distance between close-packed layers in an fcc lattice. Show that $d_0 =$ (2/3) $\sqrt{6}$) R = 1.633 R.

c) Suppose one starts with a square lattice of spheres (with neighboring spheres touching each other). We now set a second layer of spheres in the 4-fold hollows of the first layer, each sphere in the second layer touching its 4 neighbors in the first layer. (These 2 layers correspond to 2 layers of what starts as a bcc lattice, squeezed along a conventional axis, foreshadowing problem 9.) Show that the vertical distance between these 2 layers is $d_s = (\sqrt{2})\, R = 1.414\, R < d_0$.

d) If the parallel plates are squeezed a bit from part b, so they are separated by a distance less than $2R + d_0$, we can still have 2 hexagonal layers but in each the atoms will no longer touch. Suppose their centers are now separated by a distance $2R' > 2R$. Show that if the separation between the plates is reduced to $2R + d_s$, the areal packing fraction in layer is $(\pi/9)\sqrt{3} = 0.605 < 0.786$, so that more spheres fit if the layers have square symmetry! (You could, but do not need to for this problem, calculate the "critical" separation between plates that the two symmetries have the same areal packing fraction.)

7. Show that a bcc lattice may be decomposed into 2 sc lattices A, B, with the property that none of the nearest-neighbors lattice points of a lattice point on A lie on A, and similarly for the B lattice. Show that to obtain the same property, a sc lattice is. decomposed into 2 fcc lattices, and a fcc latice into 4 sc lattices. You may do this problem by citing pictures on the web. (These results are important for antiferromagnetism!)

8. Consider the CsCl structure, assuming a Cs^+ ion is at position 000 of an sc lattice.

a) Give the number of first, second, and third nearest-neighbor ions. Which are Cs^+? Cl^-?

b) Give the atomic coordinates of these neighbors, and thereby confirm your answer to a).

9. a) Show that both fcc and bcc lattices can be viewed as ABAB stackings of square lattices.

Note that iron undergoes a phase transition from the "usual" bcc to fcc at 1180 K; see http://www.fas.harvard.edu/~scdiroff/lds/CondensedMatter/BCCtoFCC/BCCtoFCC.html

b) Find the ratio of the interplanar spacings (the perpendicular distance between lattice planes) for each of these two lattices to the interatomic spacing in the square net of their lattice planes (thereby showing that they differ).

c) For arbitrary interplanar spacing between these planes, what is the Bravais structure?

Do NOT turn in this formerly-assigned problem, but its solution will be posted along with the assigned problems and we will discuss it in class: **10**. At

http://www.ill.fr/dif/3D-crystals/superconductors.html or

http://www.fhi-berlin.mpg.de/th/personal/hermann/YBaCuO.gif

you can find a graphic of the crystal structure of YBCO (i.e. $YBa_2Cu_3O_7$) associated with the high-temperature ($T_c = 90$ K) superconductor.

a) What is the underlying Bravais symmetry?

b) How many primitive cells are depicted?

c) In the basis, state how many Y, Ba, Cu, and O atoms are found.

d) Are any of the 4 sublattices formed by each of these 4 elements, respectively, Bravais? If yes, which? (If you are uncertain, what further information would you need?)

e) Find, using the web or otherwise, a high-T_c superconducting material with more atoms in the unit cell, indicating how many of each element there are in your choice. The larger, the better!