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Physics 731 **HOMEWORK ASSIGNMENT #1** **Fall 2001**

Read: A&M, Chaps. 4, 7

Due date: Thursday, Sept. 6 (so **deadline:** Tuesday, Sept. 11)

1. What is the Bravais lattice formed by all points with Cartesian coordinates (n_1, n_2, n_3) if:

a) the n_i are all even or all odd? (Consider the union of both possibilities.)

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 do old 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 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. 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 composed into 2 fcc lattices, and a fcc latice into 4 sc lattices. (These results are important for antiferromagnetism!)

7. 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).

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

b) Find the interplanar spacings for these two lattices (thereby showing that they differ).

YUK!! 10. Consider a collection of particles in **2 dimensions** with energy $E = (1/2)\,\Sigma_{i \neq j}\,\phi(r_{ij})$, where r_{ij} is the distance between particles *i* and *j* and *only nearest neighbor interactions* are considered. (In this variant of Marder, 1-5a, it is assumed in essence that $1\ \text{Å} \leq r_{ij} \leq 1.5\ \text{Å}$.)

Does a square or a hexagonal lattice have lower energy if $\phi(r) = \phi_0 \exp(-r)[1/(2r) - 1]$?