PHYSICS 731 **Department of Physics, University of Maryland, College Park**

Oct. 31, 2000 **Name: ___________________________________**

MIDTERM TEST

Budget your time. Look at all 5 pages. Do the problems you find easiest first.

1. Consider a family of hexagonal-lattice planes with $\mathbf{a_1} = \ell\,(1, 0, 0)$ and $\mathbf{a_2} = (\ell/2)\,(1, \sqrt{3}, 0)$. Now suppose that the points form an fcc crystal.

a) What is the relation between ℓ and the conventional lattice constant a ?

b) Find the distance between these planes in terms of ℓ or a .

c) Find a possible $\mathbf{a_3}$ for this fcc crystal. (You may express your answer using $\mathbf{a_1}$ and $\mathbf{a_2}$.)

d) What kind of lattice is the reciprocal lattice of this fcc crystal? (Just answer, do not derive!!)

e) To what in this reciprocal lattice does this family of planes correspond? (Be as explicit as you can.)

2. Consider a crystal lattice with a 2-atom basis on the underlying Bravais lattice. Atom 2 with form factor f_2 is at position **d** relative to atom 1 (with form factor f_1).

a) If $f_2 = f_1$ write down the condition that **d** must satisfy so that the structure factor at **K** (and thus the scattering intensity at **K**) vanishes.

b) If $f_2 \neq f_1$, with f_1 and f_2 real and positive, is there any condition under which the structure factor factor vanishes? Justify your answer briefly.

3. Recall estimating the Madelung constant α for ionic crystals using the Evjen (neutral-shell) method. Consider a CsCl lattice, i.e. a bcc lattice of sites with negative ions at the cell centers and positive ions at the corners.

a) What is the estimate of α based on just the first shell? Show your work, indicating clearly which characteristic distance you have chosen. Note that the first cube is particularly simple, containing just corner sites.

b) i) What is the critical value of the ratio of $r_>/r_<$? ii) Which of the spheres under this condition touch both its nearest and second nearest neighbors?

c) For this critical value, what is the packing fraction? (You may express your answer using $r_>$ and $r_<$, so you can answer this even if you could not do part b.)

4. Consider crystals held together predominantly by metallic (M), covalent (C), or ionic (I) bonding.

a) Which kind involves significant charge transfer? (Answer M, C, or I to this and the following.)

b) Which case has the largest angular variation in charge density about an atom (say at a distance 1/4 of the interatomic spacing from the atom)?

c) Which case has bonding dominated by the formation of bonding and antibonding orbitals?

d) Which kind has a binding energy that can be crudely deduced using the Uncertainty Principle?

e) Which kind has charge distributions that are nearly spherically symmetric around sites, but have strong radial dependence?

5a. On the square lattice of sites on the right, draw the displacement of the atoms indicated by dots, for an acoustic longitudinal phonon with **k** = (π/a) (1/2, 1/2).

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5b.On the 2-site basis square lattice on the right, draw the displacement of the two kinds of atoms for an optical transverse phonon with **k** = (π/a) (1, 0).

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6. A crystal has N cells, a p-atom basis (so Np atoms) in D dimensions, "volume" V, periodic BC's.

a) How many optical branches are there?

b) How many branches are both longitudinal and linear in $|\mathbf{k}|$ for small $|\mathbf{k}|$?

c) How many transverse branches are there?

d) How many distinct independent values of **k** are there?

e) What is the size of the primitive cell?

7. A 1D chain with lattice spacing *a* has the following dispersion relation: $\omega(k) = \omega_0[1 - (1-|k|a/\pi)^2]$

a) i) Find the group velocity. ii) What is the acoustic/sound velocity?

b) i) Find the density of states $g(\omega)$ and ii) sketch the result. iii) Indicate clearly the value[s] of ω for which a Van Hove singularity exists.

8. Do either *4* of the following *5* short-answer problems or the long problem and *1* of the short problems, all based on homework:

Short a) What is meant by a soft phonon mode?

Short b) What is the purpose of the Ewald construction? What differs when the array of scatterers has only 2D periodicity (e.g. a surface) rather than 3D periodicity (like a bulk solid)?

Short c) What is the de Boer parameter? In what context does it arise?

Short d) What is a good ansatz for a mode localized at the origin of a 1D Bravais crystal chain?

Short e) What is the effect of the Debye-Waller factor? On what parameters does it depend?

Long: In problem 3, what is the contribution to α from the second shell? Show your reasoning clearly. The second cube is more complicated, containing •100® face centers, •110® edge centers, and •111® corners. (Do not waste time summing the various contributions; just show the contribution from each type of site.)