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

Nov. 2, 1999 **Name: ___________________________________**

MIDTERM TEST

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

1. Consider a (211) plane in a cubic latttice (using conventional, Cartesian axes).

a) If the plane intersects the z-axis at A, where does it intersect the x-axis?

b) What is the volume of a primitive cell of an fcc lattice having conventional-lattice side *a* ? (Justify your answer.)

c) Show that the distance between planes in the {211} family in a cubic-family lattice is $a\sqrt{6}/12$. (For partial credit, you can instead show that the distance between planes in the {110} family in an fcc is $a\sqrt{2}/4$.)

d) What then (using b & c) is the area of a primitive cell in a {211} plane of an fcc lattice?

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

a) 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)? (Answer M, C, or I to this and the following.)

b) Which case has the largest variation in the charge density along a line connecting nearest-neighbor atoms?

c) Which kind characterizes most semiconductors?

d) Which kind characterizes materials made exclusively of an alkali element?

e) Which kind is most likely to have a crystal structure that is Bravais (with a single-atom basis)?

3. Indicate the temperature dependence of each of the following (no prefactors needed):

a) High-temperature internal energy of a solid

b) Low-temperature specific heat of a solid

c) Number of phonons of some specified $\omega_s(k)$ at high temperature

d) Number of phonons of some specified $\omega_s(k)$ at low temperature $T \ll \hbar\omega_s(k)/k_B$

e) Mean free path of phonons at very low temperature

4a. On the square lattice of sites on the right, draw the displacement of the atoms indicated by dots, for an acoustic transverse phonon with **k** = (π/a) (1/2, 0).

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4b.On the 2-site basis square lattice on the right, draw the displacement of the two kinds of atoms for an optical longitudinal phonon with **k** = (π/a) (1, 0).

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5. List two phenomena arising from the anharmonicity of lattice vibrations (i.e. that vanish in the harmonic-lattice approximations).

6. Consider a (1D) chain of atoms, spaced *a* apart, alternating between positive and negative sign.

a) What is the *periodicity* of the 1D lattice? What then are the values of the reciprocal lattice K?

b) Suppose the atomic scattering factor of the positive ions is three times that of the negative ions: $f_+ = 3 f_-$. Write down the structure factor for an arbitrary diffraction spot K.

c) What is the ratio of the *intensity* of the most intense spots to the least intense spots in the diffraction pattern? (Justify your answer; neglect Debye-Waller effects.)

d) If the spot at K = 32π/a has intensity 0.1 that at K=0, at which spot is the intensity 0.01 times that at K=0, according to the Debye-Waller factor? (Ignore the problem of using the Debye-Waller factor in 1D situations.)

7. In the linear kinetic theory of transport, why are collisions (scattering processes) necessary?

8. Consider a crystal with the rocksalt structure, e.g. NaCl.

a) Note that the first, second, and third neighbors of a Cl^- ion all lie on a cube of side 2*d* centered on the ion, with the nearest-neighbor Na^+ ions (at the face centers) a distance *d* from it. What are the distances of i) the second (at the edge centers) and ii) the third neighbor (at the corners) ions?

b) How many such i) first, ii) second, and iii) third neighboring ions are there? iv) Which are negative?

c) Write down the leading contribution to the sum for the Madelung constant, computed using the Evjen or neutral-shell method, for this cube as applied in class to the square lattice. (Your answer should be expressed as the sum of three terms; do not waste time adding them.)

9. The panels below give the phonon dispersion relations for a Bravais fcc material (Ne), diamond (C), germanium (Ge), and a mystery material with a large basis (YZ).

a) Identify which panel corresponds to which material.

b) How many atoms are in the basis of mystery material YZ?

c) On the top panel, mark clearly with arrows on the vertical axis the values of the frequency for whichone expects Van Hove singularities.

d) Again on this panel, estimate (just 1 signifcant figure, but show your work) the value of the longitudinal sound (acoustic) velocity along Γ-X, in the Δ direction, taking $X = 2\pi/a$, *a* ♠ 6Å.