

Nov. 1, 2001

Name: _____

MIDTERM TEST

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

1. a) In a simple cubic lattice, show explicitly that the $\{110\}$ planes are 2D rectangular lattices.
 - b) Now consider the (110) planes of fcc and bcc lattices. Which are also 2D rectangular lattices? For counterexamples, indicate the sort of lattice it is.
 - c) i) In a simple cubic lattice, what is the distance between a family of $(9\ 7\ 5)$ planes? (Hint: What is the length of the corresponding \mathbf{K} ?)
 - ii) What is the area of a unit cell of the 2D lattice of these planes?
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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 has nearly isotropic charge distribution near each atom but strong radial dependence?
 - c) Which kind involves hybrid orbitals?
 - d) Which kind has bonding dominated by electrostatic forces?
 - e) For which kind do atoms tend to have the fewest nearest neighbors?
 - f) Which kind must involve more than one element?

Consider X-rays, thermal neutrons, and low-energy electrons as probes of crystals:

- a) Name an important property that all have.
- b) Name a property that X-rays have but the other two lack.
- c) Name a property that low-energy electrons have but the other two lack.
- d) Name a property that thermal neutrons have but the other two lack.
- e) Why are thermal neutrons better than X-rays for probing phonon dispersion?

Perovskites such as barium titanate have a cubic crystal structure, with O at the face centers, Ba at the corners, and Ti at the body center. FIGURE

- a) Assuming that the crystal is neutral, what is the charge state (ionicity) of the Ti if the oxygen is O^{2-} and the barium is Ba^{2+} ?
- b) Using the Eyring method for the first neutral shell, estimate the cohesive energy of this crystal in terms of e/a , where a is the conventional lattice constant (the shortest distance between Ba's).
- c) Barium titanate undergoes a ferroelectric transition in which the Ba and Ti ions move in a $\langle 100 \rangle$ direction while the O ions move in the opposite direction. This transition can be described by a so-called soft mode, in which a phonon branch drops to zero around some \mathbf{k} so that the lattice can distort with no cost in energy.
 - i) Is this branch acoustic or optical? Explain.
 - ii) Which ion (Ba, Ti, or O) do you expect to move the most? Explain your reasoning.
 - iii) For what value of \mathbf{k} does this occur? (E.g. zone center, zone face center, zone corner) Explain

Consider a Debye model for a one-dimensional Bravais crystal (a chain of atoms with mass M , spring constant K , spacing a).

- a) Find the Debye wavevector k_D and the Debye frequency ω_D .
- b) Find the density of states. (Show your work.)
- c) Write an integral for the (harmonic, thermal) energy and indicate the T dependence at low-temperature.

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 longitudinal branches are there?
- c) How many distinct independent values of \mathbf{k} are there?
- d) What is the size of the Wigner-Seitz cell?
- e) In high-symmetry directions, how many distinct (non-degenerate) branches are there?

Phonon dispersion curves, DOS, etc.

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 \mathbf{d} relative to atom 1 (with form factor f_1).

a) If $f_2 = f_1$ write down the condition that \mathbf{d} must satisfy so that the structure factor at \mathbf{K} (and thus the scattering intensity at \mathbf{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 vanishes? Justify your answer briefly.

3. Recall estimating the Madelung constant α for ionic crystals using the Ewald (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.)

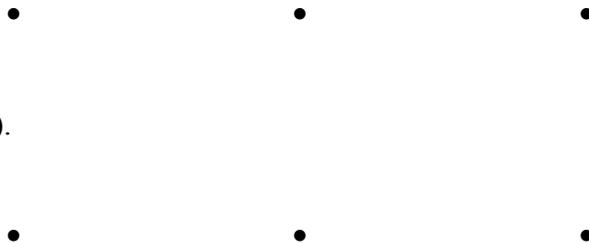
b) Which case has the largest angular variation in charge density about an atom (say at a distance $1/4$ of the interatomic spacing from the atom)?

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

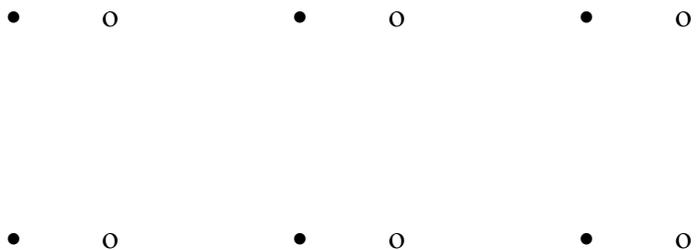
d) Which kind has a binding energy that can be crudely deduced using the Uncertainty Principle?

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 $\mathbf{k} = (\pi/a) (1/2, 1/2)$.



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 $\mathbf{k} = (\pi/a) (1, 0)$.



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 \mathbf{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: $\omega(\mathbf{k}) = \omega_0[1 - (1-|\mathbf{k}|a/\pi)^2]$

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 $\langle 100 \rangle$ face centers, $\langle 110 \rangle$ edge centers, and $\langle 111 \rangle$ corners. (Do not waste time summing the various contributions; just show the contribution from each type of site.)