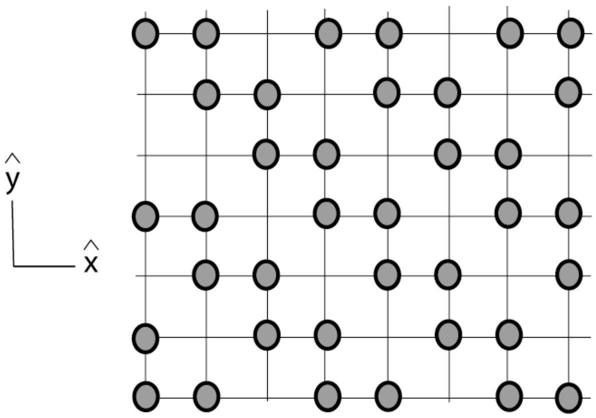
Solid State Physics Midterm Exam   Part 1   Name________________________

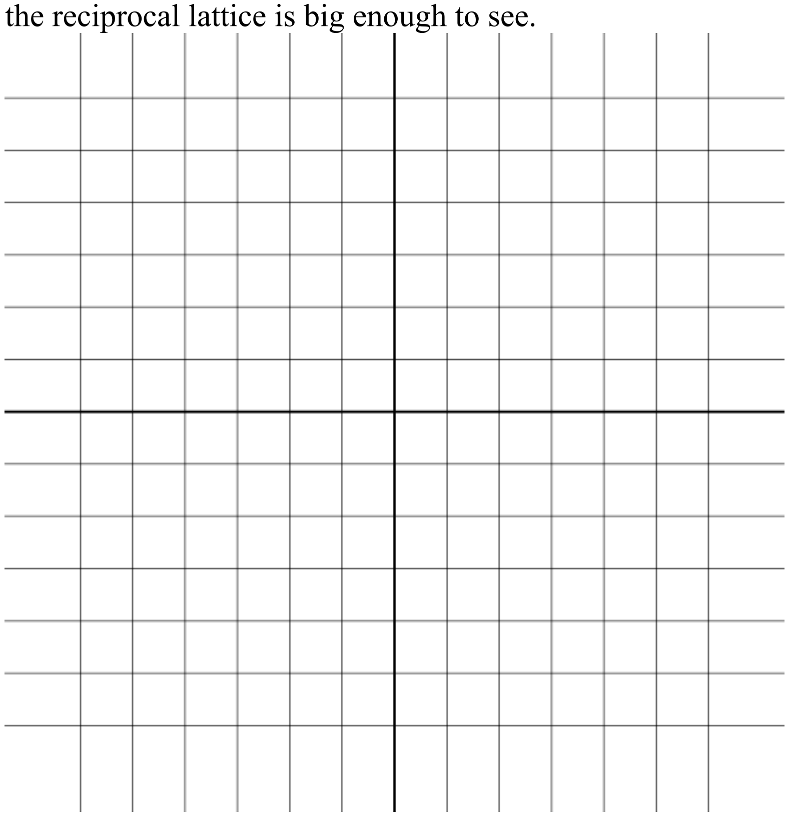
Consider the 2D arrangement of atoms shown. It's a small part of a very large crystal. The grid lines are at 2 Å separation.



a. Sketch **primitive** lattice vectors, and write them in terms of x and y. What is the basis?

b. Write the reciprocal lattice vectors in terms of x, y.
(Hint, which you may not need: you can add z as a third primitive lattice vector.)

Sketch part of the reciprocal lattice nearest the origin, showing at least 9 reciprocal lattice points, using the graph paper below. You can choose whatever scale you want for the lines on the paper, so long as the reciprocal lattice is big enough to see.



c. Add to your sketch the boundaries of the 1st Brillouin zone.

d. Add to your sketch **any pair** of initial and final k-vectors for an allowed, in-plane (elastic) x-ray diffraction.

e. If you were to shine x-rays down onto the 2D crystal, what diffraction would you expect to see? (Describe qualitatively.)

f. Find the scattered amplitude for your choice in (d). Be sure to include the structure factor appropriate to your choice of basis in (a). Assume the crystal has *N* unit cells, and the atomic form factor is *f*.

g. Consider the continuum description of plane waves traveling at 45° to the x- and y-axes (up and to the right.) Take the spring constant for closely spaced atomic planes to be 3C and for widely spaced atomic planes to be C. Take the mass of a plane of atoms to be m. Write down the equations of motion for u_s and v_s. Then, substitute in a trial solution

$$\begin{pmatrix} u_s \\ v_s \end{pmatrix} = \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} e^{i(Ksa-\omega t)}$$

and find the dispersion relation, ω(K). How many branches does it have? Sketch.
(Did you just solve for longitudinal, transverse, or unspecified polarization?)

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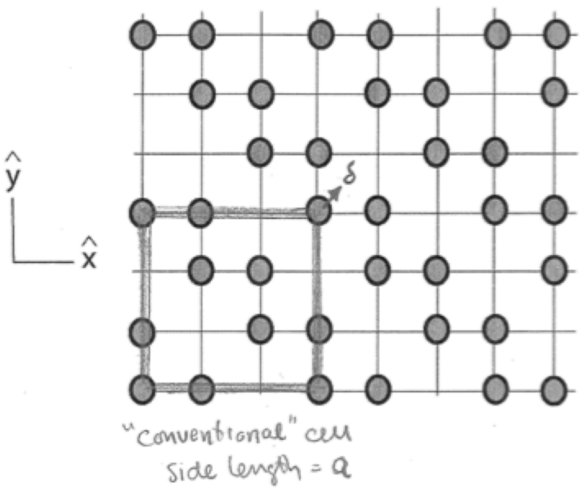
h. Measurements of wave speed can tell us about elastic constants in crystals. For this section, consider a "conventional" square cell, of side length a, shown in the figure. A longitudinal wave traveling up and right will displace the upper right atom a small distance δ. (Of course, all the atoms in the unit cell are displaced up and right, but proportionately less the closer they are to the origin.)

In terms of δ and a, what are the elastic strains e_{xx}, e_{yy}, and e_{xy} for this wave?

i. For in-plane deformations, all stress & strain terms involving z are zero. We'll also assume $C_{16} = C_{26} = C_{61}=C_{62}=0$. Write out equations 57a & b from Chapter 3 and plug in a trial longitudinal wave moving in the [11] direction. Solve for the wave speed. Is your answer consistent with what you found in part h?



Midterm Exam, part 2.

j. Suppose the 2D crystal above has a heat capacity that varies (at low temperature) like T^2. Do you expect it to be a conductor or an insulator? Why?

k. In fact, each atom of the crystal can give up one electron to the electron sea. Find the Fermi energy, and the average kinetic energy of electrons at 0K.

l. Sketch the free electron bands in the "reduced zone scheme", along the direction [10] for your choice of primitive basis vectors, $\vec{b}_1$ and $\vec{b}_2$. Sketch the lowest energy band, and also bands obtained when k is offset by $\pm\vec{b}_1$ and by $\pm\vec{b}_2$.

m. What are the largest and smallest k-vectors in the 1st Brillouin zone? (This is a geometric exercise… it may help to make use of some symmetry.

n. Suppose the smallest k-vector (for a particular choice of primitive lattice vectors) is $\frac{6\pi\sqrt{2}}{9}\mathring{A}^{-1}$ and the largest is $\frac{10\pi\sqrt{2}}{9}\mathring{A}^{-1}$. Use the nearly free electron model to estimate how large the "cosine term" in the atomic potential must be to turn this conductor into a semi-metal. (For this part, ignore the fact that there are 2 atoms in the basis. Do you think presence of the second atom would make the required atomic potential *larger* or *smaller*, for turning this material into a semi-metal?

o. Modify your sketch of the bands in (l) to include the effect of the atomic potential you found in (n).

p. Sketch the density of electronic states (or orbitals) for part o. (You should add your sketch on the right of the bands, using the vertical axis for energy and the horizontal axis for density.)

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2. A very unusual crystal has an interatomic potential given by $U=cx^2 + dx^4$. Find the thermal expansion x at temperature T in terms of c and d. You do **not** need to show your work.

3. The Debye approximation for the heat capacity (of insulators) assumes the speed of sound is independent of k, so that $\omega = v_s k$. If phonons had an electron-like dispersion relation, $\omega \sim k^2$, the heat capacity at low temperature would not vary as T^3 (in 3D). How would it vary?