Materials 200B, Winter 2008, Homework 4

Due in class on Tuesday Feb. 5th

Please turn in the two questions in separate answer packages since Alison and Bharat will grade one each.

QUESTION 1

Here we are going to continue working with our 1D chain of atoms, spaced a distance a apart, within the LCAO approximation, so that the energy is given by

$$E(k) = \alpha + 2\beta\cos(ka)$$

(a) Derive an expression for, and plot, the effective mass as a function of k. Describe what is going on physically in the top half of the band.

(b) The velocity of an electron with wavefunction Ψ_k is given by

$$v_k = \frac{1}{m}\int \Psi_k^* p \Psi_k dx$$

where m is the regular electron mass and p is the operator for momentum. (Remember $p = -i\hbar\frac{d}{dx}$.)

By substituting Bloch's theorem,

$$\Psi_k(x) = e^{ikx}u(x)$$

where $u(x) = u(x+a)$ into the Schrödinger equation for $\Psi_k(x)$, show that

$$v_k(x) = \frac{1}{\hbar}\frac{dE(k)}{dk}$$

In fact this is called the *group velocity* of the electron.

(c) Think about what your result means, and write down any insights that you have.

(d) Show that the wavefunctions labelled by k and $-k$ have equal and opposite velocities.

(e) Sketch v_k as a function of k, and indicate where it is zero.

(f) Calculate the maximum group velocity for a spacing a of 1 Å, and $\beta = -1eV$.

QUESTION 2

Polonium (Po) is the *only* element which is stable in the simple cubic structure.

(a) Sketch the unit cell of polonium and indicate the positions of the atoms.

(b) Write down the lattice vectors of the *cubic* unit cell and the primitive unit cell.

(c) How many atoms are there per simple cubic unit cell?

(d) The spacing of atoms in a solid using x-ray diffraction by applying Bragg's law,

$$2dsin\theta = n\lambda.$$

Here d is the inter-atomic spacing, θ is the angle at which a peak appears for radiation of wavelength λ, and n is any integer.

In an x-ray diffraction measurement, using x-rays of wavelength $\lambda = 0.1542$ nm, the first peak corresponding to diffraction from the $\{001\}$ planes occurs at a diffraction angle $\theta = 13.26°$. What is the unit cell edge length of Po? What is the volume of the unit cell? What is the volume per Po atom?

(e) Imagine instead that Po crystallized in the FCC structure. Sketch the conventional cubic unit cell and indicate also the primitive unit cell. Write down the lattice vectors of the primitive unit cell, and a formula for its volume in terms of the primitive lattice vectors.

(f) Taking the radius of the Po atom to be half of the inter-atomic distance in the simple cubic structure, work out the volume per Po atom in the fcc structure. Using your result, why do you think that most metals adopt the FCC structure?