Solutions for Homework 4

October 6, 2006

1 Kittel 3.8 - Young's modulus and Poison ratio

As shown in the figure stretching a cubic crystal in the x direction with a stress Xx causes a strain $e_{xx} = \delta l/l$ and $e_{yy} = e_{zz} = -\delta w/w$. (Note minus sign - defined so that $\delta w > 0$ as in the text.) The key is that the stress in the y and z directions is zero. Then $Yy = C_{12}e_{xx} + C_{12}e_{zz} + C_{11}e_{yy} = C_{12}e_{xx} + (C_{12} + C_{11})e_{yy} = 0$

Poisson ratio:

$$\frac{\delta w/w}{\delta l/l} = -\frac{e_{yy}}{e_{xx}} = \frac{C_{12}}{C_{11} + C_{12}}$$

Now consider $Xx = C_{11}e_{xx} + C_{12}e_{zz} + C_{12}e_{yy} = C_{11}e_{xx} + 2C_{12}e_{yy} = (C_{11} + 2C_{12}\frac{e_{yy}}{e_{xx}})e_{xx}$. Then Young's modulus: $Y = \frac{Xx}{e_{xx}} = C_{11} - 2C_{12}\frac{C_{12}}{C_{11}+C_{12}}$ which with a little algebra can be transformed to:

$$Y = \frac{(C_{11} - C_{12})(C_{11} + 2C_{12})}{C_{11} + C_{12}}$$

2 Kittel 4-2 Continuum elastic equation

The key to this problem is that a second derivation is the limit of the numerical difference formula

$$\frac{d^2u(x)}{dx^2} = \frac{u(x+h) + u(x-h) - 2u(x)}{h^2}$$

The expression for the lattice (Eq. 2, Ch 5) is:

$$\frac{d^2u_s}{dt^2} = (C/M)(u_{s+1} + u_{s-1} - 2u_s) = (Ca^2/M)\frac{u_{s+1} + u_{s-1} - 2u_s}{a^2}$$

In the long wave limit the change in u from one site to the next is very small compared to a. Therefore, u approaches a continuous function of position $x = sa$ and the equation becomes

$$\frac{d^2u_s}{dt^2} = (Ca^2/M)\frac{d^2u(x)}{dx^2}$$

with the sped of sound $v^2 = (Ca^2/M)$ as given in Eq. 15.

3 Kittel 4-3 Basis of two atoms

For $k = \pi/a$, $e^{ika} = -1$ and the equation 20 decouples into two independent equations:
$(2C - M_1\omega^2)u = 0$ and $(2C - M_2\omega^2)v = 0$
Thus it follows that if $2C - M_1\omega^2 = 0$, then u can be non-zero, but v must be zero, etc.

4 Kittel 4-5 Chain with C, 10C

If there are alternating force constants C and $10C$, then the lattice has the form
... $x_1 - - - C - - - x_2 - -10C - -x_1 - - - C - - - x_2 - -10C - -x_1 - - - C - - - x_2 - -10C - -x_1$ ...
where the sites are labelled 1 and 2. The displacements of the sites are u and v. The nearest-neigh. is defined to be $a/2$ and the lattice constant is a, and the BZ is $-\pi/a$ to π/a. Each site has a bond with force constant C on one side and $10C$ on the other. We can choose the cell to be $x_1 - - - C - - - x_2 - -10C - -$ (we would get the same answer with another choice). Then the equations are the ones in the text (Eq 18) modified to

$$M\frac{d^2u_s}{dt^2} = 10C(v_{s-1} - u_s) + C(v_s - u_s)$$

$$M\frac{d^2v_s}{dt^2} = 10C(u_{s+1} - v_s) + C(u_s - v_s)$$

or

$$(11C - M\omega^2)u = 10Cve^{-ika} + Cv$$

$$(11C - M\omega^2)v = 10Cue^{+ika} + Cu$$

At $k = 0$, this becomes $(11C - M\omega^2)u = 11Cv$ and $(11C - M\omega^2)v = 11Cv$, Substituting one equation into the other gives $(11C - M\omega^2)^2u = (11C)^2$, or

$$(11C - M\omega^2) = \pm 11C$$

which has two solutions $\omega = 0$ and $\omega^2 = 22C/M$

At $k = \pi/a$, $e^{+ika} = -1$ and the equations become $(11C - M\omega^2)u = -9Cv$ and $(11C - M\omega^2)v = -9Cv$, Substituting one equation into the other gives $(11C - M\omega^2)^2u = (9C)^2$, or

$$(11C - M\omega^2) = \pm 9C$$

which has two solutions $\omega = 2C/M$ and $\omega^2 = 20C/M$

The curves look like Fig. 7 in Ch. 5 of Kittel, except that there is a much larger difference in the two frequencies at the zone boundary.

5 Speed of sound in C and Au

The speed of a longitudinal wave in the [100] direction in a cubic crystal is given by $v = (C_{11}/\rho)^{1/2}$.
For diamond, $C_{11} = 10.76x10^{11} N/m^2$, $\rho = 3.52x10^3 Kg/m^3$
v = $(C_{11}/\rho)^{1/2} = 1.75x10^4 m/s$
For Au, $C_{11} = 1.92x10^{11} N/m^2$ at 300K, $\rho = 19.5x10^3 Kg/m^3$
v = $0.31x10^4 m/s$

6 Elastic properties and phonons in a simple cubic crystal

Consider a simple cubic crystal with lattice constant a and one atom per cell of mass M. Assume the atoms interact with nearest-neighbor forces $\phi(R)$ with second derivative $C = \phi''$. Answer the questions below in terms of a, M, and C.

A. Give expression for the elastic constant C_{11} and the bulk modulus B.

$$C_{11} = \frac{1}{V}\frac{d^2U}{de_{xx}^2}, \quad \text{and} \quad B = \frac{1}{V} = \frac{d^2U}{(dV/V)^2} = V\frac{d^2U}{dV^2}$$

where U is the energy of a cell with volume V. For simple cubic with one atom per cell, we can take U to be the energy per atom and $V = a^3$. There are 3 bonds per atom in the x, y and z directions and $U = [\phi(a_x) + \phi(a_y)\phi(a_z)$ as a function of the lengths in the 3 directions. For the calculation of B, the length of all three bonds change equally and it is sufficient to consider $dV = d(a^3) = 3a^2da = 3V da/a = 3(V/a)da$. Then

$$B = B = V\frac{d^2U}{dV^2} = \frac{V}{9V^2/a^2}\frac{d^2U}{da^2} = \frac{a^2}{3V}\frac{d^2\phi(a)}{da^2} = \frac{C}{3a}$$

For C_{11} only a_x changes, and $de_{xx} = da_x/a_x = da_x/a$ evaluated for $a_x = a$. Then

$$C_{11} = \frac{1}{V}\frac{d^2U}{de_{xx}^2} = \frac{a^2}{V}\frac{d^2\phi(a_x)}{da_x^2} = \frac{C}{a}$$

Note that the general relation $B = \frac{1}{3}(C_{11} + 2C_{12})$ is satisfied in the case because $C_{12} = 0$. (Check this for yourself.)

B. Give the expression for the longitudinal sound velocity v in the [100] direction in terms of the appropriate elastic constant.

$v_s = (C_{11}/\rho)^{1/2}$ as explain in the book andd class notes.

C. Give the expression for the dispersion curve $\omega(k)$ for longitudinal motion as a function of wavevector k in the [100] direction. Show that this leads to a velocity of sound in agreement with part B and give the expression for the frequency ω_{BZ} for k at the boundary of the Brillouin zone.

As given in the notes for lecture 8 (and discussed above), in this case only the $\phi(a_x)$ bond is involved in this case. The problem is exactly like a one dimensional line of atoms with spring constant C, and

$$\omega(k) = 2(C/M)^{1/2} sin(ka/2), \quad \text{and} \quad v_s = \frac{d\omega(k)}{dk} = a(C/M)^{1/2} cos(ka/2) = 2a(C/M)^{1/2} \text{forsmallk}$$

The zone boundary frequency is $\omega_{BZ} = 2(C/M)^{1/2} sin(\pi/2) = 2(C/M)^{1/2}$. The speed of sound is $v_s = a(C/M)^{1/2}$, and using $\rho = M/a^3$, this becomes $v_s = a(C/\rho a^3)^{1/2}$ which is $v_s = a(C_{11}/\rho a^2)^{1/2} = (C_{11}/\rho)^{1/2}$, which agrees with the elastic equation above.

D. Find values of each of the quantities C_{11}, B, v, and ω_{BZ}, for the case where M = mass of the Al atom, a = 0.286 nm (the nearest-neigh. distance in Al given in Kittel), and an estimate of C = 100 eV/nm^2 (This is a very crude estimate of ϕ'' based upon the idea that displacement of an atom by 0.1 nm should change the energy by of order 1 eV.)

Using the expressions above and the values $a = 0.286x10^{-9}$ m, $M = 26.981539Amu = 0.451x10^{-25}$ Kg, $C = 100eV/nm^2 = 100x1.6x10^{-19}/10^{-18} = 16.0$ J/m^2, we find

$$C_{11} = \frac{C}{a} = (16/0.286)x10^9 J/m^3 = 0.56x10^{11} J/m^3$$

$$B = C_{11}/3 = 0.18x10^{11} J/m^3$$

$$v = a(C/M)^{1/2} = 0.286x10^{-9}(16.0/0.451x10^{-25}(^{1/2} = 0.286x1.88x10^3 = 0.56x10^3 m/s$$

$$\omega_{BZ} = 2(C/M)^{1/2} = 2(16.0/0.451x10^{-25}(^{1/2} = 2x1.88x10^{12} = 3.76x10^{12} s^{-1}$$

E. Even though Al does not form the simple cubic structure and the value of C is a crude estimate, the results should be of the same order of magnitude as in real Al. Compare C_{11} and B with the actual values for Al given in Kittel.

The values are $C_{11} = 1.068x10^{11} J/m^3$ and $B = \frac{1}{3}(C_{11}+2C_{12}) = 0.761x10^{11} J/m^3$. Reasonable agreement! The reason B is too low in the calculation is that C_{12} is larger in fcc Al, whereas it is zero in the above model for simple cubic.

7 Phonons in Na

In Figure 11 (chapter 4) of Kittel, are shown the measured dispersion curves of Na, which has the bcc structure. It is a good approximation to assume the interaction $\phi(R)$ acts only between nearest neighbors.

A. From the value of the longitudinal frequency at the zone boundary in the [100] direction, find the value of the second derivative ϕ''. (Note that you must treat Na as bcc and the neighbors are not oriented along the [100] direction.)

THIS IS CORRECTED ON OCTOBER 6. THE SOLUTION POSTED OCTOBER 4 HAD A MISTAKE. The general expression for the effective force constant is given in lecture 8: $C_{eff} = Cx \sum_i (cos(\Theta_i)^2$ (here we use $C = \phi''$. For bcc one has 8 neighbors so that there are 4 neighbors in an adjacent plane. Since the neighbors are in the (111) direction for motion in the (100), (010), or (001) directions $cos^2(\Theta) = 1/3$. Thus $C_{eff} = (4/3)\phi''$ for either longitudinal or transverse motion. This leads to $\omega(k) = 2(4C/3M)^{1/2} sin(ka/2)$ and $\omega_{BZ} = 2(4C/3M)^{1/2}$ or $C = M\omega_{BZ}^2(3/16)$. Using ω_{BZ} $2\pi x 3.6 10^{12} s^{-1}$ from the graph and M = 22.98977 Amu, we find:

$$C = M\omega_{BZ}^2(3/16) = (3\pi^2/4)22.99x1.67x10^{-27}x12.96x10^{24} = 2.212 J/m^3$$

B. Give the expression for the dispersion curve for transverse motion (k in the [100] direction, displacement in the [010] direction) using the value of ϕ'' from part A. What is the value of the frequency at the Brillouin zone boundary?

For this model of bcc the transverse frequency is the same as the longitudinal frequency (because each neighbor has the same angles Θ for the motions). Note that this is very close to the observed transverse and longitudinal modes in the figure for Na.