Assignment #3

Due : 10am April 3rd 2012 (before the lecture)

1. Debye-Waller factor

In our derivation of the scattering cross-section for a crystal, we ignored the fact that the atoms are not perfectly periodic due to thermal motion of the lattice (phonon). If one takes into account the small displacement $\mathbf{u}_n$ of an atom located at $\mathbf{R}_n$, the x-ray scattering intensity should be modified to

$$I = |F|^2 = \sum_{m,n} f(\mathbf{q}) f^*(\mathbf{q}) e^{i\mathbf{q}\cdot(\mathbf{R}_m - \mathbf{R}_n)} \left\langle e^{i\mathbf{q}\cdot(\mathbf{u}_m - \mathbf{u}_n)} \right\rangle, \tag{1}$$

where $f(\mathbf{q})$ is the atomic form factor. If we define u_{qn} as the component of the displacement parallel to the wavevector for the n'th atom, bracketed factor becomes

$$\left\langle e^{i\mathbf{q}\cdot(\mathbf{u}_m - \mathbf{u}_n)} \right\rangle = \left\langle e^{iq(u_{qm} - u_{qn})} \right\rangle.$$

(a) Using the Baker-Hausdorff theorem ($\langle e^{ix} \rangle = e^{-\frac{1}{2}\langle x^2 \rangle}$), show that the scattering intensity can be written as

$$I = |f(\mathbf{q})|^2 e^{-2W} \sum_{m,n} e^{i\mathbf{q}\cdot(\mathbf{R}_m - \mathbf{R}_n)} e^{q^2 \langle u_{qm} u_{qn} \rangle}, \tag{2}$$

where $2W \equiv q^2 \left\langle u_q^2 \right\rangle = \langle (\mathbf{q}\cdot\mathbf{u})^2 \rangle$. We assume that the mean square displacement is independent of atom index, and therefore can be pulled out of the sum.

If we expand the last exponential in Taylor series, the intensity becomes

$$I = |f(\mathbf{q})|^2 e^{-2W} \sum_{m,n} e^{i\mathbf{q}\cdot(\mathbf{R}_m - \mathbf{R}_n)} (1 + q^2 \langle u_{qm} u_{qn} \rangle). \tag{3}$$

In the first term, the summation is just the square of the lattice sum, which leads to delta functions at the Bragg peak positions. Now the Bragg peak intensity is reduced by the factor e^{-2W}, called *Debye Waller factor*, which is the consequence of thermal agitation of atoms. Note that the second term in fact depends on the *correlation* between the displacements of different atoms, and therefore contributes to phonon scattering (can be probed with either inelastic scattering or thermal diffuse scattering).

(b) The mean square atomic displacement in the Debye-Waller factor, after taking thermal average using Bose statistics of phonons, becomes

$$2W = \frac{1}{Nm} \sum_{k,j} \frac{\hbar^2 (\mathbf{q}\cdot\mathbf{e}_{k,j})^2}{\hbar\omega_{k,j}} \left(n_{k,j} + \frac{1}{2} \right), \tag{4}$$

where $\omega_{k,j}$ is the phonon mode with index j and momentum $\mathbf{k}$; m is the ionic mass, and $\mathbf{e}$ is the unit vector along the direction of the displacement $\mathbf{u}$. $n_{k,j}$ is the Bose-Einstein occupation factor

$$n_{k,j} = \frac{1}{e^{\hbar\omega_{k,j}/k_B T} - 1}.$$

For simplicity, we will consider a monoatomic cubic crystal. We will further ignore the different velocities of longitudinal and transverse modes: $(\mathbf{q} \cdot \mathbf{e}_{k,j})^2 = q^2/3$. Then, the j dependence disappears, and the sum over j becomes simply a factor of 3. Following the Debye model you learned in elementary statistical physics, show that (in the high temperature limit)

$$2W = \frac{3(\hbar q)^2 T}{m k_B \Theta_D^2},$$

where Θ_D is the Debye temperature. (*Hint: Debye model only considers linear dispersion relation of acoustic phonons.*)

(c) Consider x-ray diffraction experiments using Cu Kα radiation. Evaluate the Debye-Waller factor at room temperature for the first 5 Bragg peaks of gold, whose Debye temperature is 162 K.

(d) Now consider the case of two-dimensional (square lattice) solid. Using the same approximation as in part (b), show that 2W now diverges.

2. Chaikin and Lubensky problem 7.1 (p. 411).

3. Read the following article and write a referee report of about 1 page long. You can find helpful information at the publisher's website, for example, Physical Review has information available at http://publish.aps.org/refinfo.html.

- S. M. Hayden *et al.* Phys. Rev. Lett. **76**, 1344 (1996).