Problem set 3, Due Fri. Feb. 2

Useful references for this problem set include:

- Kittel, chapters 1 & 2.
- Ziman, chapter 1.
- Numerical Recipes, chapters 7 & 12.
- Ashcroft & Mermin, chapters 4, 5, 6, 7.

1. Ibach and Lüth 3.1..

2. Ibach and Lüth 3.5..

3. Ibach and Lüth 3.9..

4. Fast Fourier Transforms. (Computer) You will need a FFT package, a random-number generator, and you will need to be able to make plots for this problem. If you write your own programs, you'll use an FFT routine like *realft* and a random–number generator like *gasdev*, described in Numerical Recipes. If you use Mathematica, your main tool will be *Fourier*; you will need to convert the uniformly–distributed output of *Random* into a Gaussian distribution. (Read about FFTs and Gaussian distributions in Numerical Recipes anyway.)

Perfect crystals are periodic, so Fourier transforms are a basic tool in this course. The numerical analysis community has provided us with excellent packages for doing fast Fourier transforms — packages whose obscure and intricate innards do everything one needs. Experimentalists and theorists use these routines often, doing everything from spectral analysis to dynamical systems. FFTs also illustrate the basic ideas of reciprocal space and diffraction particularly well.

- Perfect Crystals. The diffraction pattern of a perfect crystal is a set of δ-function peaks at the reciprocal lattice points. Consider a one-dimensional crystal with atoms centered at R_n whose electron density forms Gaussians of width σ_n

$$\rho(x) = \sum_n e^{-(x-R_n)^2/2\sigma_n^2}.$$

  To save you messing around (and us grading), let's set up a common crystal (arbitrarily). Initially, let the lattice constant a be 2.3 and σ be 0.2. Start with a matrix for ρ of 256 entries, spanning 32 lattice periods. (Really, one period suffices for part (a), but there would be only one k-vector per unit cell.) The matrix RHO should be periodic too: make RHO(256) what RHO(0) would have been. The sum over n needn't extend very far beyond the range of x. Calculate the Fourier transform $\tilde{\rho}(k)$ using the FFT routine. Examine $\rho(x)$ on the screen to make sure your electron density looks like an array of atoms. Plot the power spectrum $|\tilde{\rho}(k)|^2$ over a range which includes the first four Bragg peaks.

- Diatomic Basis. If the unit cell of a crystal doubles in size, the reciprocal lattice divides in two. Let σ_n be 0.1 if n is even, and 0.3 if n is odd. Examine your real-space density; for the same range of x (now 16 lattice periods) and the same other parameters, plot the power spectrum.

- Thermal Motion. At finite temperatures, the atoms will oscillate about their lattice positions: does the diffraction pattern get destroyed? Add a random number ϵ with standard deviation σ_ϵ to the positions ($R_n = n \cdot a + \sigma_\epsilon \cdot \mathrm{Rand(seed)}$). (Choose the random number from a normal probability distribution:

$$\mathrm{Prob(Rand)} = (1/\sqrt{2\pi}e^{-(\mathrm{Rand})^2/2}.)$$

  Keeping $\sigma_x = 0.2$, examine the real-space densities and plot the power spectrum for $\sigma_\epsilon = 0.1,\ 0.3,$ and 0.5.

- Show analytically that the reciprocal lattice peaks stay sharp, but that they are decreased in magnitude by $e^{-\sigma_\epsilon^2 k^2}$. (Start from the definition

$$\tilde{\rho}(k) = \int dx\, e^{ikx} \sum_n \rho_0(x - na - \epsilon_n);$$

pull out terms involving ϵ_n, and change the sum over n into an integral over ϵ involving Prob(ϵ). Don't forget that the power spectrum is $\tilde{\rho}^2$.) This is called the Debye-Waller factor; compare your numerical results to the analytic prediction.

- Glasses. A more realistic model of thermal motions would have the positions of the atoms vary with respect to their neighbors ($R_n - R_{n-1} = a + \sigma_\epsilon \cdot \text{Rand(seed)}$ (rather than with respect to an invisible ideal lattice). Plot the power spectrum for $\sigma_\epsilon = 0.05,\ 0.1,$ and 0.2.

  In one and two dimensions crystalline long-range translational order does not exist for $T > 0$. In three dimensions, an atom has more neighbors far away who remember where it is supposed to sit, and a reasonably high temperature is needed to destroy all remnants of periodicity. The model in part (c) is thus reasonable for 3-d crystals; it is Einstein's model for phonons in diamond. The model in part (d) gives a pretty good description of glasses and liquids: the Bragg peaks become broad when the long-range order disappears.

5. If the wavelength of the incident radiation and the scattering angle are known, then one may easily deduce the distance distance between the planes, d, responsible for each scattering peak. The following twelve lines were obtained from a crystalline powder. Data were obtained using nickel filtered Kα radiation. The powder is known to belong to a cubic system.

line	$d(\AA)$	relative intensity
1	3.157	94
2	1.931	100
3	1.647	35
4	1.366	12
5	1.253	10
6	1.1150	16
7	1.0512	7
8	0.9657	5
9	0.9233	7
10	0.9105	1
11	0.8634	9
12	0.8330	3

Index the lines in terms of their Miller indices (hkl) and calculate the lattice constant of the cubic lattice. Establish the type of cubic lattice. Explain (hint, consider the relative intensity of the lines).