Homework Assignment 1

A) Complete the Kroning-Penny Model problem 7.3 from Kittel. Refer to the text pp. 180-183 and 187-188.

(i) For the delta-function potential and with $P \leq 1$, find at $k=0$ the energy of the lowest energy band.

(ii) For the same problem find the band gap at $k=\pi/a$.

B) Radial Distribution Function. The intensity from x-ray diffraction as a function of wave number $k$, $I(k)$, for a-Ge is shown in the figure. Also note the plot shows $f^2$ for Ge. Numeric data is available in text format. Refer to Warren Ch. 10 for details.

(i) Calculate the average density of Ge atoms at room temperature, $\rho_0$, and plot the average atom-atom correlation function $4\pi^2\rho_0$, as a function of atomic separation, $r$.

(ii) Calculate the distribution of the 6 nearest neighbors for the Ge diamond (fcc with two atom basis) lattice. Plot these on the same curve.

(iii) Calculate the diffraction peak heights for crystalline Ge by weighting the nearest neighbor distribution by $f^2$. Estimate the broadening due to finite crystallite size as a gaussian distribution with FWHM given by the Scherrer equation [Warren, Eq. 13.3] $B(2\theta) = [0.94 \lambda / L \cos(\theta)]$ where $\theta$ is the scattering angle and $k=4\pi \sin(\theta)/\lambda$. Assume an average crystallite size of 3 nm and Cu Kα incident radiation with $\lambda=0.15418$ nm. Estimate a broadening due to instrumental resolution as a gaussian with FWHM of $0.03$ Å$^{-1}$. By convoluting the delta function weighted nearest neighbor distribution with the appropriate gaussian functions, calculate a scattering intensity versus scattering angle $\theta$ for the nanocrystalline. Plot this and the intensity for a-Ge as functions of scattering angle.

(iv) Calculate the radial distribution function of a-Ge based on the given intensity curve. Plot this on the same graph as the average atom-atom correlation function and the nearest neighbor distribution.

(v) Comment on the structure of a-Ge based on the results of your calculations.

C) Given the experimental curve for the specific heat at constant pressure for glassy, liquid and crystalline lithium acetate, calculate the excess entropy of the glass as a function of temperature.