Physics 375 **Fall (12) 2003**

Solid State Physics: Problem Set #4

Defects and Diffusion in Solids

Due: Friday Feb. 7 by 6 pm

Reading assignment:
- for Monday, 4.2-4.4 (dislocations and point defects)
- for Wednesday, 4.4-5.1 (diffusion in solids; Einstein model for C_v)
- for Friday, 5.2 (Debye model for heat capacity C_v)

Problem assignment:

Chapter 4 Problems:

*4.10 Vacancy concentration from diffusion data in copper (Also ... make a plot of vacancy concentration n/N vs. temperature for $0<T<T_m$) **[Peter]**

4.11 Locking in defects via a temperature quench (make a plot like Fig. 4.32)

4.13 Diffusion of carbon atoms in solid iron [Fe(α)=bcc, Fe(γ)=fcc]

A1. Estimate the relative change in density of copper due to vacancy formation at a temperature just below its melting point, 1356 K. (E_v=1.07 eV for copper).

*A2. Frenkel Defects: The simultaneous formation of a lattice vacancy and an occupied interstitial site is known as a Frenkel defect. **[Melissa]**

a) Determine the total entropy of n such defects in a crystal containing N lattice sites and N' interstitial sites.

b) Assuming it takes energy E_I to form one such defect, show that the free energy of defects of the crystal can be written as:

$$F = nE_I - k_B T\{n \ln N + n \ln N' - 2n \ln n + 2n\} \quad \text{for } n \ll N, N'$$

c) By minimizing this free energy show that the equilibrium concentration of Frenkel defects is given by:

$$n = \sqrt{NN'}\, e^{-E_I/2k_B T}$$

A3. Line widths in diffraction patterns: Consider M point scattering centers (i.e., atoms or very narrow slits) arrayed in a one-dimensional lattice with lattice vector **a**. Radiation with wave vector **k** (where **k** is perpendicular to **a**, so **k•a**=0) is incident on the lattice. We have shown that the intensity of scattered radiation is proportional to $I(x)=\sin^2(Mx/2)/\sin^2(x/2)$ where $x = \Delta\mathbf{k}\bullet\mathbf{a}$.

a) For the given geometry, show that $x = ka \sin 2\theta$ where 2θ is the scattering angle.

b) Use Maple to make plots of $I(x)$ vs. x for M=2, 3, 4, 10, and 100 (let $-8<x<8$) and estimate the full width of the main diffraction peak at half its maximum value in each case.

c) The width of the diffraction peak can also be measured from the position of the maximum to the location of the first zero. Write an expression for the peak width as a function of M using this definition and determine the peak widths for the cases plotted in (b). Compare these results with your part (b) estimates of peak width.

*To be presented in class on Friday.