Háskóli Íslands
Raunvísindadeild
Eðlisfræði

Haust 2014

Eðlisfræði þéttefnis I

Dæmablað 4

Skilafrestur 23. September 2014 kl. 15:00

1. **Scattering data** (15)

   Powder specimens of three different monatomic cubic crystals are analyzed with a Debye-Scherrer camera. It is known that one sample is face-centered cubic, one is body-centered cubic, and one has the diamond structure. The approximate positions of the first four diffraction rings (2θ) in each case are:

A	B	C
42.4	28.8	42.8
49.2	41.0	73.2
72.0	50.8	89.0
87.3	59.6	115.0

   (a) Identify the crystal structures of A, B, and C

   (b) If the wavelength of the incident X-ray beam is 1.5 Å, what is the length of the side of the conventional cubic cell in each case ?

   (c) If the diamond structure were replaced by a zincblende structure with a cubic unit cell of the same side, at what angles would the first four rings now occur ?

2. **X-ray scattering from a liquid** (15)

   A fluid is an isotropic material (i. e. it looks the same in all directions) where the form factor does not depend on the scattering wavevector $K = K_{\text{in}} - K_{\text{out}}$.

(a) Show that the scattering intensity of a liquid with N molecules has the form

$$I(\mathbf{K}) = |f_{\mathrm{a}}|^2 \left[N + N \sum_{j \neq 0} \exp\left(j\mathbf{K} \cdot \mathbf{r}_j\right) \right]$$

(b) Define the density of scatterers $n(r)$ such that

$$\sum_{j \neq 0} \exp\left(j\mathbf{K} \cdot \mathbf{r}_j\right) \equiv \int d^3 r n(\mathbf{r}) \exp\left(j\mathbf{K} \cdot \mathbf{r}\right)$$

where the integration is taken over the volume of the liquid. Suppose this density is given by $n(\mathbf{r}) = n_0 + \delta(\mathbf{r})$. Write an expression for the scattering intensity and plot as a function of the scattering wavevector K.

(c) If the density of scatterers is given by

$$n(\mathbf{r}) = n_0(g(\mathbf{r}) - 1)$$

where

$$g(\mathbf{r}) - 1 = \begin{cases} -1 & \text{if } r < (3/(4\pi n_0))^{1/3} \equiv r_0 \\ 0 & \text{otherwise} \end{cases}$$

show that:

$$I(\mathbf{K}) = N |f|^2 \left[1 + n_0 \delta(\mathbf{K}) - 3 \frac{\sin Kr_0 - Kr_0 \cos Kr_0}{(Kr_0)^3} \right]$$

Write this as a Taylor expansion in the limit $K \geq 0$ and plot.

3. **Neon** (10)

Neon can be modeled as a Lennard Jones solid with $\mathcal{E} = 3.1$ meV and $\sigma = 2.74$ Å.

(a) Calculate the nearest neighbor distance for FCC neon.

(b) Calculate the binding energy for FCC neon.

4. **Debye-Waller factor** (20)

In the early days of X-ray structure determination, people posed the following objection: Due to the thermal motion, the atoms will not be exactly at their lattice positions but rather oscillate around them. Shouldn't this destroy the sharp Bragg peaks ? To explore this question, assume that the displacement of each atom from its lattice position $\mathbf{R}_l$ is a random vector $\mathbf{u}_l$ with a Gaussian distribution

$$P(\mathbf{u}_l) = \left(\frac{1}{2\pi\Delta^2} \right)^{3/2} \exp\left(\frac{-\mathbf{u}_l^2}{2\Delta^2} \right)$$

Average the structure factor

$$S(\mathbf{q}) = \frac{1}{N}\left|\sum_l \exp(j\mathbf{q}\cdot(\mathbf{R}_l + \mathbf{u}_l))\right|^2$$

Do you still find sharp Bragg peaks ? What happens to the amplitude of the peaks ?

5. **Linear ionic crystal** (15)

Consider a one-dimensional chain of $2N$ ions of alternating charge $\pm q (N \gg 1)$. In addition to the Coulomb interaction, there is a repulsive potential A/R^n between nearest neighbors only. (R is the distance between nearest neighbor ions.)

(a) Determine the equilibrium distance R_0.

(b) Determine the cohesive energy E_0 for this distance and show that it can be written as

$$E_0 = -N2\ln 2\left(1 - \frac{1}{n}\right)\frac{q^2}{R_0}$$

(c) Determine the work necessary to compress the crystal such that $R = R_0(1-\delta)$ to leading order in the small parameter $\delta \ll 1$.