Háskóli Íslands
Raunvísindadeild
Eðlisfræði

Haust 2015

Eðlisfræði þéttefnis I

Dæmablað 4

Skilafrestur 22. September 2015 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. **Structure factor and reflections** (10)

   The atomic coordinates in a lithium unit cell are (000) and (1/2 1/2 1/2), the coordinates in LiTl are Li at (000) and Tl at (1/2 1/2 1/2).

   (a) Would you expect 100 reflection from either lithium or LiTl ? Explain.

   (b) Calculate the structure factor S for lithium and for LiTl in terms of the atomic scattering factors f_{Li} and f_{Tl}.

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 ?