

Eðlisfræði þéttefnis I

Dæmablað 4

Skilafrestur 21. September 2017 kl. 15:00

1. 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.

2. 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 ?

3. 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} .

4. 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 $\delta \ll 1$.