

Eðlisfræði þéttfnis I

Dæmablað 4

Skilafrestur 27. September 2016 kl. 15:00

1. X-ray diffraction (10)

NaCl kristallast í hliðarsetna teningsgrind þar sem grunnur Na og Cl eru aðskilinn með vegalengd sem er helmingur hornalínu teningsins. Atóm tölur Na og Cl eru 11 og 17.

- (a) Ákvarða hvaða Röntgenspeglanir koma fram (merkt vísunum fyrir dæmigerða teningsgrind).
- (b) Af þessum hópum hver hópurinn gefur sterkt merki og hver veikt ?

NaCl crystallizes in a face-centered cubic lattice with a basis of Na and Cl ions separated by half the body diagonal of the cube. The atomic numbers of Na and Cl are 11 and 17, respectively.

- (a) Determine which X-ray reflections will be observed (indexed for the conventional cubic unit cell).
- (b) Of these which group will be strong and which group weak ?

(Próf desember 2015)

2. 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.

3. 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 \AA , 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 ?

4. 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} .