

# Eðlisfræði þéttfnis I

## Dæmablað 4

Skilafrestur 25. September 2018 kl. 15:00

1. Stefnur í kristöllum – crystal directions (10)

Hve margar stefnur tilheyra  $\langle 100 \rangle$  fjölskyldunni ?

How many directions belong to the  $\langle 100 \rangle$  family ?

(Próf Desember 2017)

2. Röntgen bylgjubognun – X-ray diffraction (10)

Grindarfasti (lengd tenings) einsatóma bcc kristalls er  $a = 4.28 \text{ \AA}$ . Reikna skal bylgjubognunarhorn  $2\theta$  fyrstu fjögurra toppa (þeirra fjögurra bylgjubognunartoppa sem hafa lægstu  $2\theta$  gildi) fyrir duft sýni, þegar beitt er einlitri Röntgen geislun með bylgjulengd  $\lambda = 1.5 \text{ \AA}$ . (duft sýni þýðir að allar kristallastefnur eru mögulegar í sýninu.)

The lattice constant (length of the conventional cubic cell) of a monatomic bcc crystal is  $a = 4.28 \text{ \AA}$ . Calculate the diffraction angles  $2\theta$  of the first four diffraction peaks (the four diffraction peaks with the lowest  $2\theta$  values) from its powder specimen, using monochromatic X-ray with a wavelength  $\lambda = 1.5 \text{ \AA}$ . (Hint: powder specimen implies that all crystal orientations are possible in the specimen.)

(Próf desember 2016)

### 3. 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 vísun 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)

### 4. 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.

### 5. 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  $f_{\text{Li}}$  and  $f_{\text{Tl}}$ .