

# Eðlisfræði þéttfnis I

## Dæmablað 1

Skilafrestur 2. September 2014 kl. 15:00

### 1. Density of atoms in silicon (10)

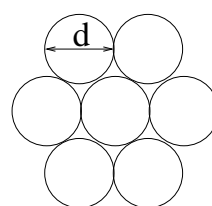
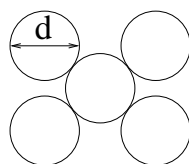
Consider the diamond structure of a Si crystal, for which the cubic lattice constant is  $a = 5.431 \text{ \AA}$ .

- Compute the distance, in  $\text{\AA}$ , between nearest-neighbor Si atoms in the crystal.
- Compute the distance, in  $\text{\AA}$ , between nearest-neighbor Si atoms in the (100), (110), and (111) planes of the Si crystal.
- Compute the density of atoms (atoms/cm<sup>3</sup>) in the Si crystal.

### 2. Pökkun í kristalli (10)

Myndin að neðan sýnir þétt pökkuð plön tveggja teningsgrinda sem hafa sömu fjarlægð milli næstu granna  $d$ .

- Hverjir eru Miller vísar plananna og í hvaða grindum finnast þau.
- Hver er frumeindapéttleikinn (frumeind/einingarflatarmál) í hvoru plani fyrir sig.



### 3. Ionic crystal KF (10)

In a single molecule of KF, the equilibrium internuclear separation is  $r_0 = 2.67 \text{ \AA}$  and the cohesive energy ( $-E_i$ ) relative to separated ions is 0.50 eV/molecule smaller than the Coulomb attractive energy, because of overlap repulsion. Given that the electron affinity of fluorine is 4.07 eV/electron and that the first ionization potential of potassium is 4.34 volts, show that the energy necessary to separate the molecule into neutral atoms is  $-0.945E_i$ .

### 4. Ionic crystals (15)

We can use the form

$$u(r) = \frac{\alpha e^2}{r} + \frac{C}{r^m}$$

of the cohesive energy per ion pair to investigate the stability of the possible crystal structure an ionic crystal may assume. Assuming that the coupling constant  $C$  characterizing the contribution of the short-range repulsion is proportional to the coordination number  $Z$ , show that the equilibrium cohesive energy for different lattice types varies as  $(\alpha^m/Z)^{1/(m-1)}$ , and use the values of the Madelung constant  $\alpha$  in the table below to construct a table of relative stability according to the value of  $m$ . (Hint: First examine the case of large or small  $m$ .)

Crystal structure	Madelung constant, $\alpha$
Cesium chloride	1.7627
Sodium chloride	1.7476
Zinchnblende	1.6381