Háskóli Íslands
Raunvísindadeild
Eðlisfræði

Haust 2014

Eðlisfræði þéttefnis 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 $a = 5.431$ Å.

   (a) Compute the distance, in Å, between nearest-neighbor Si atoms in the crystal.

   (b) Compute the distance, in Å, between nearest-neighbor Si atoms in the (100), (110), and (111) planes of the Si crystal.

   (c) Compute the density of atoms (atoms/cm^3) 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.

   (a) Hverjir eru Miller vísar plananna og í hvaða grindum finnast þau.

   (b) Hver er frumeindaþéttleikinn (frumeind/einingarflatarmál) í hvoru plani fyrir sig.

3. **Ionic crystal KF** (10)

   In a single molecule of KF, the equilibrium internuclear separation is $r_0 = 2.67$ Å and the cohesive energy ($-E_\mathrm{i}$) relative to seperated ions is 0.50 eV/molecule smaller than the Coulomb attractive energy, because of overlap repulsion. Given that the electron affinity of 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 $-0.945E_\mathrm{i}$.

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 α 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, α
Cesium chloride	1.7627
Sodium chloride	1.7476
Zinchblende	1.6381