Háskóli Íslands
Raunvísindadeild
Eðlisfræði

Haust 2016

Eðlisfræði þéttefnis I

Miðsvetrar próf

10. Október 2016 kl. 13:20 - 15:40

1. **Ge kristallur – Ge crystal** (10)

   Ge has the same crystal structure (diamond) as Si, with a lattice constant of $a = 5.64$ Å. Find the atomic density (atoms/cm^3) and the spacing between nearest-neighbor atoms in Ge.

   Ge hefur sömu kristallsgerð (demant) og Si, með grindarfasta $a = 5.64$ Å. Finna skal atómþéttleika (atoms/cm^3) og fjarægð á milli næstu granna atóma í Ge.

Number of atoms in the cubic unit cell

$$8 \times \frac{1}{8} + 6 \times \frac{1}{2} + 4 = 8$$

Atomic density

$$\frac{8}{a^3} = \frac{8}{(0.564 \times 10^{-7})^3} = 4.46 \times 10^{22} \text{ atoms/cm}^3$$

The nearest neighbor to an atom is 1/4 of the body diagonal away. The body diagonal of a cube of side a is $\sqrt{3}a$ so

$$\frac{\sqrt{3}a}{4} = 0.2441 \text{ nm}$$

2. **Mættisorka tengja – Potential energy of bonds** (40)

Tengi milli tveggja atóma í þéttefni hafa mættisorku E_{n} sem fall af fjarlægð r er gefin með jöfnunni

$$E_{\mathrm{n}}(r) = C\left[-\left(\frac{a}{r}\right)^{6} + \left(\frac{a}{r}\right)^{12}\right]$$

þar sem $C = 1.0 \times 10^{-20}$ J/tengi og $a = 0.38$ nm.

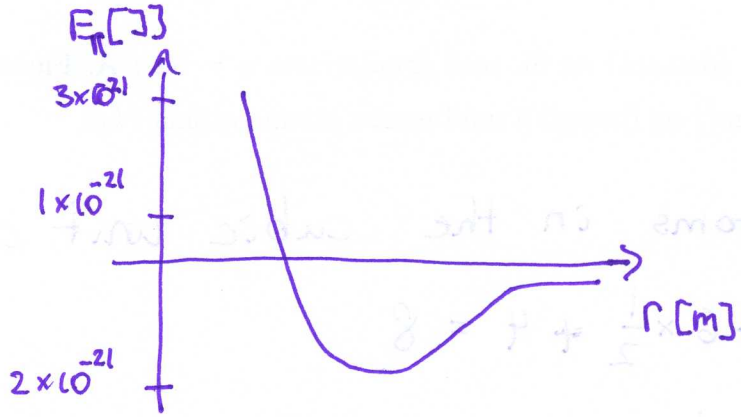
The bonds between two atoms in a solid have a potential energy E_{n} versus distance r curve given by the equation

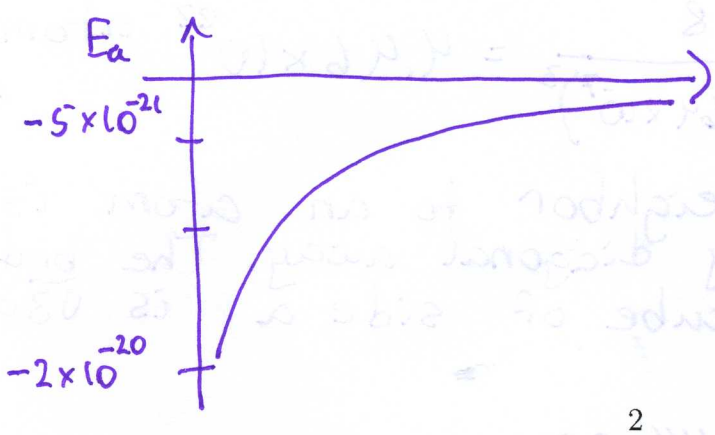
$$E_{\mathrm{n}}(r) = C\left[-\left(\frac{a}{r}\right)^{6} + \left(\frac{a}{r}\right)^{12}\right]$$

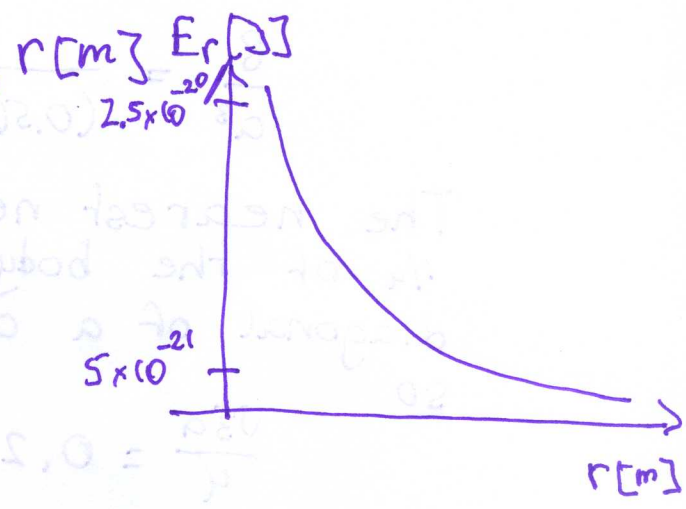
where $C = 1.0 \times 10^{-20}$ J/bond and $a = 0.38$ nm.

(a) Teiknið aðdráttar og fráhrindi liði mættisorkunnar sem fall af fjarlægð milli kjarna atómanna.

(a) Plot the attractive and repulsive terms of this potential energy versus distance between the nuclei of the atoms.







(b) Hvor liðurinn af $E_n(r)$ er ráðandi þegar mikill fjarlægð er á milli atóma ? Hvor liðurinn er ráðandi ef fjarlægð er lítil ?

(b) Which of the terms in $E_n(r)$ is dominant at large distances ? Which of the terms is dominant at short distances ?

The attractive term

$$-C\left(\frac{a}{r}\right)^6$$

is dominant at long distances, whereas the repulsive term

$$C\left(\frac{a}{r}\right)^{12}$$

is dominant at short distances

(c) Finna skal jafnvægisfjarlægðina r_o milli atóma ef enginn kraftur er lagður á tengið.

(c) Find the equilibrium distance r_o between the atoms if no force is applied to the bond.

$$\frac{dE_n}{dr} = \frac{C}{r_o}\left[-12\left(\frac{a}{r_o}\right)^{12} + 6\left(\frac{a}{r}\right)^6\right] = 0$$

or

$$2\left(\frac{a}{r_o}\right)^6 = 1 \quad \text{or} \quad r_o = a\,2^{1/6}$$

and thus

$$r_o = 0.38\,\text{nm} \times 2^{1/6} = 4.27 \times 10^{-10}\,\text{m}$$

(d) Finna skal orkuna sem leggja þarf til ef draga á atómin frá r_o og í sundur og mikla fjarlægð. Þessi orka er nefnd bindiorka táknuð með E_b.

(d) Find the energy that must be supplied to pull the two atoms from r_o to a very large distance apart. This energy is called the binding energy E_b.

$$E_b = E_n(\infty) - E_n(r_o) = 0 + 2.5 \times 10^{-21}\ \text{J}$$

(e) Bera skal saman bindiorkuna við varmaorkuna $k_B T$ við stofuhita, þar sem k_B er fasti Boltzmann. Ef $k_B T \gg E_b$ þá er þetta hvorki þéttefni eða jafnvel vökvi við stofuhita (varmatitringur rýfur tengin). Við hvaða hitastig er varmaorkan jöfn E_b ?

(e) Compare the binding energy with thermal energy $k_B T$ at room temperature, where k_B is Boltzmann's constant. If $k_B T \gg E_b$ the material will not be a solid or even a liquid at room temperature (thermal agitation will break the bond). At what temperature is will thermal energy be equal to E_b ?

Varmaorkan við stofuhita er

$$k_B T = 4.12 \times 10^{-21}\ \text{J}$$

or

$$k_B T = E_b \text{ when } T = 181\ \text{K}$$

Thus the energy from thermal agitation is not significantly greater than the binding energy of the solid. The solid will remain in a condensed state at 298K.

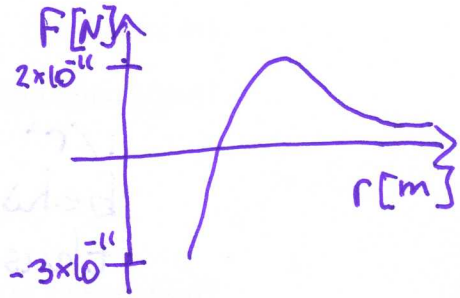
(f) Ákvarða skal kraft F sem fall of fjarlægð og teikna upp. Hver er "gormstuðull" tengisins ?

(f) Determine the force F versus distance curve for the bond and plot it. What is the "spring constant" of the bond ?

$$F = \frac{dE}{dr} = \frac{C}{r}\left[-12\left(\frac{a}{r}\right)^{12} + 6\left(\frac{a}{r}\right)^{6}\right]$$

and

$$S = \frac{d^2E_n}{dr^2} = C\left[\frac{156a^{12}}{r^{14}} - \frac{42a^6}{r^8}\right]$$



(g) Ef engin varmaorka er fyrir hendi ($T = 0$ K), hver er þá mesti kraftur sem tengið getur staðist ?

(g) If no thermal energy is available ($T = 0$ K), what is the maximum force the bond can support?

$$\frac{d^2E_n}{dr^2} = C\left[\frac{156a^{12}}{r^{14}} - \frac{42a^6}{r^8}\right] = 0$$

gives

$$r_{max} = 4.73 \times 10^{-10}\ m$$

so

$$F_{max} = 1.58 \times 10^{-11}\ N$$

3. **Tengi milli atóma í þéttefni – Bonds between pairs of atoms in a solid** (15)

Tengi á milli atóma í þéttefni geta verið

(a) jónísk tengi

(b) samgild tengi

(c) málmtengi

(d) van der Waals (tvípól-tvípól víxlverkun)

(e) vetnistengi

Hvaða tengi hafa, í mikilli fjarlægð, aðdráttarkraft sem fellur eins og $1/r^2$ milli para ?

$1/r^2$ implies Coulomb interaction between particles of opposite charge thus ionic bonding

Hvaða gerðir af tengjum geta ekki átt sér stað í þéttefni úr hreinum frumefnum ?

Ionic bonding requires dissimilar atoms. Hydrogen bonding acts between an hydrogen atom and typically one of oxygen, nitrogen or sulfur

Hvaða gerð(ir) af tengjum eru fundnar í storkinum kísli ?

Tetrahedral bonding arrangement and covalent bonds.

The bonds between pairs of atoms in a solid can be

(a) ionic bonds

(b) covalent bonds

(c) metallic bonds

(d) van der Waals (induced dipole-dipole interaction)

(e) hydrogen bonds

Which type(s) of bond has, at long distance, attractive force that varies as $1/r^2$ between pairs ?

Which type(s) of bond cannot occur in pure solid elements ?

Which type(s) of bond is found is solid Si ?

4. **2D Nykurgrind – 2D Reciprocal lattice** (10)

Finnið nykurgrind tvívíðrar grindar með $|\mathbf{a}_1| = 1.25$, $|\mathbf{a}_2| = 2.50$ og $\beta = 120°$.

Construct the reciprocal lattice for a two-dimensional lattice in which $|\mathbf{a}_1| = 1.25$, $|\mathbf{a}_2| = 2.50$ and $\beta = 120°$.

With

$$\underline{a}_1 = a(1.0)$$

$$\underline{a}_2 = a(-1, \sqrt{3})$$

using

$$\underline{b}_1 \cdot \underline{a}_1 = 2\pi \qquad \underline{b}_2 \cdot \underline{a}_2 = 2\pi$$

$$\underline{b}_2 \cdot \underline{a}_1 = 0 \qquad \underline{b}_1 \cdot \underline{a}_2 = 0$$

we find

$$\underline{b}_1 = \frac{2\pi}{a}(1, 1/\sqrt{3})$$

$$\underline{b}_2 = \frac{2\pi}{a}(0, 1/\sqrt{3})$$

5. **Línuleg keðja – Linear chain** (25)

Skoðum nú sveifluhætti línulegrar keðju, þar sem gormstuðlar milli næstu granna skiptast á að vera C of $10C$. Massarnir eru allir þeir sömu, og setjum fjarlægð milli næstu granna sem $a/2$. Finna skal $\omega(k)$ við $k = 0$ og $k = \pi/a$. Rissa skal tvístrunarsambandið. Þetta dæmi líkir eftir kristalli tvíatóma sameinda eins og H_2.

Consider the normal modes of a linear chain, in which the force constants between nearest-neighbor atoms are alternately C and 10C. Let the masses be equal, and let the nearest-neighbor separation be $a/2$. Find $\omega(k)$ at $k = 0$ and $k = \pi/a$. Sketch in the dispersion relation by eye. This problem simulates a crystal of diatomic molecules such as H_2.

We call the alternating force constants C_1 and C_2. For one type of atoms, the force constant C_1 is on the right and the force constant C_2 is on the left. For the other type of atoms, C_2 is on the right and C_1 is on the left. The equations of motion for these two sites are

$$M\frac{d^2u_s}{dt^2} = C_2(V_s - u_s) + C_1(V_{s-1} + u_s) = C_2V_s + C_1V_{s-1} - (C_1+C_2)u_s$$

$$M\frac{d^2V_s}{dt^2} = C_2(u_s - V_s) + C_1(u_{s+1} - V_s) = C_2u_s + C_1V_{s+1} - (C_1+C_2)V_s$$

Try periodic solutions of the form

$$u_s = ue^{j(ksa-\omega t)} \quad \text{and} \quad V_s = Ve^{j(ksa-\omega t)}$$

This leads to the eigenvalue equation

$$\begin{bmatrix} C_1+C_2-M\omega^2 & -(C_2+C_1e^{-jka}) \\ -(C_2-C_1e^{jka}) & C_1+C_2-M\omega^2 \end{bmatrix}\begin{bmatrix} u \\ V \end{bmatrix} = 0$$

The two solutions are

$$M\omega^2 = (C_1 + C_2) \pm \left(C_1^2 + C_2^2 + 2C_1C_2\cos ka\right)^{1/2}$$

Now set $C_1 = C$ and $C_2 = 10C$ so

$$\omega_1(k=0) = 0 \quad \text{and} \quad \omega_2(k=0) = \sqrt{22C/M}$$

$$\omega_1(k=\pi/a) = \sqrt{2C/M} \quad \text{and} \quad \omega_2(k=\pi/a) = \sqrt{\frac{20C}{M}}$$

The zero frequency mode at $k=0$ is called the Goldstone mode.