Øvinger I TMT4185, Materialteknologi, 2014, Oppgave 1.

LØSNINGSFORSLAG

Oppgave 1

a)

O: $1s^2 2s^2 2p^4$ O^{2-}
Mg: $1s^2 2s^2 2p^6 3s^2$ Mg^{2+}
Ar: $1s^2 2s^2 2p^6 3s^2 3p^6$ Danner ikke ioner
Sr: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 5s^2$ Sr^{2+}
Br: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^5$ Br^-

b)
O: Kovalent binding
Mg: Metallbinding
Ar: van der Waalsbinding
Sr: Metallbinding
Br: Kovalent binding

c)
1 cm^3 Si = 2.33 g
1 cm^3 innholder 2.33×10^{-5} g O -> 2.33×10^{-5} /16 mol O
1 cm^3 inholder $2.33 \times 10^5 \times 6.02 \times 10^{23}/16$ atomer O **= 8.8×10^{17}atomer/cm^3**

Oppgave 2

a)
i) Bindingsenergien E_0 tilsvarer minimumsenergien som finnes ved å derivere den potensielle energien E_N mhp r og deretter sette den deriverte lik 0. r settes lik r_0 som blir likevektsavstanden som gir laveste energi. r_0 uttrykkes ved A, B og n som så settes inn i uttrykket for E_N som gir E_0

$$\frac{dE_N}{dr} = \frac{d\left(-\frac{A}{r}\right)}{dr} + \frac{d\left(\frac{B}{r^n}\right)}{dr}$$

$$= \frac{A}{r^{(1+1)}} - \frac{nB}{r^{(n+1)}} = 0$$

(b) Now, solving for r ($= r_0$)

$$\frac{A}{r_0^2} = \frac{nB}{r_0^{(n+1)}}$$

or

$$r_0 = \left(\frac{A}{nB}\right)^{1/(1-n)}$$

(c) Substitution for r_0 into Equation 2.11 and solving for E ($= E_0$)

$$E_0 = -\frac{A}{r_0} + \frac{B}{r_0^n}$$

$$= -\frac{A}{\left(\frac{A}{nB}\right)^{1/(1-n)}} + \frac{B}{\left(\frac{A}{nB}\right)^{n/(1-n)}}$$

Oppgave 3

2.18 (a) The main differences between the various forms of primary bonding are:

Ionic--there is electrostatic attraction between oppositely charged ions.

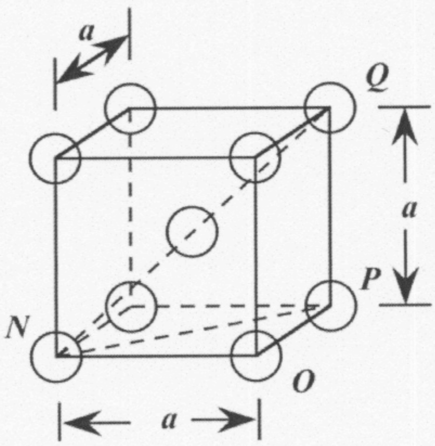
Covalent--there is electron sharing between two adjacent atoms such that each atom assumes a stable electron configuration.

Metallic--the positively charged ion cores are shielded from one another, and also "glued" together by the sea of valence electrons.

(b) The Pauli exclusion principle states that each electron state can hold no more than two electrons, which must have opposite spins.

Oppgave 4

a)



Using the triangle *NOP*

$$(\overline{NP})^2 = a^2 + a^2 = 2a^2$$

And then for triangle *NPQ*,

$$(\overline{NQ})^2 = (\overline{QP})^2 + (\overline{NP})^2$$

But $\overline{NQ} = 4R$, R being the atomic radius. Also, $\overline{QP} = a$. Therefore,

$$(4R)^2 = a^2 + 2a^2$$

or

$$a = \frac{4R}{\sqrt{3}}$$

b)

$$\text{APF} = \frac{V_S}{V_C}$$

Since there are two spheres associated with each unit cell for BCC

$$V_S = 2(\text{sphere volume}) = 2\left(\frac{4\pi R^3}{3}\right) = \frac{8\pi R^3}{3}$$

Also, the unit cell has cubic symmetry, that is $V_C = a^3$. But a depends on R according to Equation 3.3

$$V_C = \left(\frac{4R}{\sqrt{3}}\right)^3 = \frac{64\,R^3}{3\sqrt{3}}$$

Thus,

$$\text{APF} = \frac{V_S}{V_C} = \frac{8\pi\,R^3/3}{64\,R^3/3\sqrt{3}} = 0.68$$

c)

3.9 This problem asks for us to calculate the radius of a tantalum atom. For BCC, $n = 2$ atoms/unit cell, and

$$V_C = \left(\frac{4\,R}{\sqrt{3}}\right)^3 = \frac{64\,R^3}{3\sqrt{3}}$$

Since, from Equation 3.5

$$\rho = \frac{nA_{\text{Ta}}}{V_C N_{\text{A}}}$$

$$= \frac{nA_{\text{Ta}}}{\left(\frac{64\,R^3}{3\sqrt{3}}\right)N_{\text{A}}}$$

and solving for R the previous equation

$$R = \left(\frac{3\sqrt{3}nA_{\text{Ta}}}{64\rho\,N_{\text{A}}}\right)^{1/3}$$

$$= \left[\frac{(3\sqrt{3})\,(2\text{ atoms/unit cell})\,(180.9\text{ g/mol})}{(64)\,(16.6\text{ g/cm}^3)\,(6.023\times 10^{23}\text{ atoms/mol})}\right]^{1/3}$$

$$= 1.43\times 10^{-8}\text{ cm} = 0.143\text{ nm}$$