**Fundamentals of Materials Science Homework 5**

**Name: Xiao，Liyang Date: 02/8/2017 Student #: 15090215**

**Homework Problems:**

1. **(a) Using the ionic radii data in your textbook, calculate the coulombic force of attraction between Na+ and Cl- in NaCl. You may want to check the structure of NaCl to figure out the separation distance between the ions.**

**(b) What is the repulsive force in this case?**

**Solution:**

1. r(Na+)=0.102nm r(Cl-)=0.181nm r=0.102nm+0.181nm=0.283nm



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(b)

1. **(a) A common way to describe the bonding energy curve for secondary bonding is the “6–12” potential, which states that**

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**where *KA*and *KR* are constants for attraction and repulsion, respectively. This relatively simple form is a quantum mechanical result for this relatively simple bond type. Given  and , calculate the bond energy and bond length for argon.**

**(b) Plot *E* as a function of *a* over the range 0.33 to 0.80 nm.**

**Solution:**

**(a)**

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**(b)**

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| --- | --- | --- | --- | --- | --- | --- |
| a/(×10-10m) | 3.3 | 4 | 5 | 6 | 7 | 8 |
| E/J | 1.66×10-21 | -1.57×10-21 | -5.97×10-22 | -2.15×10-22 | -8.70×10-23 | -3.93×10-23 |

1. **The net potential energy between two adjacent ions, *EN*, may be represent by the sum of Equations 2.9 and 2.11, that is,**

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**Calculate the bonding energy *E0* in terms of the parameters *A*, *B*, and *n* using the following procedure:**

1. **Different *EN* with respect to *r*, and then set the resulting expression equal to zero, since the curve of *EN* versus r is a minimum at *E0.***
2. **Solve for *r* in terms *A*, *B*, and *n*, which yields *r0*, the equilibrium interionic spacing.**
3. **Determine the expression for *E0* by substitution of *r0* into Equation 2.17**

**Solution:**

**(1)**

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2. **For the Na+-Cl- ion pair, attractive and repulsive energies *EA* and *ER*, respectively, depend on the distance between the ions *r*, according to**

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**For these expressions, energies are expressed in electron volts per Na+-Cl- pair, and *r* is the distance in nanometers. The net energy *EN* is just the sum of the two expressions above.**

1. **Superimpose on a single plot *EN*, *ER*, and *EA* versus *r* up to 1.0 nm.**
2. **On the basis of this plot, determine (i) the equilibrium spacing r0 between the Na+ and Cl- ions, and (ii) the magnitude of the bonding energy E0 between the two ions.**
3. **Mathematically determine the r0 and E0 values using the solutions to Problem 2.14 and compare these with the graphical results from part (b).**

**Solution:**

**(a)**

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| r/nm | 0.15 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 | 1.0 |
| Ea/ev | -9.57 | -7.18 | -4.79 | -3.59 | -2.87 | -2.39 | -2.05 | -1.80 | -1.60 | -1.436 |
| Er/ev | 28.56 | 2.859 | 0.1116 | 0.01117 | 0.001874 | 0.0004358 | 0.0001270 | 0.00004363 | 0.00001700 | 0.000007320 |
| En/ev | 18.99 | -4.321 | -4.6784 | -3.57883 | -2.868126 | -2.3895642 | -2.049873 | -1.79995637 | -1.599983 | -1.43599268 |

**(b)** From the plots above：

r0=0.25nm ; E0=-5.5eV

**(c)**

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