CHE 350 Electronic Materials: TEST 1

Spring 2008
February 19th, 2008

Total Number of questions = 10
Maximum Points = 100
[Important Formulas on the last page]

1. CCl₄ is liquid at -180 °C because it is bonded by hydrogen bonding. (TRUE / FALSE) Circle one. [3]

2. How many atoms per unit cell are there in the FCC crystal structure?
(a.) 4,  (b.) 9,  (c.) 14,  (d.) 12. Circle one. [4]

3. FCC and HCP have the same atomic packing factor. (TRUE / FALSE). Circle one. [3]

4. An x-ray diffraction experiment is carried out on a metal which is either an FCC or a BCC structure. If you do not know either the wavelength of the X-ray or the lattice constant, but know only θ_A and θ_B, which are the first and second angles at which x-rays reflect from the diffraction planes of a crystal, which equation can be used to determine the lattice structure.

(a.) \( \sqrt{\frac{\sin(\theta_A)}{\sin^2(\theta_B)}} \),  (b.) \( \frac{\sin(\theta_A)}{\sin(\theta_B)} \),  (c.) \( \frac{\sin^2(\theta_A)}{\sqrt{\sin(\theta_B)}} \),  (d.) \( \frac{\theta_A}{\theta_B} \). Circle one. [4]

5. What is a Fluctuating Dipole? How does it explain the boiling point of He? [6]
6. What is the chemical formula of an inter-metallic compound that consists of 24.39% Cu and 75.61% Au. (Atomic Mass: Au=197; Cu=63.55). [15]

7. The material undergoes polymorphism from BCC to FCC. What is the change in its volume assuming that the radius of the atoms remains the same? [Hint: determine the volume per atom for BCC and FCC and then find the percentage change] [20]
8. What is the minimum frequency of a photon needed to ionize a Hydrogen atom? [10]

9. Determine the miller indices for these planes. Calculate the closest distance between two parallel planes for each (a=0.2 nm). [15]

![Diagrams with labeled Miller indices and distances](image-url)
10. Determine the direction indices of the two lines. [10]
11. Draw the Following Miller Indices [10]

a. [120]
b. [023]
Planks equation: $\Delta E = h\nu = \frac{hc}{\lambda}$.

**Volumes:**
For a cube = $a^3$. For a sphere = $\frac{4}{3} \pi r^3$.

**Crystal Structure:**
For FCC $a = 2\sqrt{2}R$; For BCC $a = \frac{4R}{\sqrt{3}}$.

Atomic Packing Factor = $\frac{\text{Volume of atoms in a unit cell}}{\text{Volume of unit cell}}$.

**Hydrogen Atom:**
Energy of an electron at principal quantum number, $n = -\frac{13.6}{n^2}$ eV.

**X-ray diffraction**
Bragg’s Law $2d \sin(\theta) = n\lambda$.
For crystal with cubic symmetry $d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$. 

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<table>
<thead>
<tr>
<th>Constants</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Avogadro’s number</td>
<td>$N_0$</td>
<td>$6.023 \times 10^{23}$ mol$^{-1}$</td>
</tr>
<tr>
<td>Atomic mass unit</td>
<td>$u$</td>
<td>$1.661 \times 10^{-24}$ g</td>
</tr>
<tr>
<td>Electron mass</td>
<td>$m_e$</td>
<td>$9.110 \times 10^{-28}$ g</td>
</tr>
<tr>
<td>Electronic charge (magnitude)</td>
<td>$e$</td>
<td>$1.602 \times 10^{-19}$ C</td>
</tr>
<tr>
<td>Planck’s constant</td>
<td>$h$</td>
<td>$6.626 \times 10^{-34}$ J · s</td>
</tr>
<tr>
<td>Velocity of light</td>
<td>$c$</td>
<td>$2.998 \times 10^8$ m/s</td>
</tr>
<tr>
<td>Gas constant</td>
<td>$R$</td>
<td>$1.987$ cal/(mol · K); $8.314$ J/(mol · K)</td>
</tr>
<tr>
<td>Boltzmann’s constant</td>
<td>$k$</td>
<td>$8.620 \times 10^{-5}$ eV/K</td>
</tr>
<tr>
<td>Permittivity constant</td>
<td>$\varepsilon_0$</td>
<td>$8.854 \times 10^{-12}$ C$^2$/N · m$^2$</td>
</tr>
<tr>
<td>Permeability constant</td>
<td>$\mu_0$</td>
<td>$4\pi \times 10^{-7}$ T · m/A</td>
</tr>
<tr>
<td>Bohr magneton</td>
<td>$\mu_B$</td>
<td>$9.274 \times 10^{-24}$ A · m$^2$</td>
</tr>
<tr>
<td>Faraday</td>
<td>$F$</td>
<td>$9.6485 \times 10^4$ C/mol</td>
</tr>
<tr>
<td>Gravitational acceleration</td>
<td>$g$</td>
<td>$9.806$ m/s</td>
</tr>
<tr>
<td>Density of water</td>
<td></td>
<td>$1$ g/cm$^3$ = $1$ Mg/m$^3$</td>
</tr>
</tbody>
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   (a.) \( \frac{\sqrt{\sin(\theta_A)}}{\sin^2(\theta_B)} \)  (b.) \( \frac{\sin(\theta_A)}{\sin(\theta_B)} \),  (c.) \( \frac{\sin^2(\theta_A)}{\sin(\theta_B)} \),  (d.) \( \frac{\theta_A}{\theta_B} \). Circle one. [4]

5. What is a Fluctuating Dipole? How does it explain the boiling point of He? [6]

Fluctuating dipole is a secondary bond caused by attraction between two molecules or atoms due to formation of dipole moment from instantaneous separation between electrons (negatively charged) from protons (positively charged).

If there were no fluctuating dipole bonds, He would have a boiling point of 0 K. However, due to the attraction between He atoms from fluctuating bonds, there is an increase in its boiling point.
6. What is the chemical formula of an inter-metallic compound that consists of 24.39% Cu and 75.61% Au. (Atomic Mass: Au=197; Cu=63.55). [15]

\[ 100 \text{ gm of material will have} \]
\[ 24.39 \text{ gm of Cu } = 0.3838 \text{ moles of Cu} \]
\[ 75.61 \text{ gm of Au } = 0.3858 \text{ moles of Au} \]

\[ \text{Ratio between moles of Au & Cu } = 1 \]

\[ \text{Chemical formula } = \text{AuCu} \]

7. The material undergoes polymorphism from BCC to FCC. What is the change in its volume assuming that the radius of the atoms remains the same? [Hint: determine the volume per atom for BCC and FCC and then find the percentage change] [20]

For BCC

\[ \sqrt{3} a_{\text{BCC}} = 4R \implies a_{\text{BCC}} = \frac{4R}{\sqrt{3}} \]

\[ \text{# atoms in unit cell } = 2 \]

\[ V_{\text{BCC}} = \frac{\text{Volume of unit cell}}{\text{# atoms}} = \frac{a_{\text{BCC}}^3}{2} = \frac{(\frac{4R}{\sqrt{3}})^3}{2} = 6.158R^3 \]

For FCC

\[ \sqrt{2} a_{\text{FCC}} = 4R \implies a_{\text{FCC}} = 2\sqrt{2}R \]

\[ V_{\text{FCC}} = \frac{a_{\text{FCC}}^3}{4} = \frac{(2\sqrt{2}R)^3}{4} = 5.657R^3 \]

\[ \% \text{ change in volume } = \frac{5.657R^3 - 6.158R^3}{6.158R^3} \times 100 \]

\[ = -8.138 \% \]
8. What is the minimum frequency of a photon needed to ionize a Hydrogen atom? [10]

To ionize hydrogen electron has to be removed from \( n = 2 \) to \( n = \infty \).

The energy required
\[
\left. \left( -\frac{13.6}{n^2} \right) \right|_{n=\infty} - \left. \left( -\frac{13.6}{n^2} \right) \right|_{n=1}
\]
\[= 13.6 \text{ eV} \]

\[\Delta E = h\nu = 6.626 \times 10^{-34} \text{ J} \cdot \text{s}. \nu = 13.6 \times 1.6 \times 10^{-19} \text{ J} \]
\[\Rightarrow \nu = 3.28 \times 10^{15} \text{ s}^{-1} \]

9. Determine the miller indices for these planes. Calculate the closest distance between two parallel planes for each (a=0.2 nm). [15]

(a) \[\nu \quad y \quad z\]
Intercepts \(0\infty\) \(-1\) \(\frac{1}{3}\)
reciprocal \(0\) \(-1\) \(3\)
Miller indices \(\{0\ 1\ 3\}\)

\[d_{hke} = 0.0632 \text{ nm} \]

(b) \[\nu \quad y \quad z\]
Intercepts \(-\frac{3}{2}\) \(-2\) \(1\)
reciprocal \(-2/3\) \(-1/2\) \(1\)
\(-4\) \(-3\) \(6\)

\[d_{hke} = 0.025 \text{ nm} \quad \text{Miller indices} \equiv \{4\ 3\ 6\}\]
10. Determine the direction indices of the two lines. \[ \{ \text{102} \} \]

(a) \[ \begin{array} {ccc}
3 & 0 & 0 \\
0 & 1/2 & 0 \\
-1/2 & 0 & 1 \\
\end{array} \]

(b) \[ \begin{array} {ccc}
1 & 1 & 0 \\
0 & 1/2 & 1/2 \\
1 & 1/2 & -1/2 \\
\end{array} \]

\[ \{ 211 \} \]
11. Draw the Following Miller Indices [10]

a. [120]
b. [023]