Homework Assignment #3
Solutions:

1. X-rays of an unknown wavelength are diffracted by a gold sample. The $2\Theta$ angle was 64.582° for the \{220\} planes. What is the wavelength of the X-rays used? (The lattice constant of gold = 0.40788 nm; assume first-order diffraction, $n = 1$).

   The interplanar distance is,
   \[
   d_{220} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{0.40788 \text{ nm}}{\sqrt{2^2 + 2^2 + 0^2}} = 0.1442 \text{ nm}
   \]

   The lattice constant, $a$, is then,
   \[
   \lambda = 2d_{221} \sin \theta = 2(0.1442 \text{ nm})\sin(32.291°) = 0.154 \text{ nm}
   \]

2. A sample of bcc metal with the lattice parameter $a = 0.33$ nm was placed in a X-ray diffractometer using incoming x-rays with $\lambda = 0.1541$ nm. Using Bragg’s law (assume first order diffraction, $n=1$) predict positions of the diffraction peaks (in $2\Theta$) corresponding to \{110\}, \{210\}, \{230\}, \{321\} and \{431\} planes. Which of these peaks will be observable?

   \[
a = 0.33 \text{ nm}; \lambda = 0.1541 \text{ nm}; \sin \Theta = \frac{\lambda \sqrt{h^2 + k^2 + l^2}}{2a} \quad (h+k+l)=\text{even}
   \]

   \[
   2\Theta_{\{110\}} = 38.56° \quad \text{observable}
   
   2\Theta_{\{210\}} = 61.94° \quad \text{not}
   
   2\Theta_{\{230\}} = 114.68° \quad \text{not}
   
   2\Theta_{\{321\}} = 121.76° \quad \text{observable}
   
   2\Theta_{\{431\}} = 202.0° \quad \text{observable}
   
3. Name and briefly describe three different AFM operation modes: see the lecture notes

   In which mode separation between the probe and the surface is the highest? Non-contact
The distance between atoms in a crystal are in a ~1-2 Å range, so waves with approximately this wavelength are required to explore the crystal structure. Using de Broglie law \( \lambda = \frac{h}{p} \), calculate the energies of (a) neutrons \((m=1.675\times10^{-24} \text{kg})\), (b) electrons \((m=0.911\times10^{-28} \text{kg})\) and (c) X-rays required for the structural studies?

According to the de Broglie law, any free particle with velocity \( V \), momentum \( p \), mass \( m \), and energy \( E \), has a wavelength given by:

\[
\lambda = \frac{\hbar}{p} = \frac{h}{mV} = \frac{h}{\sqrt{2mE}}; \quad E = \frac{\hbar^2}{2m\lambda^2}
\]

The distance between atoms in a crystal are ~ 1Å, so waves with a comparable wavelength are required to explore this structure. If the wavelength is much larger, structural details cannot be resolved; rather some average interaction occurs, as is found for visible light. If the wavelengths are much smaller the beam is diffracted by very small angles, making detection difficult.

For neutrons \( E = \frac{(6.626\times10^{-34})^2}{2\times1.675\times10^{-27}\times10^{-20}} = 1.31\times10^{-23} J = 0.08 eV \);

For electrons \( E = \frac{(6.626\times10^{-34})^2}{2\times0.911\times10^{-31}\times10^{-20}} = 2.41\times10^{-19} J = 150 eV \);

For X-rays \( \frac{\hbar c}{\lambda} = E; \quad E = \frac{6.626\times10^{-34} \times 3\times10^8}{10^{-10}} = 2\times10^{-19} J = 2\times10^4 eV \)

The diffusivity of Mn atoms in the fcc iron lattice is \( 1.5\times10^{-14} \text{m}^2/\text{s} \) at 1300°C and \( 1.50\times10^{-15} \text{m}^2/\text{s} \) at 400°C. Calculate the activation energy in kJ/mol for this case in this temperature range. \((R=8.314 \text{ J/(mol K)})\).

The activation energy may be calculated using the Arrhenius type equation,

\[
\frac{D_{1300°C}}{D_{400°C}} = \frac{\exp(-Q/RT_2)}{\exp(-Q/RT_1)} = \exp \left[ \frac{-Q}{R} \left( \frac{1}{T_2} - \frac{1}{T_1} \right) \right]
\]

where \( T_1 = 400°C = 673 \text{ K} \) and \( T_2 = 1300°C = 1573 \text{ K} \). Substituting,

\[
\frac{1.5\times10^{-14} \text{ m}^2/\text{s}}{1.5\times10^{-15} \text{ m}^2/\text{s}} = \exp \left[ \frac{-Q}{8.314 \text{ J/(mol K)} \left( \frac{1}{1573 \text{ K}} - \frac{1}{673 \text{ K}} \right)} \right]
\]

\[
10 = \exp \left[ (1.0226\times10^{-4})Q \right]
\]

\[
\ln(10) = (1.0226\times10^{-4})Q
\]

\[
Q = 22.518 \text{ J/mol} = 22.5 \text{ kJ/mol}
\]
6. Classify the mechanism of diffusion in first 11 solute/solvent pairs given in the Table below (interstitial or substitutional). Compare the diffusivity values and draw a conclusion.

<table>
<thead>
<tr>
<th>Solvent</th>
<th>Diffusivity (m²/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>500°C (900°F)</td>
</tr>
<tr>
<td>Carbon</td>
<td>5 x 10⁻²¹</td>
</tr>
<tr>
<td>Iron</td>
<td>3 x 10⁻²²</td>
</tr>
<tr>
<td>Nickel</td>
<td>2 x 10⁻²²</td>
</tr>
<tr>
<td>Magnesium</td>
<td>3 x 10⁻²²</td>
</tr>
<tr>
<td>Zinc</td>
<td>4 x 10⁻²²</td>
</tr>
<tr>
<td>Copper</td>
<td>4 x 10⁻²²</td>
</tr>
<tr>
<td>Aluminum</td>
<td>4 x 10⁻²²</td>
</tr>
<tr>
<td>Silver (crystalline)</td>
<td>10⁻¹⁴</td>
</tr>
<tr>
<td>Silver (grain boundary)</td>
<td>10⁻¹⁴</td>
</tr>
<tr>
<td>Carbon</td>
<td>3 x 10⁻²²</td>
</tr>
</tbody>
</table>

1 – interstitial; 2 – interstitial; 3 – substitutional; 4 - substitutional; 5 – substitutional; 6 – substitutional; 7 – substitutional; 8 – substitutional; 9 – substitutional; 10 – substitutional; 11 - substitutional

7. A stress of 2.34 MPa is applied in the [001] direction of a unit cell of the fcc copper single crystal. Calculate the resolved shear stress on the (-111) plane in the following directions: (a) [101], (b) [110], (c) [111] and (d) [0-11]

(a) $2.34 \text{ MPa} \cos 45^\circ \cos 54.7^\circ = 0.956 \text{ MPa}$

(b) $2.34 \text{ MPa} \cos 90^\circ \cos 54.7^\circ = 0 \text{ MPa}$

(c) $2.34 \text{ MPa} \cos 54.7^\circ \cos 54.7^\circ = 0.781 \text{ MPa}$

(d) $2.34 \text{ MPa} \cos 45^\circ \cos 54.7^\circ = 0.956 \text{ MPa}$
8. Calculate the engineering stress on a 0.8 cm diameter rod that is subjected to a force of 1500 kg?

\[
\sigma = \frac{F}{A} = \frac{mg}{\pi \left(\frac{d}{2}\right)^2} = \frac{1500 kg \times 9.81 m/s}{\pi \times 0.004^2 \text{ m}} = 2.93 \times 10^8 Pa = 0.293 GPa
\]

9. What is the difference between the slip and twining mechanisms of plastic deformation of metals? The slip mechanism causes all atoms on one side of the slip plane to move equal distances, such that a series of slip steps are formed. Whereas in twinning, atoms only move distances that are proportional to their respective distances from the twinning plane, and thus produce a well defined region of deformation.

10. By what mechanism do grain boundaries strengthen metals? Grain boundaries strengthen metals by acting as barriers to dislocation movement.