The University of Western Ontario
Department of Physics and Astronomy

P2800 Fall 2008

Homework Assignment #3

Solutions:

1. X-rays pf an unknown wavelength are diffracted by a gold sample. The 2Θ 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,

$$d_{220} = \frac{a}{\sqrt{h^2+k^2+l^2}} = \frac{0.40788 \text{ nm}}{\sqrt{2^2+2^2+0^2}} = \mathbf{0.1442\ nm}$$

The lattice constant, *a*, is then,

$$\lambda = 2d_{221}\sin\theta = 2(0.1442 \text{ nm})\sin(32.291^\circ) = \mathbf{0.154\ nm}$$

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

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

$2\Theta_{\{110\}}=38.56^\circ$ observable

$2\Theta_{\{210\}}=61.94^\circ$ not

$2\Theta_{\{230\}}=114.68^\circ$ not

$2\Theta_{\{321\}}=121.76^\circ$ observable

$2\Theta_{\{431\}}=202.0^\circ$ 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**

4. 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 ($\lambda = h/p$), calculate the energies of (a) neutrons (m=1.675×10-24kg), (b) electrons (m=0.911×10-28kg) 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 :

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

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.

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

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

$$\text{For X-rays} \quad hf = \frac{hc}{\lambda} = E; \quad E = \frac{6.626\times10^{-34}\times3\times10^{8}}{10^{-10}} = 2\times10^{-19}\,J = 2\times10^{4}eV$$

5. The diffusivity of Mn atoms in the *fcc* iron lattice is 1.5×10^{-14} m^2/s at 1300°C and 1.50×10^{-15} m^2/s at 400°C. Calculate the activation energy in kJ/mol for this case in this temperature range. (R=8.314 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 $T_1 = 400°C = 673$ K and $T_2 = 1300°C = 1573$ K. Substituting,

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

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

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

$$Q = 22,518\ \text{J/mol} = \mathbf{22.5\ kJ/mol}$$

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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 5.2 Diffusivities at 500°C and 1000°C for selected solute-solvent diffusion systems

Solute	Solvent (host structure)	Diffusivity (m^2/s) 500°C (930°F)	1000°C (1830°F)
1. Carbon	FCC iron	(5×10^{-15})*	3×10^{-11}
2. Carbon	BCC iron	10^{-12}	(2×10^{-9})
3. Iron	FCC iron	(2×10^{-23})	2×10^{-16}
4. Iron	BCC iron	10^{-20}	(3×10^{-14})
5. Nickel	FCC iron	10^{-23}	2×10^{-16}
6. Manganese	FCC iron	(3×10^{-24})	10^{-16}
7. Zinc	Copper	4×10^{-18}	5×10^{-13}
8. Copper	Aluminum	4×10^{-14}	10^{-10} M†
9. Copper	Copper	10^{-18}	2×10^{-13}
10. Silver	Silver (crystal)	10^{-17}	10^{-12} M
11. Silver	Silver (grain boundary)	10^{-11}	
12. Carbon	HCP titanium	3×10^{-16}	(2×10^{-11})

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) 2.34MPa cos 45° cos 54.7°=

=0.956MPa

(b) 2.34MPa cos 90° cos 54.7°=

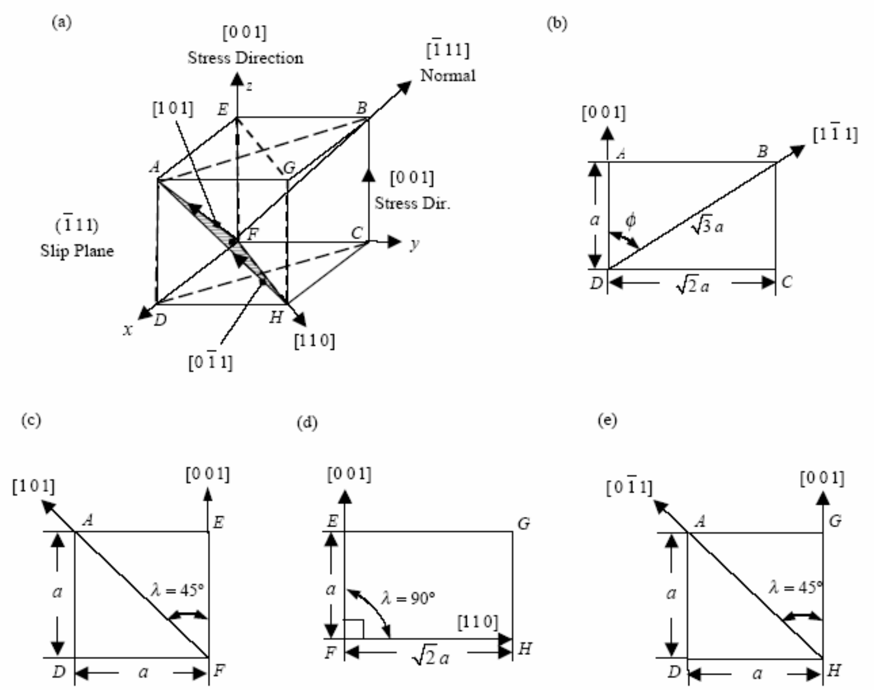
=0 MPa

(c) 2.34MPa cos 54.7° cos 54.7°=

=0.781 MPa

(d) 2.34MPa cos 45° cos 54.7°=

=0. 956 MPa



8. Calculate the engineering stress on a 0.8 cm diameter rod that is subjected to a force of 1500 kg?

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

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.**