

Problem Set # 2 Solutions and grading criteria

CHAPTERS 3 & 4

THE STRUCTURE OF CRYSTALLINE SOLIDS

And

IMPERFECTIONS IN SOLIDS

Assigned: 3.34, 3.35, 3.38 (a thru d), 3.48 (a, b), 4.2, 4.4, 4.7, 4.8, 4.26 (a), 4.28, 4.30

Graded: 3.34, 4.4, 4.8 (total points: 25)

3.34 For plane **A**, we move the origin of the coordinate system one unit cell distance upward along the **z** axis; thus, this is a $(3\bar{2}2)$ plane, as summarized below.

	$\underline{x}$	$\underline{y}$	$\underline{z}$	
Intercepts	$\frac{a}{3}$	$\frac{b}{2}$	$-\frac{c}{2}$	Components correct: 1 Reciprocals taken: 1 Enclosure and indication of negative intercept: 1 Total: 3
Intercepts in terms of a , b , and c	$\frac{1}{3}$	$\frac{1}{2}$	$-\frac{1}{2}$	
Reciprocals of intercepts	3	2	-2	
Enclosure		$(3\bar{2}2)$		

For plane **B** we move the origin of the coordinate system one unit cell distance along the **x** axis; thus, this is a $(\bar{1}01)$ plane, as summarized below.

	$\underline{x}$	$\underline{y}$	$\underline{z}$	
Intercepts	$-\frac{a}{2}$	∞b	$\frac{c}{2}$	Components correct: 1 Reciprocals taken: 1 Enclosure and indication of negative intercept: 1 Total: 3
Intercepts in terms of a , b , and c	$-\frac{1}{2}$	∞	$\frac{1}{2}$	
Reciprocals of intercepts	-2	0	2	
Reduction	-1	0	1	
Enclosure		$(\bar{1}01)$		

Maximum possible for
this problem: 6 points

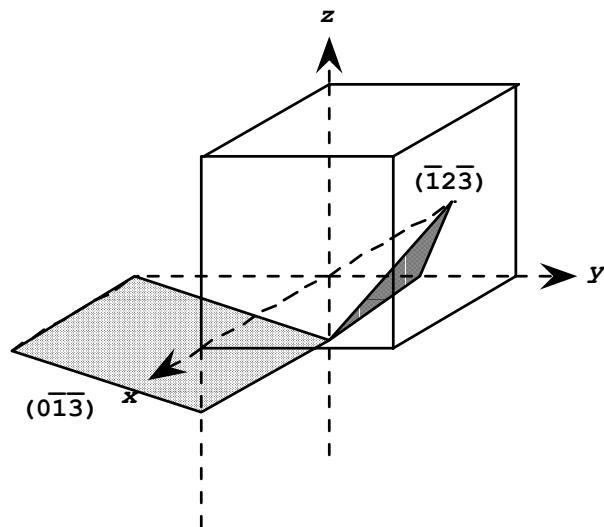
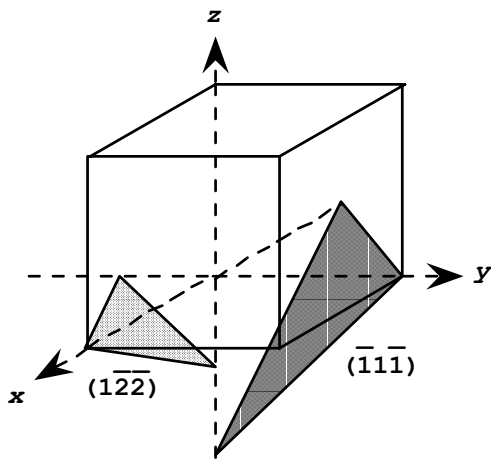
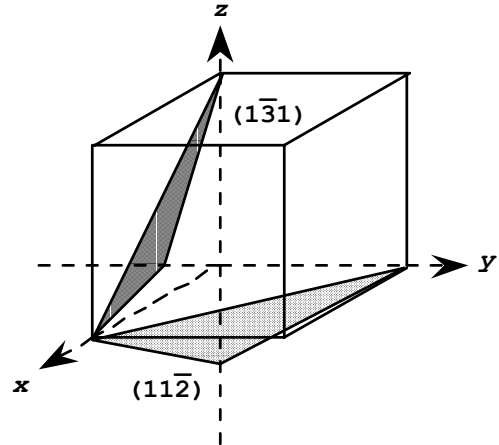
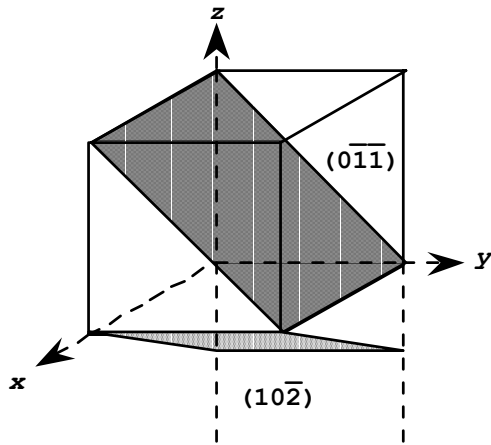
3.35 For plane **A**, since the plane passes through the origin of the coordinate system as shown, we move the origin of the coordinate system one unit cell distance to the right along the **y** axis; thus, this is a $(\bar{3}24)$ plane, as summarized below.

	<u>x</u>	<u>y</u>	<u>z</u>
Intercepts	$\frac{2a}{3}$	-b	$\frac{c}{2}$
Intercepts in terms of a , b , and c	$\frac{2}{3}$	-1	$\frac{1}{2}$
Reciprocals of intercepts	$\frac{3}{2}$	-1	2
Reduction	3	-2	4
Enclosure		$(\bar{3}24)$	

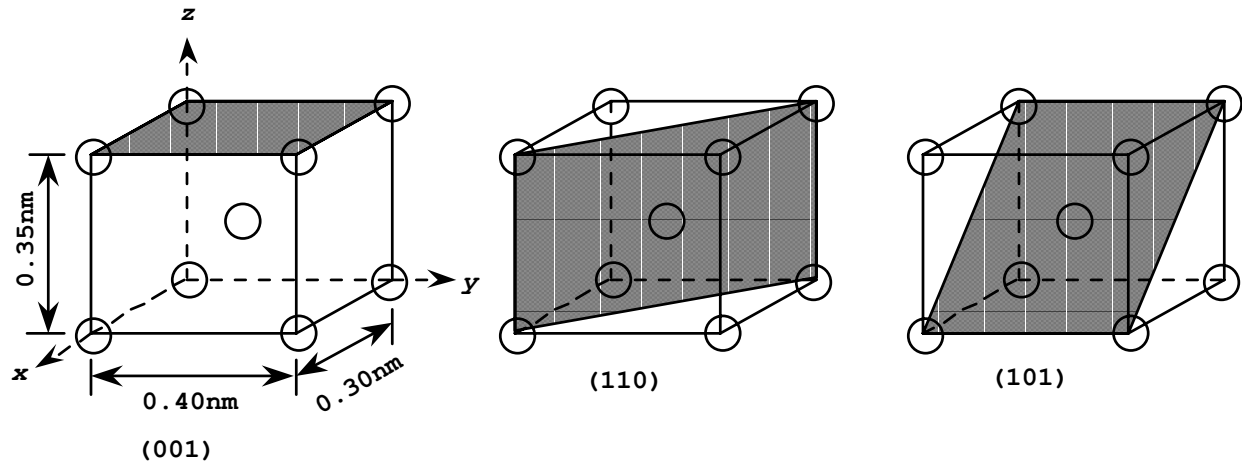
For plane **B** we leave the origin at the unit cell as shown; this is a (221) plane, as summarized below.

	<u>x</u>	<u>y</u>	<u>z</u>
Intercepts	$\frac{a}{2}$	$\frac{b}{2}$	c
Intercepts in terms of a , b , and c	$\frac{1}{2}$	$\frac{1}{2}$	1
Reciprocals of intercepts	2	2	1
Enclosure		(221)	

3.38 The planes are shown in the cubic unit cells below.



3.48 A unit cell is constructed below from the three crystallographic planes that were provided in the problem.



(a) This unit cell belongs to the **orthorhombic** crystal system since $a = 0.30 \text{ nm}$, $b = 0.40 \text{ nm}$, $c = 0.35 \text{ nm}$, and $\alpha = \beta = \gamma = 90^\circ$.

(b) This crystal structure would be called **body-centered orthorhombic** since the unit cell has orthorhombic symmetry, and an atom is located at each of the corners, as well as at the center.

4.2 Determination of the number of vacancies per cubic meter in iron at 850°C (1123 K) requires the utilization of Equations (4.1) and (4.2) as follows:

$$\begin{aligned}
 N_V &= N \exp\left(-\frac{Q_V}{kT}\right) = \frac{N_{A\rho_{\text{Fe}}}}{A_{\text{Fe}}} \exp\left(-\frac{Q_V}{kT}\right) \\
 &= \frac{(6.023 \times 10^{23} \text{ atoms/mol})(7.65 \text{ g/cm}^3)}{55.85 \text{ g/mol}} \exp\left[-\frac{1.08 \text{ eV/atom}}{(8.62 \times 10^{-5} \text{ eV/atom-K})(1123 \text{ K})}\right] \\
 &= 1.18 \times 10^{18} \text{ cm}^{-3} = 1.18 \times 10^{24} \text{ m}^{-3}
 \end{aligned}$$

4.4 In this problem we are asked to cite which of the elements listed form with Cu the three possible solid solution types. For complete substitutional solubility the following criteria must be met: 1) the difference in atomic radii between Cu and the other element ($\Delta R\%$) must be less than $\pm 15\%$, 2) the crystal structures must be the same, 3) the electronegativities must be similar, and 4) the valences

should be the same, or nearly the same. Below are tabulated, for the various elements, these criteria.

<u>Element</u>	<u>$\Delta R\%$</u>	<u>Crystal Structure</u>	<u>ΔElectro-negativity</u>	<u>Valence</u>
Cu		FCC		2+
C	-44			
H	-64			
O	-53			
Ag	+13	FCC	0	1+
Al	+12	FCC	-0.4	3+
Co	-2	HCP	-0.1	2+
Cr	-2	BCC	-0.3	3+
Fe	-3	BCC	-0.1	2+
Ni	-3	FCC	-0.1	2+
Pd	+8	FCC	+0.3	2+
Pt	+9	FCC	+0.3	2+
Zn	+4	HCP	-0.3	2+

- (a) **Ni, Pd, and Pt** meet all of the criteria and thus form substitutional solid solutions having complete solubility.
- (b) Ag, Al, Co, Cr, Fe, and Zn form substitutional solid solutions of limited solubility. All these metals have either BCC or HCP crystal structures (different than copper's FCC), and/or the difference between their atomic radii and that for Cu are greater than $\pm 15\%$, and/or have a valence different than 2+.
- (c) C, H, and O form interstitial solid solutions. These elements have atomic radii that are significantly smaller than the atomic radius of Cu.

Correct calculation of difference in atomic radius with respect to copper: 3 points

Correct calculation of difference in electronegativity with respect to copper: 3 points

(remember: it is the **difference** between these quantities that determines the solubility, not their absolute value.)

Correct identification of Ni, Pd, and Pt as completely soluble solutes: 2 point

Correct identification of Ag, Al, Co, Cr, Fe, and Zn as limited solubility solutes: 2 points

Correct identification of C, H, and O as interstitial solutes: 2 points

Maximum point total for this problem: **12 points**

4.7 In order to compute composition, in atom percent, of a 30 wt% Zn-70 wt% Cu alloy, we employ Equation (4.6) as

$$C_{Zn}' = \frac{C_{Zn}A_{Cu}}{C_{Zn}A_{Cu} + C_{Cu}A_{Zn}} \times 100$$

$$= \frac{(30)(63.55 \text{ g/mol})}{(30)(63.55 \text{ g/mol}) + (70)(65.39 \text{ g/mol})} \times 100$$

$$= 29.4 \text{ at\%}$$

$$C_{Cu}' = \frac{C_{Cu}A_{Zn}}{C_{Zn}A_{Cu} + C_{Cu}A_{Zn}} \times 100$$

$$= \frac{(70)(65.39 \text{ g/mol})}{(30)(63.55 \text{ g/mol}) + (70)(65.39 \text{ g/mol})} \times 100$$

$$= 70.6 \text{ at\%}$$

4.8 In order to compute composition, in weight percent, of a 6 at% Pb-94 at% Sn alloy, we employ Equation (4.7) as

$$C_{Pb} = \frac{C_{Pb}'A_{Pb}}{C_{Pb}'A_{Pb} + C_{Sn}'A_{Sn}} \times 100$$

$$= \frac{(6)(207.2 \text{ g/mol})}{(6)(207.2 \text{ g/mol}) + (94)(118.69 \text{ g/mol})} \times 100$$

$$10.0 \text{ wt\%}$$

$$C_{Sn} = \frac{C_{Sn}'A_{Sn}}{C_{Pb}'A_{Pb} + C_{Sn}'A_{Sn}} \times 100$$

$$= \frac{(94)(118.69 \text{ g/mol})}{(6)(207.2 \text{ g/mol}) + (94)(118.69 \text{ g/mol})} \times 100$$

$$90.0 \text{ wt\%}$$

Correct formula: 3 points

Correct substitution of known values: 2 points

Correct answer: 1 point.

(Composition of the other component can either be determined by using equation 4.7, or simply recognizing that the weight % of Pb + weight % of Sn must equal 100%. Therefore, the composition of Sn would equal (100-10.0) or 90 wt. %.)

Correct answer for the other component: 1 point

Maximum point total: 7

4.26 (a) The surface energy of a single crystal depends on crystallographic orientation because the atomic packing is different for the various crystallographic planes, and, therefore, the number of unsatisfied bonds will vary from plane to plane.

4.28 (a) A twin boundary is an interface such that atoms on one side are located at mirror image positions of those atoms situated on the other boundary side. The region on one side of this boundary is called a twin.

(b) Mechanical twins are produced as a result of mechanical deformation and generally occur in BCC and HCP metals. Annealing twins form during annealing heat treatments, most often in FCC metals.

4.30 This problem calls for a determination of the average grain size of the specimen which microstructure is shown in Figure 4.12b. Seven line segments were drawn across the micrograph, each of which was 60 mm long. The average number of grain boundary intersections for these lines was 8.7. Therefore, the average line length intersected is just

$$\frac{60 \text{ mm}}{8.7} = 6.9 \text{ mm}$$

Hence, the average grain diameter, **d**, is

$$d = \frac{\text{ave. line length intersected}}{\text{magnification}} = \frac{6.9 \text{ mm}}{100} = 6.9 \times 10^{-2} \text{ mm}$$