2.2 *Chromium has four naturally-occurring isotopes: 4.34% of* ^{50}*Cr, with an atomic weight of 49.9460 amu, 83.79% of* ^{52}*Cr, with an atomic weight of 51.9405 amu, 9.50% of* ^{53}*Cr, with an atomic weight of 52.9407 amu, and 2.37% of* ^{54}*Cr, with an atomic weight of 53.9389 amu. On the basis of these data, confirm that the average atomic weight of Cr is 51.9963 amu.*

Solution

The average atomic weight of silicon $(\overline{A}_{\mathrm{Cr}})$ is computed by adding fraction-of-occurrence/atomic weight products for the three isotopes. Thus

$$\overline{A}_{\mathrm{Cr}} = f_{^{50}\mathrm{Cr}} A_{^{50}\mathrm{Cr}} + f_{^{52}\mathrm{Cr}} A_{^{52}\mathrm{Cr}} \quad f_{^{53}\mathrm{Cr}} A_{^{53}\mathrm{Cr}} \quad f_{^{54}\mathrm{Cr}} A_{^{54}\mathrm{Cr}}$$

$$(0.0434)(49.9460 \text{ amu}) + (0.8379)(51.9405 \text{ amu}) + (0.0950)(52.9407 \text{ amu}) + (0.0237)(53.9389 \text{ amu}) = 51.9963 \text{ amu}$$

2.3 *(a) How many grams are there in one amu of a material?*

(b) Mole, in the context of this book, is taken in units of gram-mole. On this basis, how many atoms are there in a pound-mole of a substance?

Solution

(a) In order to determine the number of grams in one amu of material, appropriate manipulation of the amu/atom, g/mol, and atom/mol relationships is all that is necessary, as

$$\#\ \text{g/amu} = \left(\frac{1\ \text{mol}}{6.022 \times 10^{23}\ \text{atoms}}\right)\left(\frac{1\ \text{g/mol}}{1\ \text{amu/atom}}\right)$$

$$= 1.66 \times 10^{-24}\ \text{g/amu}$$

(b) Since there are 453.6 g/lb_m,

$$1\ \text{lb-mol} = (453.6\ \text{g/lb}_\text{m})(6.022 \times 10^{23}\ \text{atoms/g-mol})$$

$$= 2.73 \times 10^{26}\ \text{atoms/lb-mol}$$

2.4 *(a) Cite two important quantum-mechanical concepts associated with the Bohr model of the atom.*

(b) Cite two important additional refinements that resulted from the wave-mechanical atomic model.

Solution

(a) Two important quantum-mechanical concepts associated with the Bohr model of the atom are (1) that electrons are particles moving in discrete orbitals, and (2) electron energy is quantized into shells.

(b) Two important refinements resulting from the wave-mechanical atomic model are (1) that electron position is described in terms of a probability distribution, and (2) electron energy is quantized into both shells and subshells--each electron is characterized by four quantum numbers.

2.5 *Relative to electrons and electron states, what does each of the four quantum numbers specify?*

Solution

The n quantum number designates the electron shell.

The l quantum number designates the electron subshell.

The m_l quantum number designates the number of electron states in each electron subshell.

The m_s quantum number designates the spin moment on each electron.

2.6 *Allowed values for the quantum numbers of electrons are as follows:*

$$n = 1, 2, 3, \ldots$$

$$l = 0, 1, 2, 3, \ldots, n - 1$$

$$m_l = 0, \pm 1, \pm 2, \pm 3, \ldots, \pm l$$

$$m_s = \mathrm{r}\frac{1}{2}$$

The relationships between n and the shell designations are noted in Table 2.1. Relative to the subshells,

l = 0 corresponds to an s subshell

l = 1 corresponds to a p subshell

l = 2 corresponds to a d subshell

l = 3 corresponds to an f subshell

For the K shell, the four quantum numbers for each of the two electrons in the 1s state, in the order of nlm_lm_s, *are* $100(\frac{1}{2})$ *and* $100(\ \frac{1}{2})$. *Write the four quantum numbers for all of the electrons in the L and M shells, and note which correspond to the s, p, and d subshells.*

Solution

For the *L* state, *n* = 2, and eight electron states are possible. Possible *l* values are 0 and 1, while possible m_l values are 0 and ±1; and possible m_s values are $\mathrm{r}\frac{1}{2}$. Therefore, for the *s* states, the quantum numbers are $200(\frac{1}{2})$ and $200(\ \frac{1}{2})$. For the *p* states, the quantum numbers are $210(\frac{1}{2})$, $210(\ \frac{1}{2})$, $211(\frac{1}{2})$, $211(\ \frac{1}{2})$, $21(\ 1)(\frac{1}{2})$, and $21(\ 1)(\ \frac{1}{2})$.

For the *M* state, *n* = 3, and 18 states are possible. Possible *l* values are 0, 1, and 2; possible m_l values are 0, ±1, and ±2; and possible m_s values are $\mathrm{r}\frac{1}{2}$. Therefore, for the *s* states, the quantum numbers are $300(\frac{1}{2})$, $300(\ \frac{1}{2})$, for the *p* states they are $310(\frac{1}{2})$, $310(\ \frac{1}{2})$, $311(\frac{1}{2})$, $311(\ \frac{1}{2})$, $31(\ 1)(\frac{1}{2})$, and $31(\ 1)(\ \frac{1}{2})$; for the *d* states they are $320(\frac{1}{2})$, $320(\ \frac{1}{2})$, $321(\frac{1}{2})$, $321(\ \frac{1}{2})$, $32(\ 1)(\frac{1}{2})$, $32(\ 1)(\ \frac{1}{2})$, $322(\frac{1}{2})$, $322(\ \frac{1}{2})$, $32(\ 2)(\frac{1}{2})$, and $32(\ 2)(\ \frac{1}{2})$.

2.7 *Give the electron configurations for the following ions:* Fe^{2+}, Al^{3+}, Cu^{+}, Ba^{2+}, Br^{-}, *and* O^{2-}.

Solution

The electron configurations for the ions are determined using Table 2.2 (and Figure 2.6).

Fe^{2+}: From Table 2.2, the electron configuration for an atom of iron is $1s^22s^22p^63s^23p^63d^64s^2$. In order to become an ion with a plus two charge, it must lose two electrons—in this case the two 4*s*. Thus, the electron configuration for an Fe^{2+} ion is $1s^22s^22p^63s^23p^63d^6$.

Al^{3+}: From Table 2.2, the electron configuration for an atom of aluminum is $1s^22s^22p^63s^23p^1$. In order to become an ion with a plus three charge, it must lose three electrons—in this case two 3*s* and the one 3*p*. Thus, the electron configuration for an Al^{3+} ion is $1s^22s^22p^6$.

Cu^{+}: From Table 2.2, the electron configuration for an atom of copper is $1s^22s^22p^63s^23p^63d^{10}4s^1$. In order to become an ion with a plus one charge, it must lose one electron—in this case the 4*s*. Thus, the electron configuration for a Cu^{+} ion is $1s^22s^22p^63s^23p^63d^{10}$.

Ba^{2+}: The atomic number for barium is 56 (Figure 2.6), and inasmuch as it is not a transition element the electron configuration for one of its atoms is $1s^22s^22p^63s^23p^63d^{10}4s^24p^64d^{10}5s^25p^66s^2$. In order to become an ion with a plus two charge, it must lose two electrons—in this case two the 6*s*. Thus, the electron configuration for a Ba^{2+} ion is $1s^22s^22p^63s^23p^63d^{10}4s^24p^64d^{10}5s^25p^6$.

Br^{-}: From Table 2.2, the electron configuration for an atom of bromine is $1s^22s^22p^63s^23p^63d^{10}4s^24p^5$. In order to become an ion with a minus one charge, it must acquire one electron—in this case another 4*p*. Thus, the electron configuration for a Br^{-} ion is $1s^22s^22p^63s^23p^63d^{10}4s^24p^6$.

O^{2-}: From Table 2.2, the electron configuration for an atom of oxygen is $1s^22s^22p^4$. In order to become an ion with a minus two charge, it must acquire two electrons—in this case another two 2*p*. Thus, the electron configuration for an O^{2-} ion is $1s^22s^22p^6$.

2.8 *Sodium chloride (NaCl) exhibits predominantly ionic bonding. The* Na^+ *and* Cl^- *ions have electron structures that are identical to which two inert gases?*

Solution

The Na^+ ion is just a sodium atom that has lost one electron; therefore, it has an electron configuration the same as neon (Figure 2.6).

The Cl^- ion is a chlorine atom that has acquired one extra electron; therefore, it has an electron configuration the same as argon.

The Periodic Table

2.9 *With regard to electron configuration, what do all the elements in Group VIIA of the periodic table have in common?*

Solution

Each of the elements in Group VIIA has five *p* electrons.

2.10 *To what group in the periodic table would an element with atomic number 114 belong?*

<u>Solution</u>

From the periodic table (Figure 2.6) the element having atomic number 114 would belong to group IVA. According to Figure 2.6, Ds, having an atomic number of 110 lies below Pt in the periodic table and in the right-most column of group VIII. Moving four columns to the right puts element 114 under Pb and in group IVA.

2.11 *Without consulting Figure 2.6 or Table 2.2, determine whether each of the electron configurations given below is an inert gas, a halogen, an alkali metal, an alkaline earth metal, or a transition metal. Justify your choices.*

(*a*) $1s^2 2s^2 2p^6 3s^2 3p^6 3d^7 4s^2$

(*b*) $1s^2 2s^2 2p^6 3s^2 3p^6$

(*c*) $1s^2 2s^2 2p^5$

(*d*) $1s^2 2s^2 2p^6 3s^2$

(*e*) $1s^2 2s^2 2p^6 3s^2 3p^6 3d^2 4s^2$

(*f*) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$

Solution

(a) The $1s^2 2s^2 2p^6 3s^2 3p^6 3d^7 4s^2$ electron configuration is that of a transition metal because of an incomplete *d* subshell.

(b) The $1s^2 2s^2 2p^6 3s^2 3p^6$ electron configuration is that of an inert gas because of filled 3*s* and 3*p* subshells.

(c) The $1s^2 2s^2 2p^5$ electron configuration is that of a halogen because it is one electron deficient from having a filled *L* shell.

(d) The $1s^2 2s^2 2p^6 3s^2$ electron configuration is that of an alkaline earth metal because of two *s* electrons.

(e) The $1s^2 2s^2 2p^6 3s^2 3p^6 3d^2 4s^2$ electron configuration is that of a transition metal because of an incomplete *d* subshell.

(f) The $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$ electron configuration is that of an alkali metal because of a single *s* electron.

2.12 *(a) What electron subshell is being filled for the rare earth series of elements on the periodic table?*

(b) What electron subshell is being filled for the actinide series?

Solution

(a) The 4*f* subshell is being filled for the rare earth series of elements.

(b) The 5*f* subshell is being filled for the actinide series of elements.

Bonding Forces and Energies

2.13 *Calculate the force of attraction between a K^+ and an O^{2-} ion the centers of which are separated by a distance of 1.5 nm.*

Solution

The attractive force between two ions F_A is just the derivative with respect to the interatomic separation of the attractive energy expression, Equation 2.8, which is just

$$F_A = \frac{dE_A}{dr} = \frac{d\left(\frac{A}{r}\right)}{dr} = \frac{A}{r^2}$$

The constant A in this expression is defined in footnote 3. Since the valences of the K^+ and O^{2-} ions (Z_1 and Z_2) are +1 and -2, respectively, $Z_1 = 1$ and $Z_2 = 2$, then

$$F_A = \frac{(Z_1 e)(Z_2 e)}{4\pi\varepsilon_0 r^2}$$

$$= \frac{(1)(2)(1.602 \times 10^{-19}\ \text{C})^2}{(4)(\pi)(8.85 \times 10^{-12}\ \text{F/m})(1.5 \times 10^{-9}\ \text{m})^2}$$

$$= 2.05 \times 10^{-10}\ \text{N}$$

2.14 *The net potential energy between two adjacent ions, E_N, may be represented by the sum of Equations 2.8 and 2.9; that is,*

$$E_N = \frac{A}{r} \qquad \frac{B}{r^n}$$

Calculate the bonding energy E_0 in terms of the parameters A, B, and n using the following procedure:

1. Differentiate E_N with respect to r, and then set the resulting expression equal to zero, since the curve of E_N versus r is a minimum at E_0.

2. Solve for r in terms of A, B, and n, which yields r_0, the equilibrium interionic spacing.

3. Determine the expression for E_0 by substitution of r_0 into Equation 2.11.

<u>Solution</u>

(a) Differentiation of Equation 2.11 yields

$$\frac{dE_N}{dr} = \frac{d\left(\frac{A}{r}\right)}{dr} \qquad \frac{d\left(\frac{B}{r^n}\right)}{dr}$$

$$= \frac{A}{r^{(1\,+\,1)}} \qquad \frac{nB}{r^{(n\,+\,1)}} = 0$$

(b) Now, solving for r (= r_0)

$$\frac{A}{r_0^2} = \frac{nB}{r_0^{(n\,+\,1)}}$$

or

$$r_0 = \left(\frac{A}{nB}\right)^{1/(1\,-\,n)}$$

(c) Substitution for r_0 into Equation 2.11 and solving for E (= E_0)

$$E_0 = \frac{A}{r_0} + \frac{B}{r_0^n}$$

$$= \frac{A}{\left(\frac{A}{nB}\right)^{1/(1\,-\,n)}} + \frac{B}{\left(\frac{A}{nB}\right)^{n/(1\,-\,n)}}$$

2.15 *For a K^+–Cl^- ion pair, attractive and repulsive energies E_A and E_R, respectively, depend on the distance between the ions r, according to*

$$E_A \quad \frac{1.436}{r}$$

$$E_R \quad \frac{5.8 \ \text{u} \ 10^{\ 6}}{r^9}$$

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

(a) Superimpose on a single plot E_N, E_R, and E_A versus r up to 1.0 nm.

(b) On the basis of this plot, determine (i) the equilibrium spacing r_0 between the K^+ and Cl^- ions, and (ii) the magnitude of the bonding energy E_0 between the two ions.

(c) Mathematically determine the r_0 and E_0 values using the solutions to Problem 2.14 and compare these with the graphical results from part (b).

Solution

(a) Curves of E_A, E_R, and E_N are shown on the plot below.

(b) From this plot

r_0 = 0.28 nm

E_0 = – 4.6 eV

(c) From Equation 2.11 for E_N

$$A = 1.436$$

$$B = 5.86 \times 10^{-6}$$

$$n = 9$$

Thus,

$$r_0 = \left(\frac{A}{nB}\right)^{1/(1-n)}$$

$$\left[\frac{1.436}{(8)(5.86 \times 10^{-6})}\right]^{1/(1-9)} \qquad 0.279 \text{ nm}$$

and

$$E_0 = -\frac{A}{\left(\frac{A}{nB}\right)^{1/(1-n)}} + \frac{B}{\left(\frac{A}{nB}\right)^{n/(1-n)}}$$

$$= -\frac{1.436}{\left[\frac{1.436}{(9)(5.86 \times 10^{-6})}\right]^{1/(1-9)}} + \frac{5.86 \times 10^{-6}}{\left[\frac{1.436}{(9)(5.86 \times 10^{-6})}\right]^{9/(1-9)}}$$

$$= -4.57 \text{ eV}$$

2.16 *Consider a hypothetical* X^+*-*Y^- *ion pair for which the equilibrium interionic spacing and bonding energy values are 0.35 nm and -6.13 eV, respectively. If it is known that n in Equation 2.11 has a value of 10, using the results of Problem 2.14, determine explicit expressions for attractive and repulsive energies* E_A *and* E_R *of Equations 2.8 and 2.9.*

<u>Solution</u>

This problem gives us, for a hypothetical X^+-Y^- ion pair, values for r_0 (0.35 nm), E_0 (– 6.13 eV), and n (10), and asks that we determine explicit expressions for attractive and repulsive energies of Equations 2.8 and 2.9. In essence, it is necessary to compute the values of A and B in these equations. Expressions for r_0 and E_0 in terms of n, A, and B were determined in Problem 2.14, which are as follows:

$$r_0 = \left(\frac{A}{nB}\right)^{1/(1 - n)}$$

$$E_0 = \frac{A}{\left(\frac{A}{nB}\right)^{1/(1 - n)}} + \frac{B}{\left(\frac{A}{nB}\right)^{n/(1 - n)}}$$

Thus, we have two simultaneous equations with two unknowns (viz. A and B). Upon substitution of values for r_0 and E_0 in terms of n, these equations take the forms

$$0.35 \text{ nm} = \left(\frac{A}{10B}\right)^{1/(1 - 10)} = \left(\frac{A}{10B}\right)^{-1/9}$$

and

$$6.13 \text{ eV} = \frac{A}{\left(\frac{A}{10B}\right)^{1/(1 - 10)}} + \frac{B}{\left(\frac{A}{10B}\right)^{10/(1 - 10)}}$$

$$= \frac{A}{\left(\frac{A}{10B}\right)^{-1/9}} + \frac{B}{\left(\frac{A}{10B}\right)^{-10/9}}$$

We now want to solve these two equations simultaneously for values of A and B. From the first of these two equations, solving for $A/8B$ leads to

$$\frac{A}{10B} = (0.35 \text{ nm})^{-9}$$

Furthermore, from the above equation the *A* is equal to

$$A = 10B(0.35 \text{ nm})^{-9}$$

When the above two expressions for $A/10B$ and A are substituted into the above expression for E_0 (- 6.13 eV), the following results

$$6.13 \text{ eV} = = \frac{A}{\left(\frac{A}{10B}\right)^{1/9}} + \frac{B}{\left(\frac{A}{10B}\right)^{10/9}}$$

$$= \frac{10B(0.35 \text{ nm})^{-9}}{\left[(0.35 \text{ nm})^{-9}\right]^{1/9}} + \frac{B}{\left[(0.35 \text{ nm})^{-9}\right]^{10/9}}$$

$$= \frac{10B(0.35 \text{ nm})^{-9}}{0.35 \text{ nm}} + \frac{B}{(0.35 \text{ nm})^{10}}$$

Or

$$6.13 \text{ eV} = = \frac{10B}{(0.35 \text{ nm})^{10}} + \frac{B}{(0.35 \text{ nm})^{10}} = \frac{9B}{(0.35 \text{ nm})^{10}}$$

Solving for *B* from this equation yields

$$B = 1.88 \times 10^{-5} \text{ eV-nm}^{10}$$

Furthermore, the value of *A* is determined from one of the previous equations, as follows:

$$A = 10B(0.35 \text{ nm})^{-9} = (10)\left(1.88 \times 10^{-5} \text{ eV-nm}^{10}\right)(0.35 \text{ nm})^{-9}$$

$$2.39 \text{ eV-nm}$$

Thus, Equations 2.8 and 2.9 become

$$E_A = \frac{2.39}{r}$$

$$E_R = \frac{1.88 \times 10^{-5}}{r^{10}}$$

Of course these expressions are valid for *r* and *E* in units of nanometers and electron volts, respectively.

2.17 *The net potential energy E_N between two adjacent ions is sometimes represented by the expression*

$$E_N = -\frac{C}{r} + D\exp\left(-\frac{r}{\rho}\right) \tag{2.12}$$

in which r is the interionic separation and C, D, and ρ are constants whose values de

(a) Derive an expression for the bonding energy E_0 in terms of the equilibrium interionic separation r_0 and the constants D and ρ using the following procedure:

1. Differentiate E_N with respect to r and set the resulting expression equal to zero.

2. Solve for C in terms of D, ρ, and r_0.

3. Determine the expression for E_0 by substitution for C in Equation 2.12.

(b) Derive another expression for E_0 in terms of r_0, C, and ρ using a procedure analogous to the one outlined in part (a).

Solution

(a) Differentiating Equation 2.12 with respect to *r* yields

$$\frac{dE}{dr} = \frac{d\left(-\frac{C}{r}\right)}{dr} - \frac{d\left[D\exp\left(-\frac{r}{\rho}\right)\right]}{dr}$$

$$= \frac{C}{r^2} - \frac{De^{-r/\rho}}{\rho}$$

At $r = r_0$, $dE/dr = 0$, and

$$\frac{C}{r_0^2} = \frac{De^{-(r_0/\rho)}}{\rho} \tag{2.12b}$$

Solving for *C* and substitution into Equation 2.12 yields an expression for E_0 as

$$E_0 = De^{-(r_0/\rho)}\left(1 - \frac{r_0}{\rho}\right)$$

(b) Now solving for *D* from Equation 2.12b above yields

$$D = \frac{C\rho e^{(r_0/\rho)}}{r_0^2}$$

Substitution of this expression for D into Equation 2.12 yields an expression for E_0 as

$$E_0 = \frac{C}{r_0}\left(\frac{\rho}{r_0} \quad 1\right)$$

Primary Interatomic Bonds

2.18 *(a) Briefly cite the main differences between ionic, covalent, and metallic bonding.*

(b) State the Pauli exclusion principle.

Solution

(a) The main differences between the various forms of primary bonding are:

Ionic--there is electrostatic attraction between oppositely charged ions.

Covalent--there is electron sharing between two adjacent atoms such that each atom assumes a stable electron configuration.

Metallic--the positively charged ion cores are shielded from one another, and also "glued" together by the sea of valence electrons.

(b) The Pauli exclusion principle states that each electron state can hold no more than two electrons, which must have opposite spins.

2.19 *Compute the percents ionic character of the interatomic bonds for the following compounds:* TiO_2, *ZnTe, CsCl, InSb, and* $MgCl_2$.

Solution

The percent ionic character is a function of the electron negativities of the ions X_A and X_B according to Equation 2.10. The electronegativities of the elements are found in Figure 2.7.

For TiO_2, X_{Ti} = 1.5 and X_O = 3.5, and therefore,

$$\%IC = \left\{1 - e^{(-0.25)(3.5 - 1.5)^2}\right\} \times 100 = 63.2\%$$

For ZnTe, X_{Zn} = 1.6 and X_{Te} = 2.1, and therefore,

$$\%IC = \left\{1 - e^{(-0.25)(2.1 - 1.6)^2}\right\} \times 100 = 6.1\%$$

For CsCl, X_{Cs} = 0.7 and X_{Cl} = 3.0, and therefore,

$$\%IC = \left\{1 - e^{(-0.25)(3.0 - 0.7)^2}\right\} \times 100 = 73.4\%$$

For InSb, X_{In} = 1.7 and X_{Sb} = 1.9, and therefore,

$$\%IC = \left\{1 - e^{(-0.25)(1.9 - 1.7)^2}\right\} \times 100 = 1.0\%$$

For $MgCl_2$, X_{Mg} = 1.2 and X_{Cl} = 3.0, and therefore,

$$\%IC = \left\{1 - e^{(-0.25)(3.0 - 1.2)^2}\right\} \times 100 = 55.5\%$$

2.20 *Make a plot of bonding energy versus melting temperature for the metals listed in Table 2.3. Using this plot, approximate the bonding energy for copper, which has a melting temperature of 1084°C.*

Solution

Below is plotted the bonding energy versus melting temperature for these four metals. From this plot, the bonding energy for copper (melting temperature of 1084°C) should be approximately 3.6 eV. The experimental value is 3.5 eV.

2.21 *Using Table 2.2, determine the number of covalent bonds that are possible for atoms of the following elements: germanium, phosphorus, selenium, and chlorine.*

Solution

For germanium, having the valence electron structure $4s^2 4p^2$, $N' = 4$; thus, there are $8 - N' = 4$ covalent bonds per atom.

For phosphorus, having the valence electron structure $3s^2 3p^3$, $N' = 5$; thus, there is $8 - N' = 3$ covalent bonds per atom.

For selenium, having the valence electron structure $4s^2 4p^4$, $N' = 6$; thus, there are $8 - N' = 2$ covalent bonds per atom.

For chlorine, having the valence electron structure $3s^2 3p^5$, $N' = 7$; thus, there are $8 - N' = 1$ covalent bond per atom.

2.22 *What type(s) of bonding would be expected for each of the following materials: brass (a copper-zinc alloy), rubber, barium sulfide (BaS), solid xenon, bronze, nylon, and aluminum phosphide (AlP)?*

Solution

For brass, the bonding is metallic since it is a metal alloy.

For rubber, the bonding is covalent with some van der Waals. (Rubber is composed primarily of carbon and hydrogen atoms.)

For BaS, the bonding is predominantly ionic (but with some covalent character) on the basis of the relative positions of Ba and S in the periodic table.

For solid xenon, the bonding is van der Waals since xenon is an inert gas.

For bronze, the bonding is metallic since it is a metal alloy (composed of copper and tin).

For nylon, the bonding is covalent with perhaps some van der Waals. (Nylon is composed primarily of carbon and hydrogen.)

For AlP the bonding is predominantly covalent (but with some ionic character) on the basis of the relative positions of Al and P in the periodic table.

Secondary Bonding or van der Waals Bonding

2.23 *Explain why hydrogen fluoride (HF) has a higher boiling temperature than hydrogen chloride (HCl) (19.4 vs. –85°C), even though HF has a lower molecular weight.*

Solution

The intermolecular bonding for HF is hydrogen, whereas for HCl, the intermolecular bonding is van der Waals. Since the hydrogen bond is stronger than van der Waals, HF will have a higher melting temperature.

CHAPTER 3

THE STRUCTURE OF CRYSTALLINE SOLIDS

PROBLEM SOLUTIONS

Fundamental Concepts

3.1 What is the difference between atomic structure and crystal structure?

Solution

Atomic structure relates to the number of protons and neutrons in the nucleus of an atom, as well as the number and probability distributions of the constituent electrons. On the other hand, crystal structure pertains to the arrangement of atoms in the crystalline solid material.

Unit Cells

Metallic Crystal Structures

3.2 If the atomic radius of aluminum is 0.143 nm, calculate the volume of its unit cell in cubic meters.

Solution

For this problem, we are asked to calculate the volume of a unit cell of aluminum. Aluminum has an FCC crystal structure (Table 3.1). The FCC unit cell volume may be computed from Equation 3.4 as

$$V_C = 16R^3\sqrt{2} = (16)\left(0.143 \times 10^{-9}\ \text{m}\right)^3\left(\sqrt{2}\right) = 6.62 \times 10^{-29}\ \text{m}^3$$

3.3 Show for the body-centered cubic crystal structure that the unit cell edge length a and the atomic radius R are related through $a = 4R/\sqrt{3}$.

Solution

Consider the BCC unit cell shown below

Using the triangle NOP

$$(\overline{NP})^2 = a^2 + a^2 = 2a^2$$

And then for triangle NPQ,

$$(\overline{NQ})^2 = (\overline{QP})^2 + (\overline{NP})^2$$

But $\overline{NQ} = 4R$, R being the atomic radius. Also, $\overline{QP} = a$. Therefore,

$$(4R)^2 = a^2 + 2a^2$$

or

$$a = \frac{4R}{\sqrt{3}}$$

3.4 For the HCP crystal structure, show that the ideal c/a ratio is 1.633.

Solution

A sketch of one-third of an HCP unit cell is shown below.

Consider the tetrahedron labeled as JKLM, which is reconstructed as

The atom at point M is midway between the top and bottom faces of the unit cell—that is $\overline{MH}$ = c/2. And, since atoms at points J, K, and M, all touch one another,

$$\overline{JM} = \overline{JK} = 2R = a$$

where R is the atomic radius. Furthermore, from triangle JHM,

$$(\overline{JM})^2 = (\overline{JH})^2 \quad (\overline{MH})^2$$

or

$$a^2 = (\overline{JH})^2 + \left(\frac{c}{2}\right)^2$$

Now, we can determine the $\overline{JH}$ length by consideration of triangle JKL, which is an equilateral triangle,

$$\cos 30° = \frac{a/2}{JH} = \frac{\sqrt{3}}{2}$$

and

$$\overline{JH} = \frac{a}{\sqrt{3}}$$

Substituting this value for $\overline{JH}$ in the above expression yields

$$a^2 = \left(\frac{a}{\sqrt{3}}\right)^2 + \left(\frac{c}{2}\right)^2 = \frac{a^2}{3} + \frac{c^2}{4}$$

and, solving for c/a

$$\frac{c}{a} = \sqrt{\frac{8}{3}} = 1.633$$

3.5 Show that the atomic packing factor for BCC is 0.68.

Solution

The atomic packing factor is defined as the ratio of sphere volume to the total unit cell volume, or

$$\mathrm{APF} = \frac{V_S}{V_C}$$

Since there are two spheres associated with each unit cell for BCC

$$V_S = 2(\text{sphere volume}) = 2\left(\frac{4\pi R^3}{3}\right) = \frac{8\pi R^3}{3}$$

Also, the unit cell has cubic symmetry, that is $V_C = a^3$. But a depends on R according to Equation 3.3, and

$$V_C = \left(\frac{4R}{\sqrt{3}}\right)^3 = \frac{64R^3}{3\sqrt{3}}$$

Thus,

$$\mathrm{APF} = \frac{V_S}{V_C} = \frac{8\pi R^3/3}{64R^3/3\sqrt{3}} = 0.68$$

3.6 Show that the atomic packing factor for HCP is 0.74.

Solution

The APF is just the total sphere volume-unit cell volume ratio. For HCP, there are the equivalent of six spheres per unit cell, and thus

$$V_S = 6\left(\frac{4\pi R^3}{3}\right) = 8\pi R^3$$

Now, the unit cell volume is just the product of the base area times the cell height, c. This base area is just three times the area of the parallelepiped ACDE shown below.

The area of ACDE is just the length of $\overline{CD}$ times the height $\overline{BC}$. But $\overline{CD}$ is just a or 2R, and

$$\overline{BC} = 2R\cos(30°) = \frac{2R\sqrt{3}}{2}$$

Thus, the base area is just

$$\text{AREA} = (3)(\overline{CD})(\overline{BC}) = (3)(2R)\left(\frac{2R\sqrt{3}}{2}\right) = 6R^2\sqrt{3}$$

and since c = 1.633a = 2R(1.633)

$$V_C = (\text{AREA})(c) = 6R^2c\sqrt{3} \qquad (3.S1)$$

$$= \left(6R^2\sqrt{3}\right)(2)(1.633)R = 12\sqrt{3}\,(1.633)\,R^3$$

Thus,

$$\text{APF} = \frac{V_S}{V_C} = \frac{8\pi R^3}{12\sqrt{3}\,(1.633)\,R^3} = 0.74$$

Density Computations

3.7 Iron has a BCC crystal structure, an atomic radius of 0.124 nm, and an atomic weight of 55.85 g/mol. Compute and compare its theoretical density with the experimental value found inside the front cover.

Solution

This problem calls for a computation of the density of iron. According to Equation 3.5

$$\rho = \frac{nA_{Fe}}{V_C N_A}$$

For BCC, n = 2 atoms/unit cell, and

$$V_C = \left(\frac{4R}{\sqrt{3}}\right)^3$$

Thus,

$$\rho = \frac{nA_{Fe}}{\left(\frac{4R}{\sqrt{3}}\right)^3 N_A}$$

$$= \frac{(2 \text{ atoms/unit cell})(55.85 \text{ g/mol})}{\left[(4)\left(0.124 \times 10^{-7} \text{ cm}\right)/\sqrt{3}\right]^3 / (\text{unit cell}) \left(6.022 \times 10^{23} \text{ atoms/mol}\right)}$$

$$= 7.90 \text{ g/cm}^3$$

The value given inside the front cover is 7.87 g/cm^3.

3.8 Calculate the radius of an iridium atom, given that Ir has an FCC crystal structure, a density of 22.4 g/cm^3, and an atomic weight of 192.2 g/mol.

Solution

We are asked to determine the radius of an iridium atom, given that Ir has an FCC crystal structure. For FCC, n = 4 atoms/unit cell, and $V_C = 16R^3\sqrt{2}$ (Equation 3.4). Now,

$$\rho = \frac{nA_{Ir}}{V_C N_A}$$

$$= \frac{nA_{Ir}}{\left(16R^3\sqrt{2}\right)N_A}$$

And solving for R from the above expression yields

$$R = \left(\frac{nA_{Ir}}{16\rho N_A\sqrt{2}}\right)^{1/3}$$

$$= \left[\frac{(4\text{ atoms/unit cell})(192.2\text{ g/mol})}{(16)\left(22.4\text{ g/cm}^3\right)\left(6.022\times 10^{23}\text{ atoms/mol}\right)\left(\sqrt{2}\right)}\right]^{1/3}$$

$$= 1.36\times 10^{-8}\text{ cm} = 0.136\text{ nm}$$

3.9 Calculate the radius of a vanadium atom, given that V has a BCC crystal structure, a density of 5.96 g/cm^3, and an atomic weight of 50.9 g/mol.

<u>Solution</u>

This problem asks for us to calculate the radius of a vanadium atom. For BCC, $n = 2$ atoms/unit cell, and

$$V_C = \left(\frac{4R}{\sqrt{3}}\right)^3 = \frac{64R^3}{3\sqrt{3}}$$

Since, from Equation 3.5

$$\rho = \frac{nA_V}{V_C N_A}$$

$$= \frac{nA_V}{\left(\frac{64R^3}{3\sqrt{3}}\right)N_A}$$

and solving for R the previous equation

$$R = \left(\frac{3\sqrt{3}nA_V}{64\,\rho N_A}\right)^{1/3}$$

and incorporating values of parameters given in the problem statement

$$R = \left[\frac{(3\sqrt{3})\,(2 \text{ atoms/unit cell})(50.9 \text{ g/mol})}{(64)(5.96 \text{ g/cm}^3)(6.022 \times 10^{23} \text{ atoms/mol})}\right]^{1/3}$$

$$= 1.32 \times 10^{-8} \text{ cm} = 0.132 \text{ nm}$$

3.10 Some hypothetical metal has the simple cubic crystal structure shown in Figure 3.24. If its atomic weight is 70.4 g/mol and the atomic radius is 0.126 nm, compute its density.

Solution

For the simple cubic crystal structure, the value of n in Equation 3.5 is unity since there is only a single atom associated with each unit cell. Furthermore, for the unit cell edge length, $a = 2R$ (Figure 3.24). Therefore, employment of Equation 3.5 yields

$$\rho = \frac{nA}{V_C N_A} = \frac{nA}{(2R)^3 N_A}$$

and incorporating values of the other parameters provided in the problem statement leads to

$$\rho = \frac{(1 \text{ atom/unit cell})(70.4 \text{ g/mol})}{\left[(2)\left(1.26 \times 10^{-8} \text{ cm}\right)^3 \text{/(unit cell)}\right]\left(6.022 \times 10^{23} \text{ atoms/mol}\right)}$$

$$7.31 \text{ g/cm}^3$$

3.11 Zirconium has an HCP crystal structure and a density of 6.51 g/cm^3.

(a) What is the volume of its unit cell in cubic meters?

(b) If the c/a ratio is 1.593, compute the values of c and a.

Solution

(a) The volume of the Zr unit cell may be computed using Equation 3.5 as

$$V_C = \frac{nA_{Zr}}{\rho N_A}$$

Now, for HCP, n = 6 atoms/unit cell, and for Zr, A_{Zr} = 91.22 g/mol. Thus,

$$V_C = \frac{(6 \text{ atoms/unit cell})(91.22 \text{ g/mol})}{\left(6.51 \text{ g/cm}^3\right)\left(6.022 \times 10^{23} \text{ atoms/mol}\right)}$$

$$= 1.396 \times 10^{-22} \text{ cm}^3\text{/unit cell} = 1.396 \times 10^{-28} \text{ m}^3\text{/unit cell}$$

(b) From Equation 3.S1 of the solution to Problem 3.6, for HCP

$$V_C = 6R^2c\sqrt{3}$$

But, since $a = 2R$, (i.e., $R = a/2$) then

$$V_C = 6\left(\frac{a}{2}\right)^2 c\sqrt{3} = \frac{3\sqrt{3}\,a^2c}{2}$$

but, since $c = 1.593a$

$$V_C = \frac{3\sqrt{3}\,(1.593)\,a^3}{2} = 1.396 \times 10^{-22} \text{ cm}^3\text{/unit cell}$$

Now, solving for a

$$a = \left[\frac{(2)\left(1.396 \times 10^{-22} \text{ cm}^3\right)}{(3)\left(\sqrt{3}\right)(1.593)}\right]^{1/3}$$

$$= 3.23 \times 10^{-8} \text{ cm} = 0.323 \text{ nm}$$

And finally

$$c = 1.593a = (1.593)(0.323 \text{ nm}) = 0.515 \text{ nm}$$

3.12 Using atomic weight, crystal structure, and atomic radius data tabulated inside the front cover, compute the theoretical densities of lead, chromium, copper, and cobalt, and then compare these values with the measured densities listed in this same table. The c/a ratio for cobalt is 1.623.

Solution

Since Pb has an FCC crystal structure, $n = 4$, and $V_C = 16R^3\sqrt{2}$ (Equation 3.4). Also, $R = 0.175$ nm (1.75×10^{-8} cm) and $A_{Pb} = 207.2$ g/mol. Employment of Equation 3.5 yields

$$\rho = \frac{nA_{Pb}}{V_C N_A}$$

$$= \frac{(4 \text{ atoms/unit cell})(207.2 \text{ g/mol})}{\left\{(16)\left(1.75 \times 10^{-8} \text{ cm}\right)^3\left(\sqrt{2}\right)/(\text{unit cell})\right\}\left(6.022 \times 10^{23} \text{ atoms/mol}\right)}$$

$$= 11.35 \text{ g/cm}^3$$

The value given in the table inside the front cover is 11.35 g/cm^3.

Chromium has a BCC crystal structure for which $n = 2$ and $V_C = a^3 = \left(\frac{4R}{\sqrt{3}}\right)^3$ (Equation 3.3); also $A_{Cr} = 52.00$g/mol and $R = 0.125$ nm. Therefore, employment of Equation 3.5 leads to

$$\rho = \frac{(2 \text{ atoms/unit cell})(52.00 \text{ g/mol})}{\left\{\left[\frac{(4)\left(1.25 \times 10^{-8} \text{ cm}\right)}{\sqrt{3}}\right]^3/(\text{unit cell})\right\}\left(6.022 \times 10^{23} \text{ atoms/mol}\right)}$$

$$= 7.18 \text{ g/cm}^3$$

The value given in the table is 7.19 g/cm^3.

Copper also has an FCC crystal structure and therefore

$$\rho = \frac{(4 \text{ atoms/unit cell})(63.55 \text{ g/mol})}{\left[(2)\left(1.28 \times 10^{-8} \text{ cm}\right)\left(\sqrt{2}\right)\right]^3/(\text{unit cell})\left(6.022 \times 10^{23} \text{ atoms/mol}\right)}$$

$$= 8.90 \text{ g/cm}^3$$

The value given in the table is 8.90 g/cm^3.

Cobalt has an HCP crystal structure, and from the solution to Problem 3.6 (Equation 3.S1),

$$V_C = 6R^2c\sqrt{3}$$

and, since $c = 1.623a$ and $a = 2R$, $c = (1.623)(2R)$; hence

$$V_C = 6R^2(1.623)(2R)\sqrt{3} = (19.48)(\sqrt{3})R^3$$

$$= (19.48)(\sqrt{3})(1.25 \times 10^{-8}\ \text{cm})^3$$

$$= 6.59 \times 10^{-23}\ \text{cm}^3/\text{unit cell}$$

Also, there are 6 atoms/unit cell for HCP. Therefore the theoretical density is

$$\rho = \frac{nA_{\text{Co}}}{V_C N_A}$$

$$= \frac{(6\ \text{atoms/unit cell})(58.93\ \text{g/mol})}{\left(6.59 \times 10^{-23}\ \text{cm}^3/\text{unit cell}\right)\left(6.022 \times 10^{23}\ \text{atoms/mol}\right)}$$

$$= 8.91\ \text{g/cm}^3$$

The value given in the table is 8.9 g/cm^3.

3.13 Rhodium has an atomic radius of 0.1345 nm and a density of 12.41 g/cm^3. Determine whether it has an FCC or BCC crystal structure.

Solution

In order to determine whether Rh has an FCC or a BCC crystal structure, we need to compute its density for each of the crystal structures. For FCC, $n = 4$, and $a = 2R\sqrt{2}$ (Equation 3.1). Also, from Figure 2.6, its atomic weight is 102.91 g/mol. Thus, for FCC (employing Equation 3.5)

$$\rho = \frac{nA_{Rh}}{a^3 N_A} = \frac{nA_{Rh}}{\left(2R\sqrt{2}\right)^3 N_A}$$

$$= \frac{(4\ \text{atoms/unit cell})(102.91\ \text{g/mol})}{\left\{\left[(2)(1.345 \times 10^{-8}\ \text{cm})\left(\sqrt{2}\right)\right]^3/(\text{unit cell})\right\}\left(6.022 \times 10^{23}\ \text{atoms/mol}\right)}$$

$$= 12.41\ \text{g/cm}^3$$

which is the value provided in the problem statement. Therefore, Rh has the FCC crystal structure.

3.14 Below are listed the atomic weight, density, and atomic radius for three hypothetical alloys. For each determine whether its crystal structure is FCC, BCC, or simple cubic and then justify your determination. A simple cubic unit cell is shown in Figure 3.24.

Alloy	Atomic Weight (g/mol)	Density (g/cm^3)	Atomic Radius (nm)
A	77.4	8.22	0.125
B	107.6	13.42	0.133
C	127.3	9.23	0.142

Solution

For each of these three alloys we need, by trial and error, to calculate the density using Equation 3.5, and compare it to the value cited in the problem. For SC, BCC, and FCC crystal structures, the respective values of n are 1, 2, and 4, whereas the expressions for a (since $V_C = a^3$) are 2R, $2R\sqrt{2}$, and $\frac{4R}{\sqrt{3}}$.

For alloy A, let us calculate ρ assuming a simple cubic crystal structure.

$$\rho = \frac{nA_A}{V_C N_A}$$

$$= \frac{nA_A}{\left(2R\right)^3 N_A}$$

$$= \frac{(1\ \text{atom/unit cell})(77.4\ \text{g/mol})}{\left\{\left[(2)(1.25 \times 10^{-8})\right]^3 /(\text{unit cell})\right\}\left(6.022 \times 10^{23}\ \text{atoms/mol}\right)}$$

$$= 8.22\ \text{g/cm}^3$$

Therefore, its crystal structure is simple cubic.

For alloy B, let us calculate ρ assuming an FCC crystal structure.

$$\rho = \frac{nA_B}{(2R\sqrt{2})^3 N_A}$$

$$= \frac{(4\text{ atoms/unit cell})(107.6\text{ g/mol})}{\left\{\left[2\sqrt{2}\,(1.33 \times 10^{-8}\text{ cm})\right]^3/(\text{unit cell})\right\}(6.022 \times 10^{23}\text{ atoms/mol})}$$

$$= 13.42\text{ g/cm}^3$$

Therefore, its crystal structure is FCC.

For alloy C, let us calculate U assuming a simple cubic crystal structure.

$$= \frac{nA_C}{(2R)^3 N_A}$$

$$= \frac{(1\text{ atom/unit cell})(127.3\text{ g/mol})}{\left\{\left[(2)(1.42 \times 10^{-8}\text{ cm})\right]^3/(\text{unit cell})\right\}(6.022 \times 10^{23}\text{ atoms/mol})}$$

$$= 9.23\text{ g/cm}^3$$

Therefore, its crystal structure is simple cubic.

3.15 The unit cell for tin has tetragonal symmetry, with a and b lattice parameters of 0.583 and 0.318 nm, respectively. If its density, atomic weight, and atomic radius are 7.30 g/cm^3, 118.69 g/mol, and 0.151 nm, respectively, compute the atomic packing factor.

Solution

In order to determine the APF for Sn, we need to compute both the unit cell volume (V_C) which is just the a^2c product, as well as the total sphere volume (V_S) which is just the product of the volume of a single sphere and the number of spheres in the unit cell (n). The value of n may be calculated from Equation 3.5 as

$$n = \frac{\rho V_C N_A}{A_{Sn}}$$

$$= \frac{(7.30 \text{ g/cm}^3)(5.83)^2(3.18)\left(\times 10^{-24} \text{ cm}^3\right)\left(6.022 \times 10^{23} \text{ atoms/mol}\right)}{118.69 \text{ g/mol}}$$

$$= 4.00 \text{ atoms/unit cell}$$

Therefore

$$\text{APF} = \frac{V_S}{V_C} = \frac{(4)\left(\frac{4}{3}\pi R^3\right)}{(a)^2(c)}$$

$$= \frac{(4)\left[\frac{4}{3}(\pi)(1.51 \times 10^{-8} \text{ cm})^3\right]}{(5.83 \times 10^{-8} \text{ cm})^2(3.18 \times 10^{-8} \text{ cm})}$$

$$= 0.534$$

3.16 Iodine has an orthorhombic unit cell for which the a, b, and c lattice parameters are 0.479, 0.725, and 0.978 nm, respectively.

(a) If the atomic packing factor and atomic radius are 0.547 and 0.177 nm, respectively, determine the number of atoms in each unit cell.

(b) The atomic weight of iodine is 126.91 g/mol; compute its theoretical density.

Solution

(a) For indium, and from the definition of the APF

$$\mathrm{APF} = \frac{V_S}{V_C} = \frac{n\left(\frac{4}{3}\pi R^3\right)}{abc}$$

we may solve for the number of atoms per unit cell, n, as

$$n = \frac{(\mathrm{APF})\,abc}{\frac{4}{3}\pi R^3}$$

Incorporating values of the above parameters provided in the problem state leads to

$$= \frac{(0.547)(4.79 \times 10^{-8}\ \mathrm{cm})(7.25 \times 10^{-8}\ \mathrm{cm})(9.78 \times 10^{-8}\ \mathrm{cm})}{\frac{4}{3}\pi(1.77 \times 10^{-8}\ \mathrm{cm})^3}$$

= 8.0 atoms/unit cell

(b) In order to compute the density, we just employ Equation 3.5 as

$$\rho = \frac{nA_I}{abcN_A}$$

$$= \frac{(8\ \text{atoms/unit cell})(126.91\ \text{g/mol})}{\left[(4.79 \times 10^{-8}\ \mathrm{cm})(7.25 \times 10^{-8}\ \mathrm{cm})(9.78 \times 10^{-8}\ \mathrm{cm})/\text{unit cell}\right](6.022 \times 10^{23}\ \text{atoms/mol})}$$

= 4.96 g/cm^3

3. 17 Titanium has an HCP unit cell for which the ratio of the lattice parameters c/a is 1.58. If the radius of the Ti atom is 0.1445 nm, (a) determine the unit cell volume, and (b) calculate the density of Ti and compare it with the literature value.

Solution

(a) We are asked to calculate the unit cell volume for Ti. For HCP, from Equation 3.S1 (found in the solution to Problem 3.6)

$$V_C = 6R^2c\sqrt{3}$$

But for Ti, c = 1.58a, and a = 2R, or c = 3.16R, and

$$V_C = (6)(3.16)R^3\sqrt{3}$$

$$= (6)(3.16)\left(\sqrt{3}\right) \rangle 1.445 \ u \, 10^{-8} \text{ cm} \rangle^3 @ \ 9.91 \ u \, 10^{23} \text{ cm}^3\text{/unit cell}$$

(b) The theoretical density of Ti is determined, using Equation 3.5, as follows:

$$U = \frac{nA_{Ti}}{V_C N_A}$$

For HCP, n = 6 atoms/unit cell, and for Ti, A_{Ti} = 47.87 g/mol (as noted inside the front cover). Thus,

$$U = \frac{(6 \text{ atoms/unit cell})(47.87 \text{ g/mol})}{\left(9.91 \ u \, 10^{-23} \text{ cm}^3\text{/unit cell}\right)\left(6.022 \ u \, 10^{23} \text{ atoms/mol}\right)}$$

$$= 4.81 \text{ g/cm}^3$$

The value given in the literature is 4.51 g/cm^3.

3.18 Zinc has an HCP crystal structure, a c/a ratio of 1.856, and a density of 7.13 g/cm^3. Compute the atomic radius for Zn.

Solution

In order to calculate the atomic radius for Zn, we must use Equation 3.5, as well as the expression which relates the atomic radius to the unit cell volume for HCP; Equation 3.S1 (from Problem 3.6) is as follows:

$$V_C = 6R^2c\sqrt{3}$$

In this case c = 1.856a, but, for HCP, a = 2R, which means that

$$V_C = 6R^2(1.856)(2R)\sqrt{3} = (1.856)\left(12\sqrt{3}\right)R^3$$

And from Equation 3.5, the density is equal to

$$\rho = \frac{nA_{Zn}}{V_C N_A} = \frac{nA_{Zn}}{(1.856)\left(12\sqrt{3}\right)R^3 N_A}$$

And, solving for R from the above equation leads to the following:

$$R = \left[\frac{nA_{Zn}}{(1.856)\left(12\sqrt{3}\right)\rho N_A}\right]^{1/3}$$

And incorporating appropriate values for the parameters in this equation leads to

$$R = \left[\frac{(6 \text{ atoms/unit cell})(65.41 \text{ g/mol})}{(1.856)\left(12\sqrt{3}\right)\left(7.13 \text{ g/cm}^3\right)\left(6.022 \times 10^{23} \text{ atoms/mol}\right)}\right]^{1/3}$$

$$= 1.33 \times 10^{-8} \text{ cm} = 0.133 \text{ nm}$$

3.19 Rhenium has an HCP crystal structure, an atomic radius of 0.137 nm, and a c/a ratio of 1.615. Compute the volume of the unit cell for Re.

Solution

In order to compute the volume of the unit cell for Re, it is necessary to use Equation 3.S1 (found in Problem 3.6), that is

$$V_C = 6R^2 c\sqrt{3}$$

The problem states that c = 1.615a, and a = 2R. Therefore

$$V_C = (1.615)\left(12\sqrt{3}\right) R^3$$

$$= (1.615)\left(12\sqrt{3}\right)\left(1.37 \times 10^{-8}\ \text{cm}\right)^3 = 8.63 \times 10^{-23}\ \text{cm}^3 = 8.63 \times 10^{-2}\ \text{nm}^3$$

Crystal Systems

3.20 Below is a unit cell for a hypothetical metal.

(a) To which crystal system does this unit cell belong?

(b) What would this crystal structure be called?

(c) Calculate the density of the material, given that its atomic weight is 141 g/mol.

Solution

(a) The unit cell shown in the problem statement belongs to the tetragonal crystal system since $a = b = 0.30$ nm, $c = 0.40$ nm, and $\alpha = \beta = \gamma = 90°$

(b) The crystal structure would be called body-centered tetragonal

(c) As with BCC, $n = 2$ atoms/unit cell. Also, for this unit cell

$$V_C = (3.0 \times 10^{-8}\ \text{cm})^2(4.0 \times 10^{-8}\ \text{cm})$$

$$= 3.60 \times 10^{-23}\ \text{cm}^3/\text{unit cell}$$

Thus, using Equation 3.5, the density is equal to

$$\rho = \frac{nA}{V_C N_A}$$

$$= \frac{(2\ \text{atoms/unit cell})(141\ \text{g/mol})}{(3.60 \times 10^{-23}\ \text{cm}^3/\text{unit cell})(6.022 \times 10^{23}\ \text{atoms/mol})}$$

$$= 13.0\ \text{g/cm}^3$$

3.21 Sketch a unit cell for the body-centered orthorhombic crystal structure.

Solution

A unit cell for the body-centered orthorhombic crystal structure is presented below.

Point Coordinates

3.22 List the point coordinates for all atoms that are associated with the FCC unit cell (Figure 3.1).

Solution

From Figure 3.1b, the atom located of the origin of the unit cell has the coordinates 000. Coordinates for other atoms in the bottom face are 100, 110, 010, and $\frac{1}{2}\frac{1}{2}0$. (The z coordinate for all these points is zero.)

For the top unit cell face, the coordinates are 001, 101, 111, 011, and $\frac{1}{2}\frac{1}{2}1$

Coordinates for those atoms that are positioned at the centers of both side faces, and centers of both front and back faces need to be specified. For the front and back center-face atoms, the coordinates are $1\frac{1}{2}\frac{1}{2}$ and $0\frac{1}{2}\frac{1}{2}$, respectively. While for the left and right side center-face atoms, the respective coordinates are $\frac{1}{2}0\frac{1}{2}$ and $\frac{1}{2}1\frac{1}{2}$.

3.23 List the point coordinates of the titanium, barium, and oxygen ions for a unit cell of the perovskite crystal structure (Figure 12.6).

Solution

In Figure 12.6, the barium ions are situated at all corner positions. The point coordinates for these ions are as follows: 000, 100, 110, 010, 001, 101, 111, and 011.

The oxygen ions are located at all face-centered positions; therefore, their coordinates are $\frac{1}{2}\frac{1}{2}0$, $\frac{1}{2}\frac{1}{2}1$, $1\frac{1}{2}\frac{1}{2}$, $0\frac{1}{2}\frac{1}{2}$, $\frac{1}{2}0\frac{1}{2}$, and $\frac{1}{2}1\frac{1}{2}$.

And, finally, the titanium ion resides at the center of the cubic unit cell, with coordinates $\frac{1}{2}\frac{1}{2}\frac{1}{2}$.

3.24 List the point coordinates of all atoms that are associated with the diamond cubic unit cell (Figure 12.15).

Solution

First of all, one set of carbon atoms occupy all corner positions of the cubic unit cell; the coordinates of these atoms are as follows: 000, 100, 110, 010, 001, 101, 111, and 011.

Another set of atoms reside on all of the face-centered positions, with the following coordinates: $\frac{1}{2}\frac{1}{2}0$, $\frac{1}{2}\frac{1}{2}1$, $1\frac{1}{2}\frac{1}{2}$, $0\frac{1}{2}\frac{1}{2}$, $\frac{1}{2}0\frac{1}{2}$, and $\frac{1}{2}1\frac{1}{2}$.

The third set of carbon atoms are positioned within the interior of the unit cell. Using an x-y-z coordinate system oriented as in Figure 3.4, the coordinates of the atom that lies toward the lower-left-front of the unit cell has the coordinates $\frac{3}{4}\frac{1}{4}\frac{1}{4}$, whereas the atom situated toward the lower-right-back of the unit cell has coordinates of $\frac{1}{4}\frac{3}{4}\frac{1}{4}$. Also, the carbon atom that resides toward the upper-left-back of the unit cell has the $\frac{1}{4}\frac{1}{4}\frac{3}{4}$ coordinates. And, the coordinates of the final atom, located toward the upper-right-front of the unit cell, are $\frac{3}{4}\frac{3}{4}\frac{3}{4}$.

3.25 Sketch a tetragonal unit cell , and within that cell indicate locations of the $\frac{1}{2}\,1\,\frac{1}{2}$ and $\frac{1}{4}\,\frac{1}{2}\,\frac{3}{4}$ point coordinates.

Solution

A tetragonal unit in which are shown the $\frac{1}{2}\,1\,\frac{1}{2}$ and $\frac{1}{4}\frac{1}{2}\frac{3}{4}$ point coordinates is presented below.

3.26 Using the Molecule Definition Utility found in both "Metallic Crystal Structures and Crystallography" and "Ceramic Crystal Structures" modules of VMSE, located on the book's web site [www.wiley.com/college/Callister (Student Companion Site)], generate a three-dimensional unit cell for the intermetallic compound $AuCu_3$ given the following: (1) the unit cell is cubic with an edge length of 0.374 nm, (2) gold atoms are situated at all cube corners, and (3) copper atoms are positioned at the centers of all unit cell faces.

Solution

First of all, open the "Molecular Definition Utility"; it may be found in either of "Metallic Crystal Structures and Crystallography" or "Ceramic Crystal Structures" modules.

In the "Step 1" window, it is necessary to define the atom types, colors for the spheres (atoms), and specify atom sizes. Let us enter "Au" as the name for the gold atoms (since "Au" the symbol for gold), and "Cu" as the name for the copper atoms. Next it is necessary to choose a color for each atom type from the selections that appear in the pull-down menu—for example, "Yellow" for Au and "Red" for Cu. In the "Atom Size" window, it is necessary to enter an atom/ion size. In the instructions for this step, it is suggested that the atom/ion diameter in nanometers be used. From the table found inside the front cover of the textbook, the atomic radii for gold and copper are 0.144 nm and 0.128 nm, respectively, and, therefore, their ionic diameters are twice these values (i.e., 0.288 nm and 0.256 nm); therefore, we enter the values "0.288" and "0.256" for the two atom types. Now click on the "Register" button, followed by clicking on the "Go to Step 2" button.

In the "Step 2" window we specify positions for all of the atoms within the unit cell; their point coordinates are specified in the problem statement. Let's begin with gold. Click on the yellow sphere that is located to the right of the "Molecule Definition Utility" box. Again, Au atoms are situated at all eight corners of the cubic unit cell. One Au will be positioned at the origin of the coordinate system—i.e., its point coordinates are 000, and, therefore, we enter a "0" (zero) in each of the "x", "y", and "z" atom position boxes. Next we click on the "Register Atom Position" button. Now we enter the coordinates of another gold atom; let us arbitrarily select the one that resides at the corner of the unit cell that is one unit-cell length along the x-axis (i.e., at the 100 point coordinate). Inasmuch as it is located a distance of *a* units along the *x*-axis the value of "0.374" is entered in the "x" atom position box (since this is the value of *a* given in the problem statement); zeros are entered in each of the "y" and "z" position boxes. We repeat this procedure for the remaining six Au atoms.

After this step has been completed, it is necessary to specify positions for the copper atoms, which are located at all six facecentered sites. To begin, we click on the red sphere that is located next to the "Molecule Definition Utility" box. The point coordinates for some of the Cu atoms are fractional ones; in these instances, the unit cell length (i.e., 0.374) is multiplied by the fraction. For example, one Cu atom is located $1\frac{1}{2}\frac{1}{2}$ coordinate. Therefore, the x, y, and z atoms positions are (1)(0.374) = 0.374, $\frac{1}{2}$(0.374) = 0.187, and $\frac{1}{2}$(0.374) = 0.187, respectively.

For the gold atoms, the x, y, and z atom position entries for all 8 sets of point coordinates are as follows:

0, 0, and 0
0.374, 0, and 0
0, 0.374, and 0
0, 0, and 0.374
0, 0.374, 0.374
0.374, 0, 0.374
0.374, 0.374, 0
0.374, 0.374, 0.374

Now, for the copper atoms, the x, y, and z atom position entries for all 6 sets of point coordinates are as follows:

0.187, 0.187, 0
0.187, 0, 0.187
0, 0.187, 0.187
0.374, 0.187, 0.187
0.187, 0.374, 0.187
0.187, 0.187, 0.374

In Step 3, we may specify which atoms are to be represented as being bonded to one another, and which type of bond(s) to use (single solid, single dashed, double, and triple are possibilities), or we may elect to not represent any bonds at all (in which case we are finished). If it is decided to show bonds, probably the best thing to do is to represent unit cell edges as bonds. This image may be rotated by using mouse click-and-drag

Your image should appear as the following screen shot. Here the gold atoms appear lighter than the copper atoms.

[Note: Unfortunately, with this version of the Molecular Definition Utility, it is not possible to save either the data or the image that you have generated. You may use screen capture (or screen shot) software to record and store your image.]

Crystallographic Directions

3.27 Draw an orthorhombic unit cell, and within that cell a $[12\bar{1}]$ direction.

Solution

This problem calls for us to draw a $[12\bar{1}]$ direction within an orthorhombic unit cell ($a \neq b \neq c$, $\alpha = \beta = \gamma = 90°$). Such a unit cell with its origin positioned at point *O* is shown below. We first move along the +*x*-axis *a* units (from point *O* to point *A*), then parallel to the +*y*-axis 2*b* units (from point *A* to point *B*). Finally, we proceed parallel to the *z*-axis -*c* units (from point *B* to point *C*). The $[12\bar{1}]$ direction is the vector from the origin (point *O*) to point *C* as shown.

3.28 Sketch a monoclinic unit cell, and within that cell a $[0\bar{1}1]$ direction.

Solution

This problem asks that a $[0\bar{1}1]$ direction be drawn within a monoclinic unit cell ($a \neq b \neq c$, and $\alpha = \beta = 90° \neq \gamma$). One such unit cell with its origin at point O is sketched below. For this direction, there is no projection along the *x*-axis since the first index is zero; thus, the direction lies in the *y-z* plane. We next move from the origin along the minus *y*-axis *b* units (from point O to point R). Since the final index is a one, move from point R parallel to the *z*-axis, *c* units (to point P). Thus, the $[0\bar{1}1]$ direction corresponds to the vector passing from the origin (point O) to point P, as indicated in the figure.

3.29 What are the indices for the directions indicated by the two vectors in the sketch below?

Solution

For direction 1, the projection on the x-axis is zero (since it lies in the y-z plane), while projections on the y- and z-axes are b/2 and c, respectively. This is a [012] direction as indicated in the summary below.

	x	y	z
Projections	0a	b/2	c
Projections in terms of a, b, and c	0	1/2	1
Reduction to integers	0	1	2
Enclosure		[012]	

Direction 2 is $[11\bar{2}]$ as summarized below.

	x	y	z
Projections	a/2	b/2	-c
Projections in terms of a, b, and c	1/2	1/2	-1
Reduction to integers	1	1	-2
Enclosure		$[11\bar{2}]$	

3.30 Within a cubic unit cell, sketch the following directions:

(a) $[\bar{1}10]$,

(b) $[\bar{1}\bar{2}1]$,

(c) $[0\bar{1}2]$,

(d) $[1\bar{3}3]$,

(e) $[\bar{1}\bar{1}1]$,

(f) $[\bar{1}22]$,

(g) $[1\bar{2}\bar{3}]$,

(h) $[\bar{1}03]$.

Solution

The directions asked for are indicated in the cubic unit cells shown below.

3.31 Determine the indices for the directions shown in the following cubic unit cell:

Solution

Direction A is a $[0\bar{1}\bar{1}]$ direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	x	y	z
Projections	0a	–b	–c
Projections in terms of a, b, and c	0	–1	–1
Reduction to integers		not necessary	
Enclosure		$[0\bar{1}\bar{1}]$	

Direction B is a $[\bar{2}10]$ direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	x	y	z
Projections	–a	$\frac{b}{2}$	0c
Projections in terms of a, b, and c	–1	$\frac{1}{2}$	0
Reduction to integers	–2	1	0
Enclosure		$[\bar{2}10]$	

Direction C is a [112] direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	x	y	z
Projections	$\frac{a}{2}$	$\frac{b}{2}$	c
Projections in terms of a, b, and c	$\frac{1}{2}$	$\frac{1}{2}$	1
Reduction to integers	1	1	2
Enclosure		[112]	

Direction D is a $[11\bar{2}]$ direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	x	y	z
Projections	$\frac{a}{2}$	$\frac{b}{2}$	–c
Projections in terms of a, b, and c	$\frac{1}{2}$	$\frac{1}{2}$	–1
Reduction to integers	1	1	–2
Enclosure		$[11\bar{2}]$	

3.32 Determine the indices for the directions shown in the following cubic unit cell:

Solution

Direction A is a $[\bar{4}30]$ direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	x	y	z
Projections	$-\frac{2a}{3}$	$\frac{b}{2}$	0c
Projections in terms of a, b, and c	$-\frac{2}{3}$	$\frac{1}{2}$	0
Reduction to integers	–4	3	0
Enclosure		$[\bar{4}30]$	

Direction B is a $[2\bar{3}2]$ direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	x	y	z
Projections	$\frac{2a}{3}$	–b	$\frac{2c}{3}$
Projections in terms of a, b, and c	$\frac{2}{3}$	–1	$\frac{2}{3}$
Reduction to integers	2	–3	2
Enclosure		$[2\bar{3}2]$	

Direction C is a $[1\bar{3}\bar{3}]$ direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	$\underline{x}$	$\underline{y}$	$\underline{z}$
Projections	$\frac{a}{3}$	$-b$	$-c$
Projections in terms of *a*, *b*, and *c*	$\frac{1}{3}$	-1	-1
Reduction to integers	1	-3	-3
Enclosure		$[1\bar{3}\bar{3}]$	

Direction D is a $[13\bar{6}]$ direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	$\underline{x}$	$\underline{y}$	$\underline{z}$
Projections	$\frac{a}{6}$	$\frac{b}{2}$	$-c$
Projections in terms of *a*, *b*, and *c*	$\frac{1}{6}$	$\frac{1}{2}$	-1
Reduction to integers	1	3	-6
Enclosure		$[13\bar{6}]$	

3.33 For tetragonal crystals, cite the indices of directions that are equivalent to each of the following directions:

(a) [001]

(b) [110]

(c) [010]

Solution

For tetragonal crystals $a = b \neq c$ and $\alpha = \beta = \gamma = 90°$; therefore, projections along the *x* and *y* axes are equivalent, which are not equivalent to projections along the *z* axis.

(a) Therefore, for the [001] direction, there is only one equivalent direction: $[00\bar{1}]$.

(b) For the [110] direction, equivalent directions are as follows: $[\bar{1}\bar{1}0]$, $[\bar{1}10]$, and $[1\bar{1}0]$

(b) Also, for the [010] direction, equivalent directions are the following: $[0\bar{1}0]$, $[100]$, and $[\bar{1}00]$.

3.34 Convert the [100] and [111] directions into the four-index Miller–Bravais scheme for hexagonal unit cells.

Solution

For [100]

u' = 1,
v' = 0,
w' = 0

From Equations 3.6

$$u = \frac{1}{3}(2u' \quad v') = \frac{1}{3}[(2)(1) \quad 0] = \frac{2}{3}$$

$$v = \frac{1}{3}(2v' \quad u') = \frac{1}{3}[(2)(0) \quad 1] = \quad \frac{1}{3}$$

$$t = \quad (u + v) = \quad \left(\frac{2}{3} \quad \frac{1}{3}\right) = \quad \frac{1}{3}$$

$$w = w' = 0$$

It is necessary to multiply these numbers by 3 in order to reduce them to the lowest set of integers. Thus, the direction is represented as $[uvtw] = [2\bar{1}\bar{1}0]$.

For [111], u' = 1, v' = 1, and w' = 1; therefore,

$$u = \frac{1}{3}[(2)(1) \quad 1] = \frac{1}{3}$$

$$v = \frac{1}{3}[(2)(1) \quad 1] = \frac{1}{3}$$

$$t = \quad \left(\frac{1}{3} \quad \frac{1}{3}\right) \quad \frac{2}{3}$$

$$w = 1$$

If we again multiply these numbers by 3, then $u = 1$, $v = 1$, $t = -2$, and $w = 3$. Thus, the direction is represented as Thus, the direction is represented as $[uvtw] = [11\bar{2}3]$.

3.35 Determine indices for the directions shown in the following hexagonal unit cells:

Solution

(a) For this direction, projections on the $\mathbf{a}_1$, $\mathbf{a}_2$, and z axes are a, a/2, and c/2, or, in terms of a and c the projections are 1, 1/2, and 1/2, which when multiplied by the factor 2 become the smallest set of integers: 2, 1, and 1. This means that

u’ = 2

v’ = 1

w’ = 1

Now, from Equations 3.6, the u, v, t, and w indices become

$$u = \frac{1}{3}(2u' \quad v') \quad \frac{1}{3} \gt (2)(2) \quad (1) @ \frac{3}{3} \quad 1$$

$$v = \frac{1}{3}(2v\tilde{O} \quad u\tilde{O}) \quad \frac{1}{3} \gt (2)(1) \quad (2) @ \quad 0$$

$$t \quad (u \quad v) \quad 1 \quad 0 \quad 1$$

$$w = w' = 1$$

No reduction is necessary inasmuch as all of these indices are integers; therefore, this direction in the four-index scheme is $[10\bar{1}1]$

(b) For this direction, projections on the a_1, a_2, and z axes are $a/2$, a, and $0c$, or, in terms of a and c the projections are 1/2, 1, and 0, which when multiplied by the factor 2 become the smallest set of integers: 1, 2, and 0. This means that

$u' = 1$

$v' = 2$

$w' = 0$

Now, from Equations 3.6, the u, v, t, and w indices become

$$u = \frac{1}{3}(2u' - v') = \frac{1}{3}\left[(2)(1) - 2\right] = 0$$

$$v = \frac{1}{3}(2v' - u') = \frac{1}{3}\left[(2)(2) - 1\right] = 1$$

$$t = -(u + v) = -(0 + 1) = -1$$

$$w = w' = 0$$

No reduction is necessary inasmuch as all of these indices are integers; therefore, this direction in the four-index scheme is $[01\bar{1}0]$.

(c) For this direction projections on the a_1, a_2, and z axes are a, a, and c/2, or, in terms of a and c the projections are 1, 1, and 1/2, which when multiplied by the factor 2 become the smallest set of integers: 2, 2, and 1. This means that

u’ = 2

v’ = 2

w’ = 1

Now, from Equations 3.6, the u, v, t, and w indices become

$$u \quad \frac{1}{3}(2u' \quad v) \quad \frac{1}{3}(2)(\ 2) \quad (\ 2) \ @ \ \frac{2}{3}$$

$$v \quad \frac{1}{3}(2v' \quad u') \quad \frac{1}{3}(2)(\ 2) \quad (\ 2) \ @ \ \frac{2}{3}$$

$$t \qquad (u \quad v) \qquad §\ \frac{2}{3} \quad \frac{2}{3} \cdot \qquad \frac{4}{3}$$

$$w \quad w' \quad 1$$

Now, in order to get the lowest set of integers, it is necessary to multiply all indices by the factor 3, with the result that this direction is a $[\overline{2}\overline{2}43]$ direction.

(d) For this direction, projections on the a_1, $\mathbf{a}_2$, and z axes are 0, $-a$, and 0c, or, in terms of a and c the projections are 0, -1, and 0. This means that

$u' = 0$

$v' = -1$

$w' = 0$

Now, from Equations 3.6, the u, v, t, and w indices become

$$u = \frac{1}{3}(2u' - v') = \frac{1}{3}[(2)(0) - (-1)] = \frac{1}{3}$$

$$v = \frac{1}{3}(2v' - u') = \frac{1}{3}[(2)(-1) - 0] = -\frac{2}{3}$$

$$t = -(u + v) = -\left(\frac{1}{3} - \frac{2}{3}\right) = \frac{1}{3}$$

$$w = w' = 0$$

Now, in order to get the lowest set of integers, it is necessary to multiply all indices by the factor 3, with the result that this is a $[1\bar{2}10]$ direction.

3.36 Sketch the $[\bar{1}\bar{1}23]$ and $[10\bar{1}0]$ directions in a hexagonal unit cell.

Solution

The first portion of this problem asks that we plot the $[\bar{1}\bar{1}23]$ within a hexagonal unit cell. Below is shown this direction plotted within a hexagonal unit cell having a reduced-scale coordinate scheme.

For this direction, projections on the a_1, a_2, a_3, and c axes are respectively, 1, 1, 2, and 3, respectively. In plotting this direction, we begin at the origin of the coordinate system, point o. From here we proceed 1 unit distance along the a_1 axis (to point p), from here 1 unit distance parallel to a_2 axis (to point q), then 2 unit distances parallel (or along) the a_3 axis (to point r), and finally, 3 unit distances parallel to the z axis (to point s). Thus, the $[\bar{1}\bar{1}23]$ direction is that vector that extends from point o to point s as shown.

Now we are asked to plot the $[10\bar{1}0]$ within a hexagonal unit cell. In the figure below is plotted this direction within a hexagonal unit cell having a reduced-scale coordinate scheme.

For this direction, projections on the a_1, a_2, a_3, and c axes are respectively, 1, 0, -1, and 0, respectively. In plotting this direction, we begin at the origin of the coordinate system, point o. From here we proceed 1 unit distance along the a_1 axis (to point p). Since there is no projection on the a_2 axis it is not necessary to move parallel to this axis. Therefore, from point p we proceed 1 unit distance parallel to a_3 axis (to point q). And, finally, inasmuch as there is no projection along the z axis, it is not necessary to move parallel to this axis. Thus, the $[10\bar{1}0]$ direction is that vector that extends from point o to point q as shown.

3.37 Using Equations 3.6a, 3.6b, 3.6c, and 3.6d, derive expressions for each of the three primed indices set (u• Y• DQG Z• LQ WHUPV RI WKH IRXU XQSULPHG LQGLFHV X Y W

Solution

It is first necessary to do an expansion of Equation 3.6a as

$$u \quad \frac{1}{3}(2u' \quad v) \quad \frac{2u'}{3} \quad \frac{v'}{3}$$

And solving this expression for v' yields

$$v' \quad 2u' \quad 3u$$

Now, substitution of this expression into Equation 3.6b gives

$$v \quad \frac{1}{3}(2vÕ \quad uÕ) \quad \frac{1}{3}[(2)(2uÕ \quad 3u) \quad uÕ@ \quad uÕ \quad 2u$$

Or

$$u' \quad v \quad 2u$$

And, solving for v from Equation 3.6c leads to

$$v \quad (u \quad t)$$

which, when substituted into the above expression for u' yields

$$u' \quad v \quad 2u \quad u \quad t \quad 2u \quad u \quad t$$

In solving for an expression for v', we begin with the one of the above expressions for this parameter—i.e.,

$$v' \quad 2u' \quad 3u$$

Now, substitution of the above expression for u' into this equation leads to

$$vÕ \quad 2uÕ \quad 3u \quad (2)(u \quad t) \quad 3u \quad u \quad 2t$$

And solving for u from Equation 3.6c gives

$$u \qquad v \quad t$$

which, when substituted in the previous equation results in the following expression for v'

$$vÕ \qquad u \quad 2t \qquad (\; v \quad t) \quad 2t \quad v \quad t$$

And, of course from Equation 3.6d

$$w' = w$$

Crystallographic Planes

3.38 (a) Draw an orthorhombic unit cell, and within that cell a (210) plane.

(b) Draw a monoclinic unit cell, and within that cell a (002) plane.

Solution

(a) We are asked to draw a (210) plane within an orthorhombic unit cell. First remove the three indices from the parentheses, and take their reciprocals-L.H DQG ' 7KLV PHDQV x-axis WKDW WKH S at a/2, the y-axis at b, and parallels the z-axis. The plane that satisfies these requirements has been drawn within the orthorhombic unit cell below. (For orthorhombic, a • b • c, and D = E = J = 90q.)

(b) A (002) plane is drawn within the monoclinic cell shown below. We first remove the parentheses and take the reciprocals of the indices; this gives f, f, and 1/2. Thus, the (002) plane parallels both x- and y-axes, and intercepts the z-axis at a/2, as indicated in the drawing. (For monoclinic, a • b • c, and D = J = 90q • E.)

3.39 What are the indices for the two planes drawn in the sketch below?

Solution

Plane 1 is a (020) plane. The determination of its indices is summarized below.

	x	y	z
Intercepts	∞a	b/2	∞c
Intercepts in terms of a, b, and c	∞	1/2	∞
Reciprocals of intercepts	0	2	0
Enclosure		(020)	

Plane 2 is a $(2\bar{2}1)$ plane, as summarized below.

	x	y	z
Intercepts	a/2	-b/2	c
Intercepts in terms of a, b, and c	1/2	-1/2	1
Reciprocals of intercepts	2	-2	1
Enclosure		$(2\bar{2}1)$	

3.40 Sketch within a cubic unit cell the following planes:

(a) $(0\bar{1}\bar{1})$, (e) $(\bar{1}1\bar{1})$,

(b) $(11\bar{2})$, (f) $(1\bar{2}\bar{2})$,

(c) $(10\bar{2})$, (g) $(\bar{1}2\bar{3})$,

(d) $(1\bar{3}1)$, (h) $(0\bar{1}\bar{3})$

Solution

The planes called for are plotted in the cubic unit cells shown below.

3.41 Determine the Miller indices for the planes shown in the following unit cell:

Solution

For plane A we will leave the origin at the unit cell as shown; this is a (403) plane, as summarized below.

	x	y	z
Intercepts	$\frac{a}{2}$	∞b	$\frac{2c}{3}$
Intercepts in terms of a, b, and c	$\frac{1}{2}$	∞	$\frac{2}{3}$
Reciprocals of intercepts	2	0	$\frac{3}{2}$
Reduction	4	0	3
Enclosure		(403)	

For plane B we will move the origin of the unit cell one unit cell distance to the right along the y axis, and one unit cell distance parallel to the x axis; thus, this is a $(\bar{1}\bar{1}2)$ plane, as summarized below.

	x	y	z
Intercepts	– a	– b	$\frac{c}{2}$
Intercepts in terms of a, b, and c	– 1	– 1	$\frac{1}{2}$
Reciprocals of intercepts	– 1	– 1	2
Reduction		(not necessary)	
Enclosure		$(\bar{1}\bar{1}2)$	

3.42 Determine the Miller indices for the planes shown in the following unit cell:

Solution

For plane A we will move the origin of the coordinate system one unit cell distance to the upward along the z axis; thus, this is a $(32\bar{2})$ plane, as summarized below.

	x	y	z
Intercepts	$\frac{a}{3}$	$\frac{b}{2}$	$-\frac{c}{2}$
Intercepts in terms of a, b, and c	$\frac{1}{3}$	$\frac{1}{2}$	$-\frac{1}{2}$
Reciprocals of intercepts	3	2	-2
Reduction		(not necessary)	
Enclosure		$(32\bar{2})$	

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

	x	y	z
Intercepts	$-\frac{a}{2}$	∞b	$\frac{c}{2}$
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		$(\bar{1}01)$	

3.43 Determine the Miller indices for the planes shown in the following unit cell:

<u>Solution</u>

For plane *A* since the plane passes through the origin of the coordinate system as shown, we will move the origin of the coordinate system one unit cell distance to the right along the *y* axis; thus, this is a $(3\bar{2}4)$ 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		$(3\bar{2}4)$	

For plane *B* we will 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
Reduction		not necessary	
Enclosure		(221)	

3.44 Cite the indices of the direction that results from the intersection of each of the following pair of planes within a cubic crystal: (a) (100) and (010) planes, (b) (111) and $(11\bar{1})$ planes, and (c) $(10\bar{1})$ and (001) planes.

Solution

(a) In the figure below is shown (100) and (010) planes, and, as indicated, their intersection results in a [001], or equivalently, a $[00\bar{1}]$ direction.

(b) In the figure below is shown (111) and $(11\bar{1})$ planes, and, as indicated, their intersection results in a $[\bar{1}10]$, or equivalently, a $[1\bar{1}0]$ direction.

(c) In the figure below is shown $(10\bar{1})$ and (001) planes, and, as indicated, their intersection results in a [010], or equivalently, a $[0\bar{1}0]$ direction.

3.45 Sketch the atomic packing of (a) the (100) plane for the BCC crystal structure, and (b) the (201) plane for the FCC crystal structure (similar to Figures 3.10b and 3.11b).

Solution

(a) A BCC unit cell, its (100) plane, and the atomic packing of this plane are indicated below. Corresponding atom positions in the two drawings are indicated by letters W, X, Y, and Z.

(b) An FCC unit cell, its (201) plane, and the atomic packing of this plane are indicated below. Corresponding atom positions in the two drawing are indicated by letters A, B, and C.

3.46 Consider the reduced-sphere unit cell shown in Problem 3.20, having an origin of the coordinate system positioned at the atom labeled with an O. For the following sets of planes, determine which are equivalent:

(a) $(00\bar{1})$, (010), and $(\bar{1}00)$

(b) $(1\bar{1}0)$, $(10\bar{1})$, $(0\bar{1}1)$, and $(\bar{1}\bar{1}0)$

(c) $(\bar{1}\bar{1}\bar{1})$, $(\bar{1}1\bar{1})$, $(\bar{1}\bar{1}1)$, and $(1\bar{1}1)$

Solution

(a) The unit cell in Problem 3.20 is body-centered tetragonal. Of the three planes given in the problem statement the $(\bar{1}00)$ and (010) are equivalent—that is, have the same atomic packing. The atomic packing for these two planes as well as the $(00\bar{1})$ are shown in the figure below.

(b) Of the four planes cited in the problem statement, $(1\bar{1}0)$ and $(\bar{1}\bar{1}0)$ are equivalent to one another—have the same atomic packing. The atomic arrangement of these planes is shown in the left drawing below.

Furthermore, the $(10\bar{1})$ and $(0\bar{1}1)$ are equivalent to each other (but not to the other pair of planes); their atomic arrangement is represented in the other drawing. Note: the 0.424 nm dimension in the left-most drawing comes from the relationship $\left[(0.30\text{ nm})^2 + (0.30\text{ nm})^2\right]^{1/2}$. Likewise, the 0.500 nm dimension found in the right-most drawing comes from $\left[(0.30\text{ nm})^2 + (0.40\text{ nm})^2\right]^{1/2}$.

(c) All of the $(\bar{1}\bar{1}\bar{1})$, $(\bar{1}1\bar{1})$, $(\bar{1}\bar{1}1)$, and $(1\bar{1}1)$ planes are equivalent, that is, have the same atomic packing as illustrated in the following figure:

3.47 Here are shown the atomic packing schemes for several different crystallographic directions for some hypothetical metal. For each direction the circles represent only those atoms contained within a unit cell, which circles are reduced from their actual size.

(a) To what crystal system does the unit cell belong?
(b) What would this crystal structure be called?

Solution

Below is constructed a unit cell using the six crystallographic directions that were provided in the problem.

(a) This unit cell belongs to the tetragonal system since a = b = 0.40 nm, c = 0.50 nm, and $\alpha = \beta = \gamma = 90^\circ$.

(b) This crystal structure would be called face-centered tetragonal since the unit cell has tetragonal symmetry, and an atom is located at each of the corners, as well as at the centers of all six unit cell faces. In the figure above, atoms are only shown at the centers of three faces; however, atoms would also be situated at opposite faces.

3.48 Below are shown three different crystallographic planes for a unit cell of some hypothetical metal. The circles represent atoms:

(a) To what crystal system does the unit cell belong?

(b) What would this crystal structure be called?

(c) If the density of this metal is 8.95 g/cm^3, determine its atomic weight.

Solution

The unit cells constructed below show the three crystallographic planes that were provided in the problem statement.

(a) This unit cell belongs to the orthorhombic crystal system since a = 0.30 nm, b = 0.40 nm, c = 0.35 nm, and $\alpha = \beta = \gamma = 90°$

(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 cell center.

(c) In order to compute its atomic weight, we employ Equation 3.5, with n = 2; thus

$$A = \frac{\rho V_C N_A}{n}$$

$$\frac{\left(8.95\ \text{g/cm}^3\right)(3.0)(4.0)(3.5)\left(\times 10^{-24}\ \text{cm}^3\text{/unit cell}\right)\left(6.022\times 10^{23}\ \text{atoms/mol}\right)}{2\ \text{atoms/unit cell}}$$

$$= 113.2\ \text{g/mol}$$

3.49 Convert the (010) and (101) planes into the four-index Miller–Bravais scheme for hexagonal unit cells.

Solution

For (010), $h = 0$, $k = 1$, and $l = 0$, and, from Equation 3.7, the value of i is equal to

$$i \qquad (h \quad k) \qquad (0 \quad 1) \qquad 1$$

Therefore, the (010) plane becomes $(01\bar{1}0)$.

Now for the (101) plane, $h = 1$, $k = 0$, and $l = 1$, and computation of i using Equation 3.7 leads to

$$i \qquad (h \quad k) \qquad [1 \quad 0] \qquad 1$$

such that (101) becomes $(10\bar{1}1)$.

3.50 Determine the indices for the planes shown in the hexagonal unit cells below:

Solution

(a) For this plane, intersections with the a_1, a_2, and z axes are ∞a, ∞a, and $c/2$ (the plane parallels both a_1 and a_2 axes). In terms of a and c these intersections are ∞, ∞, and ½, the respective reciprocals of which are 0, 0, and 2. This means that

$h = 0$

$k = 0$

$l = 2$

Now, from Equation 3.7, the value of i is

$$i = -(h + k) = -[0 + 0] = 0$$

Hence, this is a (0002) plane.

(b) This plane passes through the origin of the coordinate axis system; therefore, we translate this plane one unit distance along the x axis, per the sketch shown below:

At this point the plane intersects the a_1, a_2, and z axes at a, ∞a, and ∞c, respectively (the plane parallels both a_2 and z axes). In terms of a and c these intersections are 1, ∞, and ∞, the respective reciprocals of which are 1, 0, and 0. This means that

$h = 1$

$k = 0$

$l = 0$

Now, from Equation 3.7, the value of i is

$$i = -(h + k) = -(1 + 0) = -1$$

Hence, this is a $(10\bar{1}0)$ plane.

(c) For this plane, intersections with the a_1, a_2, and z axes are –a, a, and c. In terms of a and c these intersections are –1, 1, and 1, the respective reciprocals of which are 0, 11, and This means that

h = –1

k = 1

l = 1

Now, from Equation 3.7, the value of i is

$$i \quad (h \quad k) \quad (\ 1 \quad 1) \quad 0$$

Hence, this is a $(\bar{1}101)$ plane.

(d) For this plane, intersections with the a_1, a_2, and z axes are –a/2, a, and c/2, respectively. In terms of a and c these intersections are –1/2, 1, and 1/2, the respective reciprocals of which are –2, 1, and 2. This means that

h = –2

k = 1

l = 2

Now, from Equation 3.7, the value of i is

$$i = -(h + k) = -(-2 + 1) = 1$$

Therefore, this is a $(\bar{2}112)$ plane.

3.51 Sketch the $(1\bar{1}01)$ and $(11\bar{2}0)$ planes in a hexagonal unit cell.

Solution

For $(1\bar{1}01)$ the reciprocals of h, k, i, and l are, respectively, 1, –1, f, and 1; thus, this plane is parallel to the a_3 axis, and intersects the a_1 axis at a, the a_2 axis at –a, and the z-axis at c. The plane having these intersections is shown in the figure below

For $(11\bar{2}0)$ the reciprocals of h, k, i, and l are, respectively, 1, 1, –1/2, and f; thus, this plane is parallel to the z axis, and intersects the a_1 axis at a, the a_2 axis at a, and the a_3 axis at –a/2. The plane having these intersections is shown in the figure below.

Linear and Planar Densities

3.52 (a) Derive linear density expressions for FCC [100] and [111] directions in terms of the atomic radius R.

(b) Compute and compare linear density values for these same two directions for silver.

Solution

(a) In the figure below is shown a [100] direction within an FCC unit cell.

For this [100] direction there is one atom at each of the two unit cell corners, and, thus, there is the equivalent of 1 atom that is centered on the direction vector. The length of this direction vector is just the unit cell edge length, $2R\sqrt{2}$ (Equation 3.1). Therefore, the expression for the linear density of this plane is

$$LD_{100} = \frac{\text{number of atoms centered on [100] direction ve}}{\text{length of [100] direction vector}}$$

$$\frac{1\text{ atom}}{2R\sqrt{2}} \quad \frac{1}{2R\sqrt{2}}$$

An FCC unit cell within which is drawn a [111] direction is shown below.

For this [111] direction, the vector shown passes through only the centers of the single atom at each of its ends, and, thus, there is the equivalence of 1 atom that is centered on the direction vector. The length of this direction vector is denoted by z in this figure, which is equal to

$$z \quad \sqrt{x^2 \quad y^2}$$

where x is the length of the bottom face diagonal, which is equal to 4R. Furthermore, y is the unit cell edge length, which is equal to $2R\sqrt{2}$ (Equation 3.1). Thus, using the above equation, the length z may be calculated as follows:

$$z \quad \sqrt{(4R)^2 \quad (2R\sqrt{2})^2} \quad \sqrt{24R^2} \quad 2R\sqrt{6}$$

Therefore, the expression for the linear density of this direction is

$$LD_{111} = \frac{\text{number of atoms centered on [111] direction ve}}{\text{length of [111] direction vector}}$$

$$\frac{1 \text{ atom}}{2R\sqrt{6}} \quad \frac{1}{2R\sqrt{6}}$$

(b) From the table inside the front cover, the atomic radius for silver is 0.144 nm. Therefore, the linear density for the [100] direction is

$$LD_{100}(\text{Ag}) \quad \frac{1}{2R\sqrt{2}} \quad \frac{1}{(2)(0.144\text{ nm})\sqrt{2}} \quad 2.46\text{ nm}^{1} \quad 2.46\ \text{u}10^{9}\ \text{m}^{1}$$

While for the [111] direction

$$LD_{111}(\text{Ag}) \quad \frac{1}{2R\sqrt{6}} \quad \frac{1}{(2)(0.144\text{ nm})\sqrt{6}} \quad 1.42\text{ nm}^{1} \quad 1.42\ \text{u}10^{9}\ \text{m}^{1}$$

3.53 (a) Derive linear density expressions for BCC [110] and [111] directions in terms of the atomic radius R.

(b) Compute and compare linear density values for these same two directions for tungsten.

Solution

(a) In the figure below is shown a [110] direction within a BCC unit cell.

For this [110] direction there is one atom at each of the two unit cell corners, and, thus, there is the equivalence of 1 atom that is centered on the direction vector. The length of this direction vector is denoted by *x* in this figure, which is equal to

$$x = \sqrt{z^2 - y^2}$$

where *y* is the unit cell edge length, which, from Equation 3.3 is equal to $\frac{4R}{\sqrt{3}}$. Furthermore, *z* is the length of the unit cell diagonal, which is equal to 4*R*. Thus, using the above equation, the length *x* may be calculated as follows:

$$x = \sqrt{(4R)^2 - \left(\frac{4R}{\sqrt{3}}\right)^2} = \sqrt{\frac{32R^2}{3}} = 4R\sqrt{\frac{2}{3}}$$

Therefore, the expression for the linear density of this direction is

$$LD_{110} = \frac{\text{number of atoms centered on [110] direction ve}}{\text{length of [110] direction vector}}$$

$$= \frac{1 \text{ atom}}{4R\sqrt{\frac{2}{3}}} = \frac{\sqrt{3}}{4R\sqrt{2}}$$

A BCC unit cell within which is drawn a [111] direction is shown below.

For although the [111] direction vector shown passes through the centers of three atoms, there is an equivalence of only two atoms associated with this unit cell—one-half of each of the two atoms at the end of the vector, in addition to the center atom belongs entirely to the unit cell. Furthermore, the length of the vector shown is equal to 4R, since all of the atoms whose centers the vector passes through touch one another. Therefore, the linear density is equal to

$$LD_{111} = \frac{\text{number of atoms centered on [111] direction ve}}{\text{length of [111] direction vector}}$$

$$= \frac{2\text{ atoms}}{4R} = \frac{1}{2R}$$

(b) From the table inside the front cover, the atomic radius for tungsten is 0.137 nm. Therefore, the linear density for the [110] direction is

$$LD_{110}(\text{W}) = \frac{\sqrt{3}}{4R\sqrt{2}} = \frac{\sqrt{3}}{(4)(0.137\text{ nm})\sqrt{2}} = 2.23\text{ nm}^{-1} = 2.23 \times 10^{9}\text{ m}^{-1}$$

While for the [111] direction

$$LD_{111}(\text{W}) = \frac{1}{2R} = \frac{1}{(2)(0.137\text{ nm})} = 3.65\text{ nm}^{-1} = 3.65 \times 10^{9}\text{ m}^{-1}$$

3.54 (a) Derive planar density expressions for FCC (100) and (111) planes in terms of the atomic radius R.

(b) Compute and compare planar density values for these same two planes for nickel.

<u>Solution</u>

(a) In the figure below is shown a (100) plane for an FCC unit cell.

For this (100) plane there is one atom at each of the four cube corners, each of which is shared with four adjacent unit cells, while the center atom lies entirely within the unit cell. Thus, there is the equivalence of 2 atoms associated with this FCC (100) plane. The planar section represented in the above figure is a square, wherein the side lengths are equal to the unit cell edge length, $2R\sqrt{2}$ (Equation 3.1); and, thus, the area of this square is just $\left(2R\sqrt{2}\right)^2 = 8R^2$. Hence, the planar density for this (100) plane is just

$$PD_{100} = \frac{\text{number of atoms centered on (100) pl}}{\text{area of (100) plane}}$$

$$\frac{2\ \text{atoms}}{8R^2} \quad \frac{1}{4R^2}$$

That portion of an FCC (111) plane contained within a unit cell is shown below.

There are six atoms whose centers lie on this plane, which are labeled A through F. Onesixth of each of atoms A, D, and F are associated with this plane (yielding an equivalence of one-half atom), with one-half of each of atoms B, C, and E (or an equivalence of one and one-half atoms) for a total equivalence of two atoms. Now, the area of the triangle shown in the above figure is equal to one-half of the product of the base length and the height h. If we consider half of the triangle, then

$$(2R)^2 \quad h^2 \quad (4R)^2$$

which leads to $h = 2R\sqrt{3}$. Thus, the area is equal to

$$\text{Area} \quad \frac{4R(h)}{2} \quad \frac{(4R)\left(2R\sqrt{3}\right)}{2} \quad 4R^2\sqrt{3}$$

And, thus, the planar density is

$$PD_{111} = \frac{\text{number of atoms centered on (111) pl}}{\text{area of (111) plane}}$$

$$\frac{2\text{ atoms}}{4R^2\sqrt{3}} \quad \frac{1}{2R^2\sqrt{3}}$$

(b) From the table inside the front cover, the atomic radius for nickel is 0.125 nm. Therefore, the planar density for the (100) plane is

$$PD_{100}(\text{Ni}) \quad \frac{1}{4R^2} \quad \frac{1}{4\,(0.125\,\text{nm})^2} \quad 16.00\,\text{nm}^{\ 2} \quad 1.600\ u10^{19}\ \text{m}^{\ 2}$$

While for the (111) plane

$$PD_{111}(\text{Ni}) \quad \frac{1}{2R^2\sqrt{3}} \quad \frac{1}{2\sqrt{3}\,(0.125\,\text{nm})^2} \quad 18.48\,\text{nm}^{\ 2} \quad 1.848\ u10^{19}\ \text{m}^{\ 2}$$

3.55 (a) Derive planar density expressions for BCC (100) and (110) planes in terms of the atomic radius R.

(b) Compute and compare planar density values for these same two planes for vanadium.

Solution

(a) A BCC unit cell within which is drawn a (100) plane is shown below.

For this (100) plane there is one atom at each of the four cube corners, each of which is shared with four adjacent unit cells. Thus, there is the equivalence of 1 atom associated with this BCC (100) plane. The planar section represented in the above figure is a square, wherein the side lengths are equal to the unit cell edge length, $\frac{4R}{\sqrt{3}}$ (Equation 3.3); and, thus, the area of this square is just $\left(\frac{4R}{\sqrt{3}}\right)^2 = \frac{16R^2}{3}$. Hence, the planar density for this (100) plane is just

$$PD_{100} = \frac{\text{number of atoms centered on (100) pl}}{\text{area of (100) plane}}$$

$$\frac{1\text{ atom}}{\frac{16\,R^2}{3}} \qquad \frac{3}{16\,R^2}$$

A BCC unit cell within which is drawn a (110) plane is shown below.

For this (110) plane there is one atom at each of the four cube corners through which it passes, each of which is shared with four adjacent unit cells, while the center atom lies entirely within the unit cell. Thus, there is the equivalence of 2 atoms associated with this BCC (110) plane. The planar section represented in the above figure is a rectangle, as noted in the figure below.

From this figure, the area of the rectangle is the product of x and y. The length x is just the unit cell edge length, which for BCC (Equation 3.3) is $\frac{4R}{\sqrt{3}}$. Now, the diagonal length z is equal to 4R. For the triangle bounded by the lengths x, y, and z

$$y = \sqrt{z^2 - x^2}$$

Or

$$y = \sqrt{(4R)^2 - \left(\frac{4R}{\sqrt{3}}\right)^2} = \frac{4R\sqrt{2}}{\sqrt{3}}$$

Thus, in terms of R, the area of this (110) plane is just

$$\text{Area}(110) = xy = \left(\frac{4R}{\sqrt{3}}\right)\left(\frac{4R\sqrt{2}}{\sqrt{3}}\right) = \frac{16R^2\sqrt{2}}{3}$$

And, finally, the planar density for this (110) plane is just

$$PD_{110} = \frac{\text{number of atoms centered on (110) pl}}{\text{area of (110) plane}}$$

$$= \frac{2\text{ atoms}}{\dfrac{16R^2\sqrt{2}}{3}} = \frac{3}{8R^2\sqrt{2}}$$

(b) From the table inside the front cover, the atomic radius for vanadium is 0.132 nm. Therefore, the planar density for the (100) plane is

$$PD_{100}(\text{V}) = \frac{3}{16R^2} = \frac{3}{16(0.132\text{ nm})^2} = 10.76\text{ nm}^{-2} = 1.076 \times 10^{19}\text{ m}^{-2}$$

While for the (110) plane

$$PD_{110}(\text{V}) = \frac{3}{8R^2\sqrt{2}} = \frac{3}{8(0.132\text{ nm})^2\sqrt{2}} = 15.22\text{ nm}^{-2} = 1.522 \times 10^{19}\text{ m}^{-2}$$

3.56 (a) Derive the planar density expression for the HCP (0001) plane in terms of the atomic radius R.

(b) Compute the planar density value for this same plane for magnesium.

Solution

(a) A (0001) plane for an HCP unit cell is show below.

Each of the 6 perimeter atoms in this plane is shared with three other unit cells, whereas the center atom is shared with no other unit cells; this gives rise to three equivalent atoms belonging to this plane.

In terms of the atomic radius R, the area of each of the 6 equilateral triangles that have been drawn is $R^2\sqrt{3}$, or the total area of the plane shown is $6R^2\sqrt{3}$. And the planar density for this (0001) plane is equal to

$$PD_{0001} \quad \frac{\text{number of atoms centered on (0001) pl}}{\text{area of (0001) plane}}$$

$$\frac{3\text{ atoms}}{6R^2\sqrt{3}} \quad \frac{1}{2R^2\sqrt{3}}$$

(b) From the table inside the front cover, the atomic radius for magnesium is 0.160 nm. Therefore, the planar density for the (0001) plane is

$$PD_{0001}(\text{Mg}) \quad \frac{1}{2R^2\sqrt{3}} \quad \frac{1}{2(0.160\text{ nm})^2\sqrt{3}} \quad 11.28\text{ nm}^{2} \quad 1.128\text{ u}10^{19}\text{ m}^{2}$$

Polycrystalline Materials

3.57 Explain why the properties of polycrystalline materials are most often isotropic.

Solution

Although each individual grain in a polycrystalline material may be anisotropic, if the grains have random orientations, then the solid aggregate of the many anisotropic grains will behave isotropically.

X-ray Diffraction: Determination of Crystal Structures

3.58 Using the data for molybdenum in Table 3.1, compute the interplanar spacing for the (111) set of planes.

Solution

From the Table 3.1, molybdenum has a BCC crystal structure and an atomic radius of 0.1363 nm. Using Equation (3.3), the lattice parameter *a* may be computed as

$$a = \frac{4R}{\sqrt{3}} = \frac{(4)(0.1363\ \text{nm})}{\sqrt{3}} = 0.3148\ \text{nm}$$

Now, the interplanar spacing d_{111} maybe determined using Equation 3.14 as

$$d_{111} = \frac{a}{\sqrt{(1)^2 + (1)^2 + (1)^2}} = \frac{0.3148\ \text{nm}}{\sqrt{3}} = 0.1817\ \text{nm}$$

3.59 Determine the expected diffraction angle for the first-order reflection from the (113) set of planes for FCC platinum when monochromatic radiation of wavelength 0.1542 nm is used.

Solution

We first calculate the lattice parameter using Equation 3.1 and the value of *R* (0.1387 nm) cited in Table 3.1, as follows:

$$a = 2R\sqrt{2} = (2)(0.1387\ \text{nm})(\sqrt{2}) = 0.3923\ \text{nm}$$

Next, the interplanar spacing for the (113) set of planes may be determined using Equation 3.14 according to

$$d_{113} = \frac{a}{\sqrt{(1)^2 + (1)^2 + (3)^2}} = \frac{0.3923\ \text{nm}}{\sqrt{11}} = 0.1183\ \text{nm}$$

And finally, employment of Equation 3.13 yields the diffraction angle as

$$\sin\theta = \frac{n\lambda}{2d_{113}} = \frac{(1)(0.1542\ \text{nm})}{(2)(0.1183\ \text{nm})} = 0.652$$

Which leads to

$$\theta = \sin^{-1}(0.652) = 40.69^\circ$$

And, finally

$$2\theta = (2)(40.69^\circ) = 81.38$$

3.60 Using the data for aluminum in Table 3.1, compute the interplanar spacings for the (110) and (221) sets of planes.

Solution

From the table, aluminum has an FCC crystal structure and an atomic radius of 0.1431 nm. Using Equation 3.1 the lattice parameter, *a*, may be computed as

$$a = 2R\sqrt{2} = (2)(0.1431\ \text{nm})(\sqrt{2}) = 0.4047\ \text{nm}$$

Now, the d_{110} interplanar spacing may be determined using Equation 3.14 as

$$d_{110} = \frac{a}{\sqrt{(1)^2 + (1)^2 + (0)^2}} = \frac{0.4047\ \text{nm}}{\sqrt{2}} = 0.2862\ \text{nm}$$

And, similarly for d_{221}

$$d_{221} = \frac{a}{\sqrt{(2)^2 + (2)^2 + (1)^2}} = \frac{0.4047\ \text{nm}}{\sqrt{9}} = 0.1349\ \text{nm}$$

3.61 The metal iridium has an FCC crystal structure. If the angle of diffraction for the (220) set of planes occurs at 69.22° (first-order reflection) when monochromatic x-radiation having a wavelength of 0.1542 nm is used, compute (a) the interplanar spacing for this set of planes, and (b) the atomic radius for an iridium atom.

Solution

(a) From the data given in the problem, and realizing that 69.22° = 2θ, the interplanar spacing for the (220) set of planes for iridium may be computed using Equation 3.13 as

$$d_{220} = \frac{n\lambda}{2\sin\theta} = \frac{(1)(0.1542\ \text{nm})}{(2)\left(\sin\frac{69.22^\circ}{2}\right)} = 0.1357\ \text{nm}$$

(b) In order to compute the atomic radius we must first determine the lattice parameter, *a*, using Equation 3.14, and then *R* from Equation 3.1 since Ir has an FCC crystal structure. Therefore,

$$a = d_{220}\sqrt{(2)^2 + (2)^2 + (0)^2} = (0.1357\ \text{nm})\left(\sqrt{8}\right) = 0.3838\ \text{nm}$$

And, from Equation 3.1

$$R = \frac{a}{2\sqrt{2}} = \frac{0.3838\ \text{nm}}{2\sqrt{2}} = 0.1357\ \text{nm}$$

3.62 The metal rubidium has a BCC crystal structure. If the angle of diffraction for the (321) set of planes occurs at 27.00° (first-order reflection) when monochromatic x-radiation having a wavelength of 0.0711 nm is used, compute (a) the interplanar spacing for this set of planes, and (b) the atomic radius for the rubidium atom.

<u>Solution</u>

(a) From the data given in the problem, and realizing that 27.00° = 2θ, the interplanar spacing for the (321) set of planes for Rb may be computed using Equation 3.13 as follows:

$$d_{321} = \frac{n\lambda}{2\sin\theta} = \frac{(1)(0.0711\ \text{nm})}{(2)\left(\sin\dfrac{27.00°}{2}\right)} = 0.1523\ \text{nm}$$

(b) In order to compute the atomic radius we must first determine the lattice parameter, *a*, using Equation 3.14, and then *R* from Equation 3.3 since Rb has a BCC crystal structure. Therefore,

$$a = d_{321}\sqrt{(3)^2 + (2)^2 + (1)^2} = (0.1523\ \text{nm})\left(\sqrt{14}\right) = 0.5700\ \text{nm}$$

And, from Equation 3.3

$$R = \frac{a\sqrt{3}}{4} = \frac{(0.5700\ \text{nm})\sqrt{3}}{4} = 0.2468\ \text{nm}$$

3.63 For which set of crystallographic planes will a first-order diffraction peak occur at a diffraction angle of 46.21° for BCC iron when monochromatic radiation having a wavelength of 0.0711 nm is used?

Solution

The first step to solve this problem is to compute the interplanar spacing using Equation 3.13. Thus,

$$d_{hkl} = \frac{n\lambda}{2\sin\theta} = \frac{(1)(0.0711\ \text{nm})}{(2)\left(\sin\frac{46.21°}{2}\right)} = 0.0906\ \text{nm}$$

Now, employment of both Equations 3.14 and 3.3 (since Fe's crystal structure is BCC), and the value of R for iron from Table 3.1 (0.1241 nm) leads to

$$\sqrt{h^2 + k^2 + l^2} = \frac{a}{d_{hkl}} = \frac{4R}{d_{hkl}\sqrt{3}}$$

$$= \frac{(4)(0.1241\ \text{nm})}{(0.0906\ \text{nm})(\sqrt{3})} = 3.163$$

This means that

$$h^2 + k^2 + l^2 = (3.163)^2 = 10.0$$

By trial and error, the only three integers having a sum that is even, and the sum of the squares of which equals 10.0 are 3, 1, and 0. Therefore, the set of planes responsible for this diffraction peak are the (310) ones.

3.64 Figure 3.22 shows an x-ray diffraction pattern for α-iron taken using a diffractometer and monochromatic x-radiation having a wavelength of 0.1542 nm; each diffraction peak on the pattern has been indexed. Compute the interplanar spacing for each set of planes indexed; also determine the lattice parameter of Fe for each of the peaks.

Solution

For each peak, in order to compute the interplanar spacing and the lattice parameter we must employ Equations 3.14 and 3.13, respectively. The first peak of Figure 3.22, which results from diffraction by the (110) set of planes, occurs at $\theta =$ °; the corresponding interplanar spacing for this set of planes, using Equation 3.13, is equal to

$$d_{110} = \frac{n\lambda}{2\sin\theta} = \frac{(1)(0.1542\ \text{nm})}{(2)\sin\left(\frac{45.0°}{2}\right)} = 0.2015\ \text{nm}$$

And, from Equation 3.14, the lattice parameter *a* is determined as

$$a = d_{hkl}\sqrt{(h)^2 + (k)^2 + (l)^2} = d_{110}\sqrt{(1)^2 + (1)^2 + (0)^2}$$

$$= (0.2015\ \text{nm})\sqrt{2} = 0.2850\ \text{nm}$$

Similar computations are made for the other peaks which results are tabulated below:

Peak Index	2 T	d_{hkl}(nm)	a (nm)
200	65.1	0.1433	0.2866
211	82.8	0.1166	0.2856

3.65 The diffraction peaks shown in Figure 3.22 are indexed according to the reflection rules for BCC (i.e., the sum h + k + l must be even). Cite the h, k, and l indices for the first four diffraction peaks for FCC crystals consistent with h, k, and l all being either odd or even.

Solution

The first four diffraction peaks that will occur for FCC consistent with h, k, and l all being odd or even are (111), (200), (220), and (311).

3.66 Figure 3.25 shows the first four peaks of the x-ray diffraction pattern for copper, which has an FCC crystal structure; monochromatic x-radiation having a wavelength of 0.1542 nm was used.

(a) Index (i.e., give h, k, and l indices) for each of these peaks.

(b) Determine the interplanar spacing for each of the peaks.

(c) For each peak, determine the atomic radius for Cu and compare these with the value presented in Table 3.1.

Solution

(a) Since Cu has an FCC crystal structure, only those peaks for which h, k, and l are all either odd or even will appear. Therefore, the first peak results by diffraction from (111) planes.

(b) For each peak, in order to calculate the interplanar spacing we must employ Equation 3.13. For the first peak which occurs at 43.8°

$$d_{111} = \frac{n\lambda}{2\sin\theta} = \frac{(1)(0.1542\text{ nm})}{(2)\sin\left(\frac{43.8°}{2}\right)} = 0.2067\text{ nm}$$

(c) Employment of Equations 3.14 and 3.1 is necessary for the computation of R for Cu as

$$R = \frac{a}{2\sqrt{2}} = \frac{(d_{hkl})\sqrt{(h)^2 + (k)^2 + (l)^2}}{2\sqrt{2}}$$

$$= \frac{(0.2067\text{nm})\sqrt{(1)^2 + (1)^2 + (1)^2}}{2\sqrt{2}}$$

$$= 0.1266\text{ nm}$$

Similar computations are made for the other peaks which results are tabulated below:

Peak Index	2 T	d_{hkl}(nm)	R (nm)
200	50.8	0.1797	0.1271
220	74.4	0.1275	0.1275
311	90.4	0.1087	0.1274

Noncrystalline Solids

3.67 Would you expect a material in which the atomic bonding is predominantly ionic in nature to be more or less likely to form a noncrystalline solid upon solidification than a covalent material? Why? (See Section 2.6.)

Solution

A material in which atomic bonding is predominantly ionic in nature is less likely to form a noncrystalline solid upon solidification than a covalent material because covalent bonds are directional whereas ionic bonds are nondirectional; it is more difficult for the atoms in a covalent material to assume positions giving rise to an ordered structure.

CHAPTER 4

IMPERFECTIONS IN SOLIDS

PROBLEM SOLUTIONS

Vacancies and Self-Interstitials

4.1 Calculate the fraction of atom sites that are vacant for lead at its melting temperature of 327°C (600 K). Assume an energy for vacancy formation of 0.55 eV/atom.

Solution

In order to compute the fraction of atom sites that are vacant in lead at 600 K, we must employ Equation 4.1. As stated in the problem, Q_v = 0.55 eV/atom. Thus,

$$\frac{N_v}{N} = \exp\left(-\frac{Q_v}{kT}\right) = \exp\left[-\frac{0.55\ \text{eV/atom}}{(8.62 \times 10^{-5}\ \text{eV/atom-K})(600\ \text{K})}\right]$$

$$= 2.41 \times 10^{-5}$$

4.2 Calculate the number of vacancies per cubic meter in iron at 850°C. The energy for vacancy formation is 1.08 eV/atom. Furthermore, the density and atomic weight for Fe are 7.65 g/cm^3 and 55.85 g/mol, respectively.

Solution

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:

$$N_v = N \exp\left(-\frac{Q_v}{kT}\right) = \frac{N_A\,\rho_{Fe}}{A_{Fe}} \exp\left(-\frac{Q_v}{kT}\right)$$

And incorporation of values of the parameters provided in the problem statement into the above equation leads to

$$N_v = \frac{(6.022 \times 10^{23}\ \text{atoms/mol})(7.65\ \text{g/cm}^3)}{55.85\ \text{g/mol}} \exp\left[-\frac{1.08\ \text{eV/atom}}{(8.62 \times 10^{-5}\ \text{eV/atom-K})(850^\circ\text{C} + 273\ \text{K})}\right]$$

$$= 1.18 \times 10^{18}\ \text{cm}^{-3} = 1.18 \times 10^{24}\ \text{m}^{-3}$$

4.3 Calculate the activation energy for vacancy formation in aluminum, given that the equilibrium number of vacancies at 500°C (773 K) is 7.57×10^{23} m^{-3}. The atomic weight and density (at 500°C) for aluminum are, respectively, 26.98 g/mol and 2.62 g/cm^3.

Solution

Upon examination of Equation 4.1, all parameters besides Q_v are given except N, the total number of atomic sites. However, N is related to the density, (ρ_{Al}), Avogadro's number (N_A), and the atomic weight (A_{Al}) according to Equation 4.2 as

$$N = \frac{N_A \rho_{Al}}{A_{Al}}$$

$$= \frac{(6.022 \times 10^{23} \text{ atoms/mol})(2.62 \text{ g/cm}^3)}{26.98 \text{ g/mol}}$$

$$= 5.85 \times 10^{22} \text{ atoms/cm}^3 = 5.85 \times 10^{28} \text{ atoms/m}^3$$

Now, taking natural logarithms of both sides of Equation 4.1,

$$\ln N_v = \ln N - \frac{Q_v}{kT}$$

and, after some algebraic manipulation

$$Q_v = -kT \ln\left(\frac{N_v}{N}\right)$$

$$= -(8.62 \times 10^{-5} \text{ eV/atom-K})(500°\text{C} + 273 \text{ K}) \ln\left[\frac{7.57 \times 10^{23} \text{ m}^{-3}}{5.85 \times 10^{28} \text{ m}^{-3}}\right]$$

$$= 0.75 \text{ eV/atom}$$

Impurities in Solids

4.4 Below, atomic radius, crystal structure, electronegativity, and the most common valence are tabulated, for several elements; for those that are nonmetals, only atomic radii are indicated.

Element	Atomic Radius (nm)	Crystal Structure	Electronegativity	Valence
Cu	0.1278	FCC	1.9	+2
C	0.071			
H	0.046			
O	0.060			
Ag	0.1445	FCC	1.9	+1
Al	0.1431	FCC	1.5	+3
Co	0.1253	HCP	1.8	+2
Cr	0.1249	BCC	1.6	+3
Fe	0.1241	BCC	1.8	+2
Ni	0.1246	FCC	1.8	+2
Pd	0.1376	FCC	2.2	+2
Pt	0.1387	FCC	2.2	+2
Zn	0.1332	HCP	1.6	+2

Which of these elements would you expect to form the following with copper:

(a) A substitutional solid solution having complete solubility

(b) A substitutional solid solution of incomplete solubility

(c) An interstitial solid solution

Solution

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 ('R%) must be less than ±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.

Element	'R%	Crystal Structure	'Electro-negativity	Valence
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. At elevated temperatures Co and Fe experience allotropic transformations to the FCC crystal structure, and thus display complete solid solubility at these temperatures.

(b) Ag, Al, Co, Cr, Fe, and Zn form substitutional solid solutions of incomplete solubility. All these metals have either BCC or HCP crystal structures, and/or the difference between their atomic radii and that for Cu are greater than ±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.

4.5 For both FCC and BCC crystal structures, there are two different types of interstitial sites. In each case, one site is larger than the other, and is normally occupied by impurity atoms. For FCC, this larger one is located at the center of each edge of the unit cell; it is termed an octahedral interstitial site. On the other hand, with BCC the larger site type is found at $0\frac{1}{2}\frac{1}{4}$ positions—that is, lying on {100} faces, and situated midway between two unit cell edges on this face and one-quarter of the distance between the other two unit cell edges; it is termed a tetrahedral interstitial site. For both FCC and BCC crystal structures, compute the radius r of an impurity atom that will just fit into one of these sites in terms of the atomic radius R of the host atom.

Solution

In the drawing below is shown the atoms on the (100) face of an FCC unit cell; the interstitial site is at the center of the edge.

The diameter of an atom that will just fit into this site (2r) is just the difference between that unit cell edge length (a) and the radii of the two host atoms that are located on either side of the site (R); that is

$$2r = a - 2R$$

However, for FCC a is related to R according to Equation 3.1 as $a = 2R\sqrt{2}$; therefore, solving for r from the above equation gives

$$r = \frac{a - 2R}{2} = \frac{2R\sqrt{2} - 2R}{2} = 0.41R$$

A (100) face of a BCC unit cell is shown below.

The interstitial atom that just fits into this interstitial site is shown by the small circle. It is situated in the plane of this (100) face, midway between the two vertical unit cell edges, and one quarter of the distance between the bottom and top cell edges. From the right triangle that is defined by the three arrows we may write

$$\left(\frac{a}{2}\right)^2 + \left(\frac{a}{4}\right)^2 = (R \quad r)^2$$

However, from Equation 3.3, $a = \frac{4R}{\sqrt{3}}$, and, therefore, making this substitution, the above equation takes the form

$$\left(\frac{4R}{2\sqrt{3}}\right)^2 + \left(\frac{4R}{4\sqrt{3}}\right)^2 = R^2 + 2Rr + r^2$$

After rearrangement the following quadratic equation results:

$$r^2 + 2Rr \quad 0.667R^2 = 0$$

And upon solving for **r**:

$$r = \frac{-(2R) \pm \sqrt{(2R)^2 - (4)(1)(-0.667R^2)}}{2}$$

$$= \frac{-2R \pm 2.582R}{2}$$

And, finally

$$r(+) = \frac{-2R + 2.582R}{2} = 0.291R$$

$$r(-) = \frac{-2R - 2.582R}{2} = -2.291R$$

Of course, only the r(+) root is possible, and, therefore, r = 0.291R.

Thus, for a host atom of radius R, the size of an interstitial site for FCC is approximately 1.4 times that for BCC.

Specification of Composition

4.6 Derive the following equations:

(a) Equation 4.7a

(b) Equation 4.9a

(c) Equation 4.10a

(d) Equation 4.11b

Solution

(a) This problem asks that we derive Equation 4.7a. To begin, C_1 is defined according to Equation 4.3 as

$$C_1 = \frac{m_1}{m_1 + m_2} \times 100$$

or, equivalently

$$C_1 = \frac{m_1'}{m_1' + m_2'} \times 100$$

where the primed m's indicate masses in grams. From Equation 4.4 we may write

$$m_1' = n_{m1} A_1$$

$$m_2' = n_{m2} A_2$$

And, substitution into the C_1 expression above

$$C_1 = \frac{n_{m1} A_1}{n_{m1} A_1 + n_{m2} A_2} \times 100$$

From Equation 4.5 it is the case that

$$n_{m1} = \frac{C_1' (n_{m1} + n_{m2})}{100}$$

$$n_{m2} = \frac{C_2'\left(n_{m1} \quad n_{m2}\right)}{100}$$

And substitution of these expressions into the above equation leads to

$$C_1 = \frac{C_1' A_1}{C_1' A_1 \quad C_2' A_2} \; u \; 100$$

which is just Equation 4.7a.

(b) This problem asks that we derive Equation 4.9a. To begin, C_1'' is defined as the mass of component 1 per unit volume of alloy, or

$$C_1'' = \frac{m_1}{V}$$

If we assume that the total alloy volume V is equal to the sum of the volumes of the two constituents--i.e., $V = V_1 + V_2$--then

$$C_1'' = \frac{m_1}{V_1 \quad V_2}$$

Furthermore, the volume of each constituent is related to its density and mass as

$$V_1 = \frac{m_1}{U_1}$$

$$V_2 = \frac{m_2}{U_2}$$

This leads to

$$C_1'' = \frac{m_1}{\dfrac{m_1}{U_1} \quad \dfrac{m_2}{U_2}}$$

From Equation 4.3, m_1 and m_2 may be expressed as follows:

$$m_1 = \frac{C_1(m_1 + m_2)}{100}$$

$$m_2 = \frac{C_2(m_1 + m_2)}{100}$$

Substitution of these equations into the preceding expression yields

$$C_1'' = \frac{\dfrac{C_1(m_1 + m_2)}{100}}{\dfrac{\dfrac{C_1(m_1 + m_2)}{100}}{\rho_1} + \dfrac{\dfrac{C_2(m_1 + m_2)}{100}}{\rho_2}}$$

$$= \frac{C_1}{\dfrac{C_1}{\rho_1} + \dfrac{C_2}{\rho_2}}$$

If the densities ρ_1 and ρ_2 are given in units of g/cm^3, then conversion to units of kg/m^3 requires that we multiply this equation by 10^3, inasmuch as

$$1 \text{ g/cm}^3 = 10^3 \text{ kg/m}^3$$

Therefore, the previous equation takes the form

$$C_1'' = \frac{C_1}{\dfrac{C_1}{\rho_1} + \dfrac{C_2}{\rho_2}} \times 10^3$$

which is the desired expression.

(c) Now we are asked to derive Equation 4.10a. The density of an alloy ρ_{ave} is just the total alloy mass M divided by its volume V

$$\rho_{ave} = \frac{M}{V}$$

Or, in terms of the component elements 1 and 2

$$U_{ave} = \frac{m_1 \quad m_2}{V_1 \quad V_2}$$

[Note: here it is assumed that the total alloy volume is equal to the separate volumes of the individual components, which is only an approximation; normally V will not be exactly equal to (V_1 + V_2)].

Each of V_1 and V_2 may be expressed in terms of its mass and density as,

$$V_1 \quad \frac{m_1}{U_1}$$

$$V_2 \quad \frac{m_2}{U_2}$$

When these expressions are substituted into the above equation, we get

$$U_{ave} = \frac{m_1 \quad m_2}{\dfrac{m_1}{U_1} \quad \dfrac{m_2}{U_2}}$$

Furthermore, from Equation 4.3

$$m_1 = \frac{C_1 (m_1 \quad m_2)}{100}$$

$$m_2 = \frac{C_2 (m_1 \quad m_2)}{100}$$

Which, when substituted into the above U_{ave} expression yields

$$U_{ave} = \frac{m_1 \quad m_2}{\dfrac{\dfrac{C_1 (m_1 \quad m_2)}{100}}{U_1} \quad \dfrac{\dfrac{C_2 (m_1 \quad m_2)}{100}}{U_2}}$$

And, finally, this equation reduces to

$$= \frac{100}{\frac{C_1}{U_1} \quad \frac{C_2}{U_2}}$$

(d) And, finally, the derivation of Equation 4.11b for A_{ave} is requested. The alloy average molecular weight is just the ratio of total alloy mass in grams M' and the total number of moles in the alloy N_m. That is

$$A_{ave} = \frac{MÕ}{N_m} = \frac{m_1' \quad m_2'}{n_{m1} \quad n_{m2}}$$

But using Equation 4.4 we may write

$$m_1' = n_{m1} A_1$$

$$m_2' = n_{m2} A_2$$

Which, when substituted into the above A_{ave} expression yields

$$A_{ave} = \frac{M'}{N_m} = \frac{n_{m1} A_1 \quad n_{m2} A_2}{n_{m1} \quad n_{m2}}$$

Furthermore, from Equation 4.5

$$n_{m1} = \frac{C_1' (n_{m1} \quad n_{m2})}{100}$$

$$n_{m2} = \frac{C_2' (n_{m1} \quad n_{m2})}{100}$$

Thus, substitution of these expressions into the above equation for A_{ave} yields

$$A_{ave} = \frac{\frac{C_1' A_1 (n_{m1} \quad n_{m2})}{100} \quad \frac{C_2' A_2 (n_{m1} \quad n_{m2})}{100}}{n_{m1} \quad n_{m2}}$$

$$= \frac{C_1' A_1 \quad C_2' A_2}{100}$$

which is the desired result.

4.7 What is the composition, in atom percent, of an alloy that consists of 30 wt% Zn and 70 wt% Cu?

Solution

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

$$C'_{Zn} = \frac{C_{Zn}A_{Cu}}{C_{Zn}A_{Cu} \quad C_{Cu}A_{Zn}} \times 100$$

$$= \frac{(30)(63.55 \text{ g/mol})}{(30)(63.55 \text{ g/mol}) \quad (70)(65.41 \text{ g/mol})} \times 100$$

= 29.4 at%

$$C'_{Cu} = \frac{C_{Cu}A_{Zn}}{C_{Zn}A_{Cu} \quad C_{Cu}A_{Zn}} \times 100$$

$$= \frac{(70)(65.41 \text{ g/mol})}{(30)(63.55 \text{ g/mol}) \quad (70)(65.41 \text{ g/mol})} \times 100$$

= 70.6 at%

4.8 What is the composition, in weight percent, of an alloy that consists of 6 at% Pb and 94 at% Sn?

Solution

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

$$C_{Pb} = \frac{C'_{Pb}A_{Pb}}{C'_{Pb}A_{Pb} \quad C'_{Sn}A_{Sn}} \times 100$$

$$= \frac{(6)(207.2\ \mathrm{g/mol})}{(6)(207.2\ \mathrm{g/mol}) \quad (94)(118.71\ \mathrm{g/mol})} \times 100$$

$$= 10.0\ \mathrm{wt\%}$$

$$C_{Sn} = \frac{C'_{Sn}A_{Sn}}{C'_{Pb}A_{Pb} \quad C'_{Sn}A_{Sn}} \times 100$$

$$= \frac{(94)(118.71\ \mathrm{g/mol})}{(6)(207.2\ \mathrm{g/mol}) \quad (94)(118.71\ \mathrm{g/mol})} \times 100$$

$$= 90.0\ \mathrm{wt\%}$$

4.9 Calculate the composition, in weight percent, of an alloy that contains 218.0 kg titanium, 14.6 kg of aluminum, and 9.7 kg of vanadium.

Solution

The concentration, in weight percent, of an element in an alloy may be computed using a modified form of Equation 4.3. For this alloy, the concentration of titanium (C_{Ti}) is just

$$C_{Ti} = \frac{m_{Ti}}{m_{Ti} \quad m_{Al} \quad m_V} \times 100$$

$$= \frac{218\,\text{kg}}{218\,\text{kg} \quad 14.6\,\text{kg} \quad 9.7\,\text{kg}} \times 100 = 89.97\ \text{wt\%}$$

Similarly, for aluminum

$$C_{Al} = \frac{14.6\,\text{kg}}{218\,\text{kg} \quad 14.6\,\text{kg} \quad 9.7\,\text{kg}} \times 100 = 6.03\ \text{wt\%}$$

And for vanadium

$$C_V = \frac{9.7\,\text{kg}}{218\,\text{kg} \quad 14.6\,\text{kg} \quad 9.7\,\text{kg}} \times 100 = 4.00\ \text{wt\%}$$

4.10 What is the composition, in atom percent, of an alloy that contains 98 g tin and 65 g of lead?

Solution

The concentration of an element in an alloy, in atom percent, may be computed using Equation 4.5. However, it first becomes necessary to compute the number of moles of both Sn and Pb, using Equation 4.4. Thus, the number of moles of Sn is just

$$n_{m_{Sn}} = \frac{m'_{Sn}}{A_{Sn}} = \frac{98\text{ g}}{118.71\text{ g/mol}} = 0.826\text{ mol}$$

Likewise, for Pb

$$n_{m_{Pb}} = \frac{65\text{ g}}{207.2\text{ g/mol}} = 0.314\text{ mo}$$

Now, use of Equation 4.5 yields

$$C'_{Sn} = \frac{n_{m_{Sn}}}{n_{m_{Sn}} + n_{m_{Pb}}} \times 100$$

$$= \frac{0.826\text{ mol}}{0.826\text{ mol} + 0.314\text{ mol}} \times 100 = 72.5\text{ at\%}$$

Also,

$$C'_{Pb} = \; = \frac{0.314\text{ mol}}{0.826\text{ mol} + 0.314\text{ mol}} \times 100 = 27.5\text{ at\%}$$

4.11 What is the composition, in atom percent, of an alloy that contains 99.7 lb_m copper, 102 lb_m zinc, and 2.1 lb_m lead?

Solution

In this problem we are asked to determine the concentrations, in atom percent, of the Cu-Zn-Pb alloy. It is first necessary to convert the amounts of Cu, Zn, and Pb into grams.

$$m'_{Cu} = (99.7\ \text{lb}_m)(453.6\ \text{g/lb}_m) = 45{,}224\ \text{g}$$

$$m'_{Zn} = (102\ \text{lb}_m)(453.6\ \text{g/lb}_m) = 46{,}267\ \text{g}$$

$$m'_{Pb} = (2.1\ \text{lb}_m)(453.6\ \text{g/lb}_m) = 953\ \text{g}$$

These masses must next be converted into moles (Equation 4.4), as

$$n_{m_{Cu}} = \frac{m'_{Cu}}{A_{Cu}} = \frac{45{,}224\ \text{g}}{63.55\ \text{g/mol}} = 711.6\ \text{mo}$$

$$n_{m_{Zn}} = \frac{46{,}267\ \text{g}}{65.41\ \text{g/mol}} = 707.3\ \text{mo}$$

$$n_{m_{Pb}} = \frac{953\ \text{g}}{207.2\ \text{g/mol}} = 4.6\ \text{mo}$$

Now, employment of a modified form of Equation 4.5, gives

$$C'_{Cu} = \frac{n_{m_{Cu}}}{n_{m_{Cu}} \quad n_{m_{Zn}} \quad n_{m_{Pb}}} \times 100$$

$$= \frac{711.6\ \text{mol}}{711.6\ \text{mol} \quad 707.3\ \text{mol} \quad 4.6\ \text{mol}} \times 100 = 50.0\ \text{at\%}$$

$$C'_{Zn} = \frac{707.3\ \text{mol}}{711.6\ \text{mol} \quad 707.3\ \text{mol} \quad 4.6\ \text{mol}} \times 100 = 49.7\ \text{at\%}$$

$$C'_{Pb} = \frac{4.6\,\text{mol}}{711.6\,\text{mol} \quad 707.3\,\text{mol} \quad 4.6\,\text{mol}} \times 100 = 0.3\ \text{at\%}$$

4.12 What is the composition, in atom percent, of an alloy that consists of 97 wt% Fe and 3 wt% Si?

Solution

We are asked to compute the composition of an Fe-Si alloy in atom percent. Employment of Equation 4.6 leads to

$$C'_{Fe} = \frac{C_{Fe}A_{Si}}{C_{Fe}A_{Si} + C_{Si}A_{Fe}} \times 100$$

$$= \frac{97(28.09\ g/mol)}{97(28.09\ g/mol) + 3(55.85\ g/mol)} \times 100$$

$$= 94.2\ \text{at\%}$$

$$C'_{Si} = \frac{C_{Si}A_{Fe}}{C_{Si}A_{Fe} + C_{Fe}A_{Si}} \times 100$$

$$= \frac{3(55.85\ g/mol)}{3(55.85\ g/mol) + 97(28.09\ g/mol)} \times 100$$

$$= 5.8\ \text{at\%}$$

4.13 Convert the atom percent composition in Problem 4.11 to weight percent.

Solution

The composition in atom percent for Problem 4.11 is 50.0 at% Cu, 49.7 at% Zn, and 0.3 at% Pb. Modification of Equation 4.7 to take into account a three-component alloy leads to the following

$$C_{Cu} = \frac{C'_{Cu}A_{Cu}}{C'_{Cu}A_{Cu} \quad C'_{Zn}A_{Zn} \quad C'_{Pb}A_{Pb}} \times 100$$

$$= \frac{(50.0)(63.55\text{ g/mol})}{(50.0)(63.55\text{ g/mol}) \quad (49.7)(65.41\text{ g/mol}) \quad (0.3)(207.2\text{ g/mol})} \times 100$$

= 49.0 wt%

$$C_{Zn} = \frac{C'_{Zn}A_{Zn}}{C'_{Cu}A_{Cu} \quad C'_{Zn}A_{Zn} \quad C'_{Pb}A_{Pb}} \times 100$$

$$= \frac{(49.7)(65.41\text{ g/mol})}{(50.0)(63.55\text{ g/mol}) \quad (49.7)(65.41\text{ g/mol}) \quad (0.3)(207.2\text{ g/mol})} \times 100$$

= 50.1 wt%

$$C_{Pb} = \frac{C'_{Pb}A_{Pb}}{C'_{Cu}A_{Cu} \quad C'_{Zn}A_{Zn} \quad C'_{Pb}A_{Pb}} \times 100$$

$$= \frac{(0.3)(207.2\text{ g/mol})}{(50.0)(63.55\text{ g/mol}) \quad (49.7)(65.41\text{ g/mol}) \quad (0.3)(207.2\text{ g/mol})} \times 100$$

= 1.0 wt%

4.14 Calculate the number of atoms per cubic meter in aluminum.

Solution

In order to solve this problem, one must employ Equation 4.2,

$$N = \frac{N_A \; U_{Al}}{A_{Al}}$$

The density of Al (from the table inside of the front cover) is 2.71 g/cm^3, while its atomic weight is 26.98 g/mol. Thus,

$$N = \frac{(6.022 \; u \, 10^{23} \; \text{atoms/mol})(2.71 \, \text{g/cm}^3)}{26.98 \, \text{g/mol}}$$

$$= 6.05 \; u 10^{22} \; \text{atoms/cm}^3 = 6.05 \; u 10^{28} \; \text{atoms/m}^3$$

4.15 The concentration of carbon in an iron-carbon alloy is 0.15 wt%. What is the concentration in kilograms of carbon per cubic meter of alloy?

Solution

In order to compute the concentration in kg/m^3 of C in a 0.15 wt% C-99.85 wt% Fe alloy we must employ Equation 4.9 as

$$C''_C = \frac{C_C}{\dfrac{C_C}{\rho_C} + \dfrac{C_{Fe}}{\rho_{Fe}}} \times 10^3$$

From inside the front cover, densities for carbon and iron are 2.25 and 7.87 g/cm^3, respectively; and, therefore

$$C''_C = \frac{0.15}{\dfrac{0.15}{2.25\,\text{g/cm}^3} + \dfrac{99.85}{7.87\,\text{g/cm}^3}} \times 10^3$$

$$= 11.8\ \text{kg/m}^3$$

4.16 Determine the approximate density of a high-leaded brass that has a composition of 64.5 wt% Cu, 33.5 wt% Zn, and 2.0 wt% Pb.

Solution

In order to solve this problem, Equation 4.10a is modified to take the following form:

$$\rho_{ave} = \frac{100}{\dfrac{C_{Cu}}{\rho_{Cu}} + \dfrac{C_{Zn}}{\rho_{Zn}} + \dfrac{C_{Pb}}{\rho_{Pb}}}$$

And, using the density values for Cu, Zn, and Pb—i.e., 8.94 g/cm^3, 7.13 g/cm^3, and 11.35 g/cm^3—(as taken from inside the front cover of the text), the density is computed as follows:

$$\rho_{ave} = \frac{100}{\dfrac{64.5\,\text{wt\%}}{8.94\,\text{g/cm}^3} + \dfrac{33.5\,\text{wt\%}}{7.13\,\text{g/cm}^3} + \dfrac{2.0\,\text{wt\%}}{11.35\,\text{g/cm}^3}}$$

$$= 8.27\ \text{g/cm}^3$$

4.17 Calculate the unit cell edge length for an 85 wt% Fe-15 wt% V alloy. All of the vanadium is in solid solution, and, at room temperature the crystal structure for this alloy is BCC.

Solution

In order to solve this problem it is necessary to employ Equation 3.5; in this expression density and atomic weight will be averages for the alloy—that is

$$\rho_{ave} = \frac{nA_{ave}}{V_C N_A}$$

Inasmuch as the unit cell is cubic, then $V_C = a^3$, then

$$\rho_{ave} = \frac{nA_{ave}}{a^3 N_A}$$

And solving this equation for the unit cell edge length, leads to

$$a = \left(\frac{nA_{ave}}{\rho_{ave} N_A}\right)^{1/3}$$

Expressions for A_{ave} and ρ_{ave} are found in Equations 4.11a and 4.10a, respectively, which, when incorporated into the above expression yields

$$a = \left[\frac{n\left(\dfrac{100}{\dfrac{C_{Fe}}{A_{Fe}} + \dfrac{C_V}{A_V}}\right)}{\left(\dfrac{100}{\dfrac{C_{Fe}}{\rho_{Fe}} + \dfrac{C_V}{\rho_V}}\right) N_A}\right]^{1/3}$$

Since the crystal structure is BCC, the value of n in the above expression is 2 atoms per unit cell. The atomic weights for Fe and V are 55.85 and 50.94 g/mol, respectively (Figure 2.6), whereas the densities for the Fe and V are 7.87 g/cm^3 and 6.10 g/cm^3 (from inside the front cover). Substitution of these, as well as the concentration values stipulated in the problem statement, into the above equation gives

$$a = \left[\frac{(2\ \text{atoms/unit cell})\left(\dfrac{100}{\dfrac{85\ \text{wt\%}}{55.85\ \text{g/mol}} + \dfrac{15\ \text{wt\%}}{50.94\ \text{g/mol}}}\right)}{\left(\dfrac{100}{\dfrac{85\ \text{wt\%}}{7.87\ \text{g/cm}^3} + \dfrac{15\ \text{wt\%}}{6.10\ \text{g/cm}^3}}\right)\left(6.022 \times 10^{23}\ \text{atoms/mol}\right)}\right]^{1/3}$$

$$= 2.89 \times 10^{-8}\ \text{cm} = 0.289\ \text{nm}$$

4.18 Some hypothetical alloy is composed of 12.5 wt% of metal A and 87.5 wt% of metal B. If the densities of metals A and B are 4.27 and 6.35 g/cm^3, respectively, whereas their respective atomic weights are 61.4 and 125.7 g/mol, determine whether the crystal structure for this alloy is simple cubic, face-centered cubic, or body-centered cubic. Assume a unit cell edge length of 0.395 nm.

Solution

In order to solve this problem it is necessary to employ Equation 3.5; in this expression density and atomic weight will be averages for the alloy—that is

$$\rho_{ave} = \frac{nA_{ave}}{V_C N_A}$$

Inasmuch as for each of the possible crystal structures, the unit cell is cubic, then $V_C = a^3$, or

$$\rho_{ave} = \frac{nA_{ave}}{a^3 N_A}$$

And, in order to determine the crystal structure it is necessary to solve for n, the number of atoms per unit cell. For $n=1$, the crystal structure is simple cubic, whereas for values of 2 and 4, the crystal structure will be either BCC or FCC, respectively. When we solve the above expression for n the result is as follows:

$$n = \frac{\rho_{ave} a^3 N_A}{A_{ave}}$$

Expressions for A_{ave} and ρ_{ave} are found in Equations 4.11a and 4.10a, respectively, which, when incorporated into the above expression yields

$$n = \frac{\left(\dfrac{100}{\dfrac{C_A}{\rho_A} + \dfrac{C_B}{\rho_B}}\right) a^3 N_A}{\left(\dfrac{100}{\dfrac{C_A}{A_A} + \dfrac{C_B}{A_B}}\right)}$$

Substitution of the concentration values (i.e., C_A = 12.5 wt% and C_B = 87.5 wt%) as well as values for the other parameters given in the problem statement, into the above equation gives

$$n = \frac{\left[\dfrac{100}{\dfrac{12.5\text{ wt\%}}{4.27\text{ g/cm}^3} + \dfrac{87.5\text{ wt\%}}{6.35\text{ g/cm}^3}}\right]\left(3.95 \times 10^{-8}\text{ nm}\right)^3\left(6.022 \times 10^{23}\text{ atoms/mol}\right)}{\left[\dfrac{100}{\dfrac{12.5\text{ wt\%}}{61.4\text{ g/mol}} + \dfrac{87.5\text{ wt\%}}{125.7\text{ g/mol}}}\right]}$$

$$= 2.00 \text{ atoms/unit cell}$$

Therefore, on the basis of this value, the crystal structure is body-centered cubic.

4.19 For a solid solution consisting of two elements (designated as 1 and 2), sometimes it is desirable to determine the number of atoms per cubic centimeter of one element in a solid solution, N_1, given the concentration of that element specified in weight percent, C_1. This computation is possible using the following expression:

$$N_1 \quad \frac{N_A C_1}{\frac{C_1 A_1}{U_1} \quad \frac{A_1}{U_2} 100 \quad C_1} \tag{4.18}$$

where

N_A = Avogadro's number

$!_1$ D Q G_2 = densities of the two elements

A_1 = the atomic weight of element 1

Derive Equation 4.18 using Equation 4.2 and expressions contained in Section 4.4.

Solution

This problem asks that we derive Equation 4.18, using other equations given in the chapter. The concentration of component 1 in atom percent $(C_1^{'})$ is just $100c_1^{'}$ where $c_1^{'}$ is the atom fraction of component 1. Furthermore, $c_1^{'}$ is defined as $c_1^{'} = N_1/N$ where N_1 and N are, respectively, the number of atoms of component 1 and total number of atoms per cubic centimeter. Thus, from the above discussion the following holds:

$$N_1 = \frac{C_1^{'} N}{100}$$

Substitution into this expression of the appropriate form of N from Equation 4.2 yields

$$N_1 = \frac{C_1^{'} N_A U_{ave}}{100 A_{ave}}$$

And, finally, substitution into this equation expressions for $C_1^{'}$ (Equation 4.6a), U_{ave} (Equation 4.10a), A_{ave} (Equation 4.11a), and realizing that C_2 € $(C_1 – 100)$, and after some algebraic manipulation we obtain the desired expression:

$$N_1 = \frac{N_A C_1}{\frac{C_1 A_1}{U_1} \quad \frac{A_1}{U_2}\left(100 \quad C_1\right)}$$

4.20 Gold forms a substitutional solid solution with silver. Compute the number of gold atoms per cubic centimeter for a silver-gold alloy that contains 10 wt% Au and 90 wt% Ag. The densities of pure gold and silver are 19.32 and 10.49 g/cm^3, respectively.

<u>Solution</u>

To solve this problem, employment of Equation 4.18 is necessary, using the following values:

$C_1 = C_{Au} = 10$ wt%
$\rho_1 = \rho_{Au} = 19.32$ g/cm^3
$\rho_2 = \rho_{Ag} = 10.49$ g/cm^3
$A_1 = A_{Au} = 196.97$ g/mol

Thus

$$N_{Au} = \frac{N_A C_{Au}}{\dfrac{C_{Au} A_{Au}}{\rho_{Au}} + \dfrac{A_{Au}}{\rho_{Ag}}\left(100 - C_{Au}\right)}$$

$$= \frac{\left(6.022 \times 10^{23} \text{ atoms/mol}\right)(10 \text{ wt\%})}{\dfrac{(10 \text{ wt\%})(196.97 \text{ g/mol})}{19.32 \text{ g/cm}^3} + \dfrac{196.97 \text{ g/mol}}{10.49 \text{ g/cm}^3}\left(100 - 10 \text{ wt\%}\right)}$$

$$= 3.36 \times 10^{21} \text{ atoms/cm}^3$$

4.21 Germanium forms a substitutional solid solution with silicon. Compute the number of germanium atoms per cubic centimeter for a germanium-silicon alloy that contains 15 wt% Ge and 85 wt% Si. The densities of pure germanium and silicon are 5.32 and 2.33 g/cm^3, respectively.

Solution

To solve this problem, employment of Equation 4.18 is necessary, using the following values:

$C_1 = C_{Ge} = 15$ wt%
$\rho_1 = \rho_{Ge} = 5.32$ g/cm^3
$\rho_2 = \rho_{Si} = 2.33$ g/cm^3
$A_1 = A_{Ge} = 72.64$ g/mol

Thus

$$N_{Ge} = \frac{N_A C_{Ge}}{\dfrac{C_{Ge} A_{Ge}}{\rho_{Ge}} + \dfrac{A_{Ge}}{\rho_{Si}}(100 - C_{Ge})}$$

$$= \frac{(6.022 \times 10^{23}\ \text{atoms/mol})\,(15\ \text{wt\%})}{\dfrac{(15\ \text{wt\%})(72.64\ \text{g/mol})}{5.32\ \text{g/cm}^3} + \dfrac{72.64\ \text{g/mol}}{2.33\ \text{g/cm}^3}(100 - 15\ \text{wt\%})}$$

$$= 3.16 \times 10^{21}\ \text{atoms/cm}^3$$

4.22 Sometimes it is desirable to be able to determine the weight percent of one element, C_1, that will produce a specified concentration in terms of the number of atoms per cubic centimeter, N_1, for an alloy composed of two types of atoms. This computation is possible using the following expression:

$$C_1 = \frac{100}{1 + \frac{N_A \rho_2}{N_1 A_1} - \frac{\rho_2}{\rho_1}} \tag{4.19}$$

where

N_A = Avogadro’s number

ρ_1 and ρ_2 = densities of the two elements

A_1 and A_2 = the atomic weights of the two elements

Derive Equation 4.19 using Equation 4.2 and expressions contained in Section 4.4.

Solution

The number of atoms of component 1 per cubic centimeter is just equal to the atom fraction of component 1 (c_1') times the total number of atoms per cubic centimeter in the alloy (N). Thus, using the equivalent of Equation 4.2, we may write

$$N_1 = c_1' N = \frac{c_1' N_A \rho_{ave}}{A_{ave}}$$

Realizing that

$$c_1' = \frac{C_1'}{100}$$

and

$$C_2' = 100 - C_1'$$

and substitution of the expressions for ρ_{ave} and A_{ave}, Equations 4.10b and 4.11b, respectively, leads to

$$N_1 = \frac{c_1' N_A \rho_{ave}}{A_{ave}}$$

$$= \frac{N_A C_1^{'} \; U_1 \; U_2}{C_1^{'} \; U_2 A_1 \quad \left(100 \quad C_1^{'}\right) U_1 A_2}$$

And, solving for $C_1^{'}$

$$C_1^{'} = \frac{100 \, N_1 \, U_1 \, A_2}{N_A \; U_1 \; U_2 \quad N_1 \; U_2 \, A_1 \quad N_1 \; U_1 \, A_2}$$

Substitution of this expression for $C_1^{'}$ into Equation 4.7a, which may be written in the following form

$$C_1 = \frac{C_1^{'} \, A_1}{C_1^{'} \, A_1 \quad C_2^{'} \, A_2} \; u \; 100$$

$$= \frac{C_1^{'} \, A_1}{C_1^{'} A_1 \quad \left(100 \quad C_1^{'}\right) A_2} \; u \; 100$$

yields

$$C_1 = \frac{100}{1 \quad \frac{N_A \; U_2}{N_1 \, A_1} \quad \frac{U_2}{U_1}}$$

the desired expression.

4.23 Molybdenum forms a substitutional solid solution with tungsten. Compute the weight percent of molybdenum that must be added to tungsten to yield an alloy that contains 1.0×10^{22} Mo atoms per cubic centimeter. The densities of pure Mo and W are 10.22 and 19.30 g/cm^3, respectively.

<u>Solution</u>

To solve this problem, employment of Equation 4.19 is necessary, using the following values:

$N_1 = N_{Mo} = 10^{22}$ atoms/cm^3
$\rho_1 = \rho_{Mo} = 10.22$ g/cm^3
$\rho_2 = \rho_W = 19.30$ g/cm^3
$A_1 = A_{Mo} = 95.94$ g/mol
$A_2 = A_W = 183.84$ g/mol

Thus

$$C_{Mo} = \frac{100}{1 + \dfrac{N_A \rho_W}{N_{Mo} A_{Mo}} - \dfrac{\rho_W}{\rho_{Mo}}}$$

$$= \frac{100}{1 + \dfrac{(6.022 \times 10^{23}\ \text{atoms/mol})(19.30\ \text{g/cm}^3)}{(10^{22}\ \text{atoms/cm}^3)(95.94\ \text{g/mol})} - \left(\dfrac{19.30\ \text{g/cm}^3}{10.22\ \text{g/cm}^3}\right)}$$

$$= 8.91\ \text{wt\%}$$

4.24 Niobium forms a substitutional solid solution with vanadium. Compute the weight percent of niobium that must be added to vanadium to yield an alloy that contains 1.55×10^{22} Nb atoms per cubic centimeter. The densities of pure Nb and V are 8.57 and 6.10 g/cm^3, respectively.

Solution

To solve this problem, employment of Equation 4.19 is necessary, using the following values:

$N_1 = N_{Nb} = 1.55 \times 10^{22}$ atoms/cm^3
$\rho_1 = \rho_{Nb} = 8.57$ g/cm^3
$\rho_2 = \rho_V = 6.10$ g/cm^3
$A_1 = A_{Nb} = 92.91$ g/mol
$A_2 = A_V = 50.94$ g/mol

Thus

$$C_{Nb} = \frac{100}{1 + \frac{N_A \rho_V}{N_{Nb} A_{Nb}} - \frac{\rho_V}{\rho_{Nb}}}$$

$$= \frac{100}{1 + \frac{(6.022 \times 10^{23} \text{ atoms/mol})(6.10 \text{ g/cm}^3)}{(1.55 \times 10^{22} \text{ atoms/cm}^3)(92.91 \text{ g/mol})} - \left(\frac{6.10 \text{ g/cm}^3}{8.57 \text{ g/cm}^3}\right)}$$

$$= 35.2 \text{ wt\%}$$

4.25 Silver and palladium both have the FCC crystal structure, and Pd forms a substitutional solid solution for all concentrations at room temperature. Compute the unit cell edge length for a 75 wt% Ag–25 wt% Pd alloy. The room-temperature density of Pd is 12.02 g/cm^3, and its atomic weight and atomic radius are 106.4 g/mol and 0.138 nm, respectively.

Solution

First of all, the atomic radii for Ag (using the table inside the front cover) and Pd are 0.144 and 0.138 nm, respectively. Also, using Equation 3.5 it is possible to compute the unit cell volume, and inasmuch as the unit cell is cubic, the unit cell edge length is just the cube root of the volume. However, it is first necessary to calculate the density and average atomic weight of this alloy using Equations 4.10a and 4.11a. Inasmuch as the densities of silver and palladium are 10.49 g/cm^3 (as taken from inside the front cover) and 12.02 g/cm^3, respectively, the average density is just

$$\rho_{ave} = \frac{100}{\dfrac{C_{Ag}}{\rho_{Ag}} + \dfrac{C_{Pd}}{\rho_{Pd}}}$$

$$= \frac{100}{\dfrac{75\ \text{wt\%}}{10.49\ \text{g/cm}^3} + \dfrac{25\ \text{wt\%}}{12.02\ \text{g/cm}^3}}$$

$$= 10.83\ \text{g/cm}^3$$

And for the average atomic weight

$$A_{ave} = \frac{100}{\dfrac{C_{Ag}}{A_{Ag}} + \dfrac{C_{Pd}}{A_{Pd}}}$$

$$= \frac{100}{\dfrac{75\ \text{wt\%}}{107.9\ \text{g/mol}} + \dfrac{25\ \text{wt\%}}{106.4\ \text{g/mol}}}$$

$$= 107.5\ \text{g/mol}$$

Now, V_C is determined from Equation 3.5 as

$$V_C = \frac{nA_{ave}}{\rho_{ave}N_A}$$

$$= \frac{(4 \text{ atoms/unit cell})(107.5 \text{ g/mol})}{\left(10.83 \text{ g/cm}^3\right)\left(6.022 \times 10^{23} \text{ atoms/mol}\right)}$$

$$= 6.59 \times 10^{-23} \text{ cm}^3\text{/unit cell}$$

And, finally

$$a = \left(V_C\right)^{1/3}$$

$$= \left(6.59 \times 10^{-23} \text{cm}^3\text{/unit cell}\right)^{1/3}$$

$$= 4.04 \times 10^{-8} \text{ cm} = 0.404 \text{ nm}$$

Dislocations—Linear Defects

4.26 Cite the relative Burgers vector–dislocation line orientations for edge, screw, and mixed dislocations.

Solution

The Burgers vector and dislocation line are perpendicular for edge dislocations, parallel for screw dislocations, and neither perpendicular nor parallel for mixed dislocations.

Interfacial Defects

4.27 For an FCC single crystal, would you expect the surface energy for a (100) plane to be greater or less than that for a (111) plane? Why? (Note: You may want to consult the solution to Problem 3.54 at the end of Chapter 3.)

Solution

The surface energy for a crystallographic plane will depend on its packing density [i.e., the planar density (Section 3.11)]—that is, the higher the packing density, the greater the number of nearest-neighbor atoms, and the more atomic bonds in that plane that are satisfied, and, consequently, the lower the surface energy. From the solution to Problem 3.54, planar densities for FCC (100) and (111) planes are $\frac{1}{4R^2}$ and $\frac{1}{2R^2\sqrt{3}}$, respectively—that is $\frac{0.25}{R^2}$ and $\frac{0.29}{R^2}$ (where R is the atomic radius). Thus, since the planar density for (111) is greater, it will have the lower surface energy.

4.28 For a BCC single crystal, would you expect the surface energy for a (100) plane to be greater or less than that for a (110) plane? Why? (Note: You may want to consult the solution to Problem 3.55 at the end of Chapter 3.)

Solution

The surface energy for a crystallographic plane will depend on its packing density [i.e., the planar density (Section 3.11)]—that is, the higher the packing density, the greater the number of nearest-neighbor atoms, and the more atomic bonds in that plane that are satisfied, and, consequently, the lower the surface energy. From the solution to Problem 3.55, the planar densities for BCC (100) and (110) are $\frac{3}{16R^2}$ and $\frac{3}{8R^2\sqrt{2}}$, respectively—that is $\frac{0.19}{R^2}$ and $\frac{0.27}{R^2}$. Thus, since the planar density for (110) is greater, it will have the lower surface energy.

4.29 (a) For a given material, would you expect the surface energy to be greater than, the same as, or less than the grain boundary energy? Why?

(b) The grain boundary energy of a small-angle grain boundary is less than for a high-angle one. Why is this so?

Solution

(a) The surface energy will be greater than the grain boundary energy. For grain boundaries, some atoms on one side of a boundary will bond to atoms on the other side; such is not the case for surface atoms. Therefore, there will be fewer unsatisfied bonds along a grain boundary.

(b) The small-angle grain boundary energy is lower than for a high-angle one because more atoms bond across the boundary for the small-angle, and, thus, there are fewer unsatisfied bonds.

4.30 (a) Briefly describe a twin and a twin boundary.

(b) Cite the difference between mechanical and annealing twins.

Solution

(a) A twin boundary is an interface such that atoms on one side are located in 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.

4.31 For each of the following stacking sequences found in FCC metals, cite the type of planar defect that exists:

(a) . . . A B C A B C B A C B A . . .

(b) . . . A B C A B C B C A B C . . .

Now, copy the stacking sequences and indicate the position(s) of planar defect(s) with a vertical dashed line.

Solution

(a) The interfacial defect that exists for this stacking sequence is a twin boundary, which occurs at the indicated position.

The stacking sequence on one side of this position is mirrored on the other side.

(b) The interfacial defect that exists within this FCC stacking sequence is a stacking fault, which occurs between the two lines.

Within this region, the stacking sequence is HCP.

Grain Size Determination

4.32 (a) Using the intercept method, determine the average grain size, in millimeters, of the specimen whose microstructure is shown in Figure 4.14(b); use at least seven straight-line segments.

(b) Estimate the ASTM grain size number for this material.

Solution

(a) Below is shown the photomicrograph of Figure 4.14(b), on which seven straight line segments, each of which is 60 mm long has been constructed; these lines are labeled "1" through "7".

In order to determine the average grain diameter, it is necessary to count the number of grains intersected by each of these line segments. These data are tabulated below.

Line Number	No. Grains Intersected
1	11
2	10
3	9
4	8.5
5	7
6	10
7	8

The average number of grain boundary intersections for these lines was 9.1. Therefore, the average line length intersected is just

$$\frac{60 \text{ mm}}{9.1} = 6.59 \text{ mm}$$

Hence, the average grain diameter, d, is

$$d = \frac{\text{ave. line length intersected}}{\text{magnification}} = \frac{6.59 \text{ mm}}{100} = 6.59 \times 10^{-2} \text{ mm}$$

(b) This portion of the problem calls for us to estimate the ASTM grain size number for this same material. The average grain size number, n, is related to the number of grains per square inch, N, at a magnification of 100 × according to Equation 4.16. Inasmuch as the magnification is 100 ×, the value of N is measured directly from the micrograph. The photomicrograph on which has been constructed a square 1 in. on a side is shown below.

The total number of complete grains within this square is approximately 10 (taking into account grain fractions). Now, in order to solve for n in Equation 4.16, it is first necessary to take logarithms as

$$\log N = (n - 1) \log 2$$

From which n equals

$$n = \frac{\log N}{\log 2} + 1$$

$$\frac{\log 10}{\log 2} \quad 1 \quad 4.3$$

4.33 (a) Employing the intercept technique, determine the average grain size for the steel specimen whose microstructure is shown in Figure 9.25(a); use at least seven straight-line segments.

(b) Estimate the ASTM grain size number for this material.

Solution

(a) Below is shown the photomicrograph of Figure 9.25(a), on which seven straight line segments, each of which is 60 mm long has been constructed; these lines are labeled “1” through “7”.

In order to determine the average grain diameter, it is necessary to count the number of grains intersected by each of these line segments. These data are tabulated below.

Line Number	No. Grains Intersected
1	7
2	7
3	7
4	8
5	10
6	7
7	8

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

$$d = \frac{\text{ave. line length intersected}}{\text{magnification}} = \frac{6.9\text{ mm}}{90} = 0.077\text{ mm}$$

(b) This portion of the problem calls for us to estimate the ASTM grain size number for this same material. The average grain size number, n, is related to the number of grains per square inch, N, at a magnification of 100× according to Equation 4.16. However, the magnification of this micrograph is not 100×, but rather 90×. Consequently, it is necessary to use Equation 4.17

$$N_M \left(\frac{M}{100}\right)^2 = 2^{n-1}$$

where N_M = the number of grains per square inch at magnification M, and n is the ASTM grain size number. Taking logarithms of both sides of this equation leads to the following:

$$\log N_M + 2\log\left(\frac{M}{100}\right) = (n - 1)\log 2$$

Solving this expression for n gives

$$n = \frac{\log N_M + 2\log\left(\frac{M}{100}\right)}{\log 2} + 1$$

The photomicrograph on which has been constructed a square 1 in. on a side is shown below.

From Figure 9.25(a), N_M is measured to be approximately 7, which leads to

$$n \qquad \frac{\log 7 \quad 2\log\left(\frac{90}{100}\right)}{\log 2} \qquad 1$$

$$= 3.5$$

4.34 For an ASTM grain size of 8, approximately how many grains would there be per square inch at

(a) a magnification of 100, and

(b) without any magnification?

Solution

(a) This part of problem asks that we compute the number of grains per square inch for an ASTM grain size of 8 at a magnification of 100. All we need do is solve for the parameter N in Equation 4.16, inasmuch as n = 8. Thus

$$N = 2^{n-1}$$

$$= 2^{8-1} = 128 \text{ grains/in.}^2$$

(b) Now it is necessary to compute the value of N for no magnification. In order to solve this problem it is necessary to use Equation 4.17:

$$N_M \left(\frac{M}{100}\right)^2 = 2^{n-1}$$

where N_M = the number of grains per square inch at magnification M, and n is the ASTM grain size number. Without any magnification, M in the above equation is 1, and therefore,

$$N_1 \left(\frac{1}{100}\right)^2 = 2^{8-1} = 128$$

And, solving for N_1, N_1 = 1,280,000 grains/in.^{2}.

4.35 Determine the ASTM grain size number if 25 grains per square inch are measured at a magnification of 600.

Solution

This problem asks that we determine the ASTM grain size number if 8 grains per square inch are measured at a magnification of 600. In order to solve this problem we make use of Equation 4.17:

$$N_M \left(\frac{M}{100}\right)^2 = 2^{n-1}$$

where N_M = the number of grains per square inch at magnification M, and n is the ASTM grain size number. Solving the above equation for n, and realizing that N_M = 8, while M = 600, we have

$$n = \frac{\log N_M + 2 \log \left(\frac{M}{100}\right)}{\log 2} + 1$$

$$= \frac{\log 8 + 2 \log \left(\frac{600}{100}\right)}{\log 2} + 1 = 9.2$$

4.36 Determine the ASTM grain size number if 20 grains per square inch are measured at a magnification of 50.

Solution

This problem asks that we determine the ASTM grain size number if 20 grains per square inch are measured at a magnification of 50. In order to solve this problem we make use of Equation 4.17—viz.

$$N_M \left(\frac{M}{100}\right)^2 = 2^{n-1}$$

where N_M = the number of grains per square inch at magnification M, and n is the ASTM grain size number. Solving the above equation for n, and realizing that N_M = 20, while M = 50, we have

$$n = \frac{\log N_M + 2 \log \left(\frac{M}{100}\right)}{\log 2} + 1$$

$$= \frac{\log 20 + 2 \log \left(\frac{50}{100}\right)}{\log 2} + 1 = 3.3$$

DESIGN PROBLEMS

Specification of Composition

4.D1 Aluminum-lithium alloys have been developed by the aircraft industry to reduce the weight and improve the performance of its aircraft. A commercial aircraft skin material having a density of 2.55 g/cm^3 is desired. Compute the concentration of Li (in wt%) that is required.

Solution

Solution of this problem requires the use of Equation 4.10a, which takes the form

$$\rho_{ave} = \frac{100}{\frac{C_{Li}}{\rho_{Li}} + \frac{100 - C_{Li}}{\rho_{Al}}}$$

inasmuch as $C_{Li} + C_{Al} = 100$. According to the table inside the front cover, the respective densities of Li and Al are 0.534 and 2.71 g/cm^3. Upon solving for C_{Li} from the above equation, we get

$$C_{Li} = \frac{100\,\rho_{Li}\left(\rho_{Al} - \rho_{ave}\right)}{\rho_{ave}\left(\rho_{Al} - \rho_{Li}\right)}$$

And incorporating specified values into the above equation leads to

$$C_{Li} = \frac{(100)\left(0.534\ \mathrm{g/cm^3}\right)\left(2.71\ \mathrm{g/cm^3} - 2.55\ \mathrm{g/cm^3}\right)}{\left(2.55\ \mathrm{g/cm^3}\right)\left(2.71\ \mathrm{g/cm^3} - 0.534\ \mathrm{g/cm^3}\right)}$$

$$= 1.540\ \mathrm{wt\%}$$

4.D2 Iron and vanadium both have the BCC crystal structure and V forms a substitutional solid solution in Fe for concentrations up to approximately 20 wt% V at room temperature. Determine the concentration in weight percent of V that must be added to iron to yield a unit cell edge length of 0.289 nm.

Solution

To begin, it is necessary to employ Equation 3.5, and solve for the unit cell volume, V_C, as

$$V_C = \frac{nA_{ave}}{\rho_{ave} N_A}$$

where A_{ave} and ρ_{ave} are the atomic weight and density, respectively, of the Fe-V alloy. Inasmuch as both of these materials have the BCC crystal structure, which has cubic symmetry, V_C is just the cube of the unit cell length, a. That is

$$V_C = a^3 = (0.289 \text{ nm})^3$$

$$(2.89 \times 10^{-8} \text{ cm})^3 = 2.414 \times 10^{-23} \text{ cm}^3$$

It is now necessary to construct expressions for A_{ave} and ρ_{ave} in terms of the concentration of vanadium, C_V, using Equations 4.11a and 4.10a. For A_{ave} we have

$$A_{ave} = \frac{100}{\dfrac{C_V}{A_V} + \dfrac{(100 - C_V)}{A_{Fe}}}$$

$$= \frac{100}{\dfrac{C_V}{50.94 \text{ g/mol}} + \dfrac{(100 - C_V)}{55.85 \text{ g/mol}}}$$

whereas for ρ_{ave}

$$\rho_{ave} = \frac{100}{\dfrac{C_V}{\rho_V} + \dfrac{(100 - C_V)}{\rho_{Fe}}}$$

$$= \frac{100}{\dfrac{C_V}{6.10 \text{ g/cm}^3} + \dfrac{(100 - C_V)}{7.87 \text{ g/cm}^3}}$$

Within the BCC unit cell there are 2 equivalent atoms, and thus, the value of n in Equation 3.5 is 2; hence, this expression may be written in terms of the concentration of V in weight percent as follows:

$$V_C = 2.414 \times 10^{-23}\ \text{cm}^3$$

$$= \frac{nA_{\text{ave}}}{\rho_{\text{ave}} N_A}$$

$$= \frac{(2\ \text{atoms/unit cell})\left[\dfrac{100}{\dfrac{C_V}{50.94\ \text{g/mol}} + \dfrac{(100 - C_V)}{55.85\ \text{g/mol}}}\right]}{\left[\dfrac{100}{\dfrac{C_V}{6.10\ \text{g/cm}^3} + \dfrac{(100 - C_V)}{7.87\ \text{g/cm}^3}}\right](6.022 \times 10^{23}\ \text{atoms/mol})}$$

And solving this expression for C_V leads to C_V = 12.9 wt%.

CHAPTER 5

DIFFUSION

PROBLEM SOLUTIONS

Introduction

5.1 Briefly explain the difference between self-diffusion and interdiffusion.

<u>Solution</u>

Self-diffusion is atomic migration in pure metals--i.e., when all atoms exchanging positions are of the same type. Interdiffusion is diffusion of atoms of one metal into another metal.

5.2 Self-diffusion involves the motion of atoms that are all of the same type; therefore it is not subject to observation by compositional changes, as with interdiffusion. Suggest one way in which self-diffusion may be monitored.

Solution

Self-diffusion may be monitored by using radioactive isotopes of the metal being studied. The motion of these isotopic atoms may be monitored by measurement of radioactivity level.

Diffusion Mechanisms

5.3 (a) Compare interstitial and vacancy atomic mechanisms for diffusion.

(b) Cite two reasons why interstitial diffusion is normally more rapid than vacancy diffusion.

Solution

(a) With vacancy diffusion, atomic motion is from one lattice site to an adjacent vacancy. Self-diffusion and the diffusion of substitutional impurities proceed via this mechanism. On the other hand, atomic motion is from interstitial site to adjacent interstitial site for the interstitial diffusion mechanism.

(b) Interstitial diffusion is normally more rapid than vacancy diffusion because: (1) interstitial atoms, being smaller, are more mobile; and (2) the probability of an empty adjacent interstitial site is greater than for a vacancy adjacent to a host (or substitutional impurity) atom.

Steady-State Diffusion

5.4 Briefly explain the concept of steady state as it applies to diffusion.

Solution

Steady-state diffusion is the situation wherein the rate of diffusion into a given system is just equal to the rate of diffusion out, such that there is no net accumulation or depletion of diffusing species—i.e., the diffusion flux is independent of time.

5.5 (a) Briefly explain the concept of a driving force.

(b) What is the driving force for steady-state diffusion?

Solution

(a) The driving force is that which compels a reaction to occur.

(b) The driving force for steady-state diffusion is the concentration gradient.

5.6 The purification of hydrogen gas by diffusion through a palladium sheet was discussed in Section 5.3. Compute the number of kilograms of hydrogen that pass per hour through a 5-mm-thick sheet of palladium having an area of 0.20 m^2 at 500°C. Assume a diffusion coefficient of 1.0×10^{-8} m^2/s, that the concentrations at the high- and low-pressure sides of the plate are 2.4 and 0.6 kg of hydrogen per cubic meter of palladium, and that steady-state conditions have been attained.

Solution

This problem calls for the mass of hydrogen, per hour, that diffuses through a Pd sheet. It first becomes necessary to employ both Equations 5.1a and 5.3. Combining these expressions and solving for the mass yields

$$M = JAt = -DAt\frac{\Delta C}{\Delta x}$$

$$= -(1.0 \times 10^{-8}\ \text{m}^2/\text{s})(0.20\ \text{m}^2)(3600\ \text{s/h})\left[\frac{0.6 - 2.4\ \text{kg/m}^3}{5 \times 10^{-3}\ \text{m}}\right]$$

$$= 2.6 \times 10^{-3}\ \text{kg/h}$$

5.7 A sheet of steel 1.5 mm thick has nitrogen atmospheres on both sides at 1200°C and is permitted to achieve a steady-state diffusion condition. The diffusion coefficient for nitrogen in steel at this temperature is 6×10^{-11} m^2/s, and the diffusion flux is found to be 1.2×10^{-7} kg/m^2-s. Also, it is known that the concentration of nitrogen in the steel at the high-pressure surface is 4 kg/m^3. How far into the sheet from this high-pressure side will the concentration be 2.0 kg/m^3? Assume a linear concentration profile.

Solution

This problem is solved by using Equation 5.3 in the form

$$J = -D\frac{C_A - C_B}{x_A - x_B}$$

If we take C_A to be the point at which the concentration of nitrogen is 4 kg/m^3, then it becomes necessary to solve for x_B, as

$$x_B = x_A + D\left[\frac{C_A - C_B}{J}\right]$$

Assume x_A is zero at the surface, in which case

$$x_B = 0 + (6 \times 10^{-11}\ \mathrm{m^2/s})\left[\frac{4\ \mathrm{kg/m^3} - 2\ \mathrm{kg/m^3}}{1.2 \times 10^{-7}\ \mathrm{kg/m^2\text{-}s}}\right]$$

$$= 1 \times 10^{-3}\ \mathrm{m} = 1\ \mathrm{mm}$$

5.8 A sheet of BCC iron 1 mm thick was exposed to a carburizing gas atmosphere on one side and a decarburizing atmosphere on the other side at 725°C. After having reached steady state, the iron was quickly cooled to room temperature. The carbon concentrations at the two surfaces of the sheet were determined to be 0.012 and 0.0075 wt%. Compute the diffusion coefficient if the diffusion flux is 1.4×10^{-8} kg/m^2-s. Hint: Use Equation 4.9 to convert the concentrations from weight percent to kilograms of carbon per cubic meter of iron.

Solution

Let us first convert the carbon concentrations from weight percent to kilograms carbon per meter cubed using Equation 4.9a. For 0.012 wt% C

$$C_C'' = \frac{C_C}{\dfrac{C_C}{\rho_C} \quad \dfrac{C_{Fe}}{\rho_{Fe}}} \times 10^3$$

$$= \frac{0.012}{\dfrac{0.012}{2.25\,\text{g/cm}^3} \quad \dfrac{99.988}{7.87\,\text{g/cm}^3}} \times 10^3$$

$$0.944 \text{ kg C/m}^3$$

Similarly, for 0.0075 wt% C

$$C_C'' = \frac{0.0075}{\dfrac{0.0075}{2.25\,\text{g/cm}^3} \quad \dfrac{99.9925}{7.87\text{ g/cm}^3}} \times 10^3$$

$$= 0.590 \text{ kg C/m}^3$$

Now, using a rearranged form of Equation 5.3

$$D = \quad J\left[\frac{x_A \quad x_B}{C_A \quad C_B}\right]$$

$$= \quad (1.40 \times 10^{-8} \text{ kg/m}^2\text{-s})\left[\frac{10^{3}\text{ m}}{0.944\,\text{kg/m}^3 \quad 0.590\text{ kg/m}^3}\right]$$

$$= 3.95 \times 10^{-11}\ \text{m}^2/\text{s}$$

5.9 When α-iron is subjected to an atmosphere of hydrogen gas, the concentration of hydrogen in the iron, C_H (in weight percent), is a function of hydrogen pressure, p_{H_2} (in MPa), and absolute temperature (T) according to

$$C_H = 1.34 \times 10^{-2} \sqrt{p_{H_2}} \exp\left(-\frac{27.2 \text{ kJ/mol}}{RT}\right) \qquad (5.14)$$

Furthermore, the values of D_0 and Q_d for this diffusion system are 1.4×10^{-7} m^2/s and 13,400 J/mol, respectively. Consider a thin iron membrane 1 mm thick that is at 250°C. Compute the diffusion flux through this membrane if the hydrogen pressure on one side of the membrane is 0.15 MPa (1.48 atm), and on the other side 7.5 MPa (74 atm).

Solution

Ultimately we will employ Equation 5.3 to solve this problem. However, it first becomes necessary to determine the concentration of hydrogen at each face using Equation 5.14. At the low pressure (or B) side

$$C_{H(B)} = \left(1.34 \times 10^{-2}\right)\sqrt{0.15 \text{ MPa}} \exp\left[-\frac{27{,}200 \text{ J/mol}}{(8.31 \text{ J/mol-K})(250 + 273 \text{ K})}\right]$$

$$= 9.93 \times 10^{-6} \text{ wt\%}$$

Whereas, for the high pressure (or A) side

$$C_{H(A)} = \left(1.34 \times 10^{-2}\right)\sqrt{7.5 \text{ MPa}} \exp\left[-\frac{27{,}200 \text{ J/mol}}{(8.31 \text{ J/mol-K})(250 + 273 \text{ K})}\right]$$

$$= 7.02 \times 10^{-5} \text{ wt\%}$$

We now convert concentrations in weight percent to mass of nitrogen per unit volume of solid. At face B there are 9.93×10^{-6} g (or 9.93×10^{-9} kg) of hydrogen in 100 g of Fe, which is virtually pure iron. From the density of iron (7.87 g/cm^3), the volume iron in 100 g (V_B) is just

$$V_B = \frac{100 \text{ g}}{7.87 \text{ g/cm}^3} = 12.7 \text{ cm}^3 = 1.27 \times 10^{-5} \text{ m}^3$$

Therefore, the concentration of hydrogen at the B face in kilograms of H per cubic meter of alloy [$C''_{H(B)}$] is just

$$C''_{H(B)} = \frac{C_{H(B)}}{V_B}$$

$$= \frac{9.93 \times 10^{9}\ \text{kg}}{1.27 \times 10^{5}\ \text{m}^3} = 7.82 \times 10^{-4}\ \text{kg/m}^3$$

At the A face the volume of iron in 100 g (V_A) will also be $1.27 \times 10^{-5}\ \text{m}^3$, and

$$C''_{H(A)} = \frac{C_{H(A)}}{V_A}$$

$$= \frac{7.02 \times 10^{8}\ \text{kg}}{1.27 \times 10^{5}\ \text{m}^3} = 5.53 \times 10^{-3}\ \text{kg/m}^3$$

Thus, the concentration gradient is just the difference between these concentrations of nitrogen divided by the thickness of the iron membrane; that is

$$\frac{\Delta C}{\Delta x} = \frac{C''_{H(B)} \quad C''_{H(A)}}{x_B \quad x_A}$$

$$= \frac{7.82 \times 10^{4}\ \text{kg/m}^3 \quad 5.53 \times 10^{3}\ \text{kg/m}^3}{10^{3}\ \text{m}} = \quad 4.75\ \text{kg/m}^4$$

At this time it becomes necessary to calculate the value of the diffusion coefficient at 250°C using Equation 5.8. Thus,

$$D = D_0 \exp\left(\frac{Q_d}{RT}\right)$$

$$= \left(1.4 \times 10^{7}\ \text{m}^2/\text{s}\right) \exp\left[\frac{13{,}400\ \text{J/mol}}{(8.31\ \text{J/mol} \quad \text{K})(250 \quad 273\ \text{K})}\right]$$

$$= 6.41 \times 10^{-9}\ \text{m}^2/\text{s}$$

And, finally, the diffusion flux is computed using Equation 5.3 by taking the negative product of this diffusion coefficient and the concentration gradient, as

$$J = D\frac{\Delta C}{\Delta x}$$

$$= \left(6.41 \times 10^{-9}\ \mathrm{m^2/s}\right)\left(4.75\ \mathrm{kg/m^4}\right) = 3.05 \times 10^{-8}\ \mathrm{kg/m^2\text{-}s}$$

Nonsteady-State Diffusion

5.10 Show that

$$C_x = \frac{B}{\sqrt{Dt}} \exp\left(\frac{x^2}{4Dt}\right)$$

is also a solution to Equation 5.4b. The parameter B is a constant, being independent of both x and t.

Solution

It can be shown that

$$C_x = \frac{B}{\sqrt{Dt}} \exp\left(\frac{x^2}{4Dt}\right)$$

is a solution to

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

simply by taking appropriate derivatives of the C_x expression. When this is carried out,

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} = \frac{B}{2D^{1/2}t^{3/2}}\left(\frac{x^2}{2Dt} \quad 1\right)\exp\left(\frac{x^2}{4Dt}\right)$$

5.11 Determine the carburizing time necessary to achieve a carbon concentration of 0.45 wt% at a position 2 mm into an iron-carbon alloy that initially contains 0.20 wt% C. The surface concentration is to be maintained at 1.30 wt% C, and the treatment is to be conducted at 1000°C. Use the diffusion data for γ-Fe in Table 5.2.

Solution

In order to solve this problem it is first necessary to use Equation 5.5:

$$\frac{C_x - C_0}{C_s - C_0} = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

wherein, $C_x = 0.45$, $C_0 = 0.20$, $C_s = 1.30$, and $x = 2\ \text{mm} = 2 \times 10^{-3}$ m. Thus,

$$\frac{C_x - C_0}{C_s - C_0} = \frac{0.45 - 0.20}{1.30 - 0.20} = 0.2273 = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

or

$$\operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) = 1 - 0.2273 = 0.7727$$

By linear interpolation using data from Table 5.1

z	erf(z)
0.85	0.7707
z	0.7727
0.90	0.7970

$$\frac{z - 0.850}{0.900 - 0.850} = \frac{0.7727 - 0.7707}{0.7970 - 0.7707}$$

From which

$$z = 0.854 = \frac{x}{2\sqrt{Dt}}$$

Now, from Table 5.2, at 1000°C (1273 K)

$$D = \left(2.3 \times 10^{-5}\ \text{m}^2/\text{s}\right) \exp\left[\frac{148{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(1273\ \text{K})}\right]$$

$$= 1.93 \times 10^{-11}\ \text{m}^2/\text{s}$$

Thus,

$$0.854 = \frac{2 \times 10^{-3}\ \text{m}}{(2)\sqrt{\left(1.93 \times 10^{-11}\ \text{m}^2/\text{s}\right)(t)}}$$

Solving for t yields

$$t = 7.1 \times 10^4\ \text{s} = 19.7\ \text{h}$$

5.12 An FCC iron-carbon alloy initially containing 0.35 wt% C is exposed to an oxygen-rich and virtually carbon-free atmosphere at 1400 K (1127°C). Under these circumstances the carbon diffuses from the alloy and reacts at the surface with the oxygen in the atmosphere; that is, the carbon concentration at the surface position is maintained essentially at 0 wt% C. (This process of carbon depletion is termed decarburization.) At what position will the carbon concentration be 0.15 wt% after a 10-h treatment? The value of D at 1400 K is 6.9 × 10^{-11} m^2/s.

Solution

This problem asks that we determine the position at which the carbon concentration is 0.15 wt% after a 10-h heat treatment at 1325 K when C_0 = 0.35 wt% C. From Equation 5.5

$$\frac{C_x - C_0}{C_s - C_0} = \frac{0.15 - 0.35}{0 - 0.35} = 0.5714 = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

Thus,

$$\operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) = 0.4286$$

Using data in Table 5.1 and linear interpolation

z	erf (z)
0.40	0.4284
z	0.4286
0.45	0.4755

$$\frac{z - 0.40}{0.45 - 0.40} = \frac{0.4286 - 0.4284}{0.4755 - 0.4284}$$

And,

$$z = 0.4002$$

Which means that

$$\frac{x}{2\sqrt{Dt}} = 0.4002$$

And, finally

$$x = 2(0.4002)\sqrt{Dt} = (0.8004)\sqrt{\left(6.9 \times 10^{-11}\ \text{m}^2/\text{s}\right)\left(3.6 \times 10^{4}\ \text{s}\right)}$$

$$= 1.26 \times 10^{-3}\ \text{m} = 1.26\ \text{mm}$$

Note: this problem may also be solved using the “Diffusion” module in the VMSE software. Open the “Diffusion” module, click on the “Diffusion Design” submodule, and then do the following:

1. Enter the given data in left-hand window that appears. In the window below the label “D Value” enter the value of the diffusion coefficient—viz. “6.9e-11”.

2. In the window just below the label “Initial, C_0” enter the initial concentration—viz. “0.35”.

3. In the window the lies below “Surface, C_s” enter the surface concentration—viz. “0”.

4. Then in the “Diffusion Time t” window enter the time in seconds; in 10 h there are (60 s/min)(60 min/h)(10 h) = 36,000 s—so enter the value “3.6e4”.

5. Next, at the bottom of this window click on the button labeled “Add curve”.

6. On the right portion of the screen will appear a concentration profile for this particular diffusion situation. A diamond-shaped cursor will appear at the upper left-hand corner of the resulting curve. Click and drag this cursor down the curve to the point at which the number below “Concentration:” reads “0.15 wt%”. Then read the value under the “Distance:”. For this problem, this value (the solution to the problem) is ranges between 1.24 and 1.30 mm.

5.13 Nitrogen from a gaseous phase is to be diffused into pure iron at 700°C. If the surface concentration is maintained at 0.1 wt% N, what will be the concentration 1 mm from the surface after 10 h? The diffusion coefficient for nitrogen in iron at 700°C is 2.5 × 10^{-11} m^2/s.

Solution

This problem asks us to compute the nitrogen concentration (C_x) at the 1 mm position after a 10 h diffusion time, when diffusion is nonsteady-state. From Equation 5.5

$$\frac{C_x - C_0}{C_s - C_0} = \frac{C_x - 0}{0.1 - 0} = 1 - \mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

$$= 1 - \mathrm{erf}\left[\frac{10^{-3}\ \mathrm{m}}{(2)\sqrt{(2.5 \times 10^{-11}\ \mathrm{m^2/s})(10\ \mathrm{h})(3600\ \mathrm{s/h})}}\right]$$

$$= 1 - \mathrm{erf}\ (0.527)$$

Using data in Table 5.1 and linear interpolation

z	erf (z)
0.500	0.5205
0.527	y
0.550	0.5633

$$\frac{0.527 - 0.500}{0.550 - 0.500} = \frac{y - 0.5205}{0.5633 - 0.5205}$$

from which

$$y = \mathrm{erf}\ (0.527) = 0.5436$$

Thus,

$$\frac{C_x - 0}{0.1 - 0} = 1.0 - 0.5436$$

This expression gives

$$C_x = 0.046 \text{ wt\% N}$$

Note: this problem may also be solved using the “Diffusion” module in the VMSE software. Open the “Diffusion” module, click on the “Diffusion Design” submodule, and then do the following:

1. Enter the given data in left-hand window that appears. In the window below the label “D Value” enter the value of the diffusion coefficient—viz. “2.5e-11”.

2. In the window just below the label “Initial, C_0” enter the initial concentration—viz. “0”.

3. In the window the lies below “Surface, C_s” enter the surface concentration—viz. “0.1”.

4. Then in the “Diffusion Time t” window enter the time in seconds; in 10 h there are (60 s/min)(60 min/h)(10 h) = 36,000 s—so enter the value “3.6e4”.

5. Next, at the bottom of this window click on the button labeled “Add curve”.

6. On the right portion of the screen will appear a concentration profile for this particular diffusion situation. A diamond-shaped cursor will appear at the upper-left-hand corner of the resulting curve. Click and drag this cursor down the curve to the point at which the number below “Distance:” reads “1.00 mm”. Then read the value under the “Concentration:”. For this problem, this value (the solution to the problem) is 0.05 wt%.

5.14 Consider a diffusion couple composed of two semi-infinite solids of the same metal, and that each side of the diffusion couple has a different concentration of the same elemental impurity; furthermore, assume each impurity level is constant throughout its side of the diffusion couple. For this situation, the solution to Fick's second law (assuming that the diffusion coefficient for the impurity is independent of concentration), is as follows:

$$C_x = \left(\frac{C_1 + C_2}{2}\right) - \left(\frac{C_1 - C_2}{2}\right)\operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \qquad (5.15)$$

In this expression, when the x = 0 position is taken as the initial diffusion couple interface, then C_1 is the impurity concentration for x < 0; likewise, C_2 is the impurity content for x > 0.

A diffusion couple composed of two silver-gold alloys is formed; these alloys have compositions of 98 wt% Ag–2 wt% Au and 95 wt% Ag–5 wt% Au. Determine the time this diffusion couple must be heated at 750ºC (1023 K) in order for the composition to be 2.5 wt% Au at the 50 μm position into the 2 wt% Au side of the diffusion couple. Preexponential and activation energy values for Au diffusion in Ag are 8.5×10^{-5} m^2/s and 202,100 J/mol, respectively.

Solution

For this platinum-gold diffusion couple for which C_1 = 5 wt% Au and C_2 = 2 wt% Au, we are asked to determine the diffusion time at 750°C that will give a composition of 2.5 wt% Au at the 50 μm position. Thus, for this problem, Equation 5.15 takes the form

$$2.5 = \left(\frac{5 + 2}{2}\right) - \left(\frac{5 - 2}{2}\right)\operatorname{erf}\left(\frac{50 \times 10^{-6}\ \text{m}}{2\sqrt{Dt}}\right)$$

It now becomes necessary to compute the diffusion coefficient at 750°C (1023 K) given that $D_0 = 8.5 \times 10^{-5}$ m^2/s and Q_d = 202,100 J/mol. From Equation 5.8 we have

$$D = D_0 \exp\left(-\frac{Q_d}{RT}\right)$$

$$= \left(8.5 \times 10^{-5}\ \text{m}^2/\text{s}\right) \exp\left[-\frac{202{,}100\ \text{J/mol}}{(8.31\ \text{J/mol-K})(1023\ \text{K})}\right]$$

$$= 4.03 \times 10^{-15}\ \text{m}^2/\text{s}$$

Substitution of this value into the above equation leads to

$$2.5 = \left(\frac{5+2}{2}\right) - \left(\frac{5-2}{2}\right)\text{erf}\left[\frac{50 \times 10^{-6}\text{ m}}{2\sqrt{(4.03 \times 10^{-15}\text{ m}^2/\text{s})(t)}}\right]$$

This expression reduces to the following form:

$$0.6667 = \text{erf}\left(\frac{393.8\sqrt{\text{s}}}{\sqrt{t}}\right)$$

Using data in Table 5.1, it is necessary to determine the value of z for which the error function is 0.6667 We use linear interpolation as follows:

z	erf (z)
0.650	0.6420
y	0.6667
0.700	0.6778

$$\frac{y - 0.650}{0.700 - 0.650} = \frac{0.6667 - 0.6420}{0.6778 - 0.6420}$$

from which

$$y = 0.6844 = \frac{393.8\sqrt{\text{s}}}{\sqrt{t}}$$

And, solving for t gives

$$t = 3.31 \times 10^{5}\text{ s} = 92\text{ h}$$

5.15 For a steel alloy it has been determined that a carburizing heat treatment of 10-h duration will raise the carbon concentration to 0.45 wt% at a point 2.5 mm from the surface. Estimate the time necessary to achieve the same concentration at a 5.0-mm position for an identical steel and at the same carburizing temperature.

Solution

This problem calls for an estimate of the time necessary to achieve a carbon concentration of 0.45 wt% at a point 5.0 mm from the surface. From Equation 5.6b,

$$\frac{x^2}{Dt} = \text{constant}$$

But since the temperature is constant, so also is D constant, and

$$\frac{x^2}{t} = \text{constant}$$

or

$$\frac{x_1^2}{t_1} = \frac{x_2^2}{t_2}$$

Thus,

$$\frac{(2.5\ \text{mm})^2}{10\ \text{h}} = \frac{(5.0\ \text{mm})^2}{t_2}$$

from which

$$t_2 = 40\ \text{h}$$

Factors That Influence Diffusion

5.16 Cite the values of the diffusion coefficients for the interdiffusion of carbon in both -iron (BCC) and -iron (FCC) at 900°C. Which is larger? Explain why this is the case.

Solution

We are asked to compute the diffusion coefficients of C in both D and J iron at 900 q C. Using the data in Table 5.2,

$$D_D = \left(6.2\ u\ 10^{-7}\ m^2/s\right) \exp \frac{80,000\ J/mol}{(8.31\ J/mol-K)(1173\ K)}$$

$$= 1.69\ u 10^{-10}\ m^2/s$$

$$D_J = \left(2.3\ u\ 10^{-5}\ m^2/s\right) \exp \frac{148,000\ J/mol}{(8.31\ J/mol-K)(1173\ K)}$$

$$= 5.86\ u 10^{-12}\ m^2/s$$

The D for diffusion of C in BCC D iron is larger, the reason being that the atomic packing factor is smaller than for FCC J iron (0.68 versus 0.74—Section 3.4); this means that there is slightly more interstitial void space in the BCC Fe, and, therefore, the motion of the interstitial carbon atoms occurs more easily.

5.17 Using the data in Table 5.2, compute the value of D for the diffusion of zinc in copper at 650ºC.

Solution

Incorporating the appropriate data from Table 5.2 into Equation 5.8 leads to

$$D = (2.4 \times 10^{-5}\ \mathrm{m^2/s})\exp\left[-\frac{189{,}000\ \mathrm{J/mol}}{(8.31\ \mathrm{J/mol\text{-}K})(650 + 273\ \mathrm{K})}\right]$$

$$= 4.8 \times 10^{-16}\ \mathrm{m^2/s}$$

Note: this problem may also be solved using the "Diffusion" module in the VMSE software. Open the "Diffusion" module, click on the "D vs 1/T Plot" submodule, and then do the following:

1. In the left-hand window that appears, click on the "Zn-Cu" pair under the "Diffusing Species"-"Host Metal" headings.

2. Next, at the bottom of this window, click the "Add Curve" button.

3. A log D versus 1/T plot then appears, with a line for the temperature dependence of the diffusion coefficient for Zn in Cu. Now under "Temp Range" in the boxes appearing below "T Max" change the temperature to either "650" C or "923" K. At the top of this curve is a diamond-shaped cursor. Click-and-drag this cursor down the line to the point at which the entry under the "Temperature (T):" label reads 923 K (inasmuch as this is the Kelvin equivalent of 650ºC). Finally, the diffusion coefficient value at this temperature is given under the label "Diff Coeff (D):". For this problem, the value is $4.7 \times 10^{-16}\ \mathrm{m^2/s}$.

5.18 At what temperature will the diffusion coefficient for the diffusion of copper in nickel have a value of 6.5×10^{-17} m^2/s. Use the diffusion data in Table 5.2.

Solution

Solving for T from Equation 5.9a

$$T = -\frac{Q_d}{R(\ln D - \ln D_0)}$$

and using the data from Table 5.2 for the diffusion of Cu in Ni (i.e., $D_0 = 2.7 \times 10^{-5}$ m^2/s and Q_d = 256,000 J/mol) , we get

$$T = -\frac{256{,}000 \text{ J/mol}}{(8.31 \text{ J/mol-K})\left[\ln\left(6.5 \times 10^{-17} \text{ m}^2\text{/s}\right) - \ln\left(2.7 \times 10^{-5} \text{ m}^2\text{/s}\right)\right]}$$

$$= 1152 \text{ K} = 879°\text{C}$$

Note: this problem may also be solved using the “Diffusion” module in the VMSE software. Open the “Diffusion” module, click on the “D vs 1/T Plot” submodule, and then do the following:

1. In the left-hand window that appears, there is a preset set of data for several diffusion systems. Click on the box for which Cu is the diffusing species and Ni is the host metal. Next, at the bottom of this window, click the “Add Curve” button.

2. A log D versus 1/T plot then appears, with a line for the temperature dependence of the diffusion coefficient for Cu in Ni. At the top of this curve is a diamond-shaped cursor. Click-and-drag this cursor down the line to the point at which the entry under the “Diff Coeff (D):” label reads 6.5×10^{-17} m^2/s. The temperature at which the diffusion coefficient has this value is given under the label “Temperature (T):”. For this problem, the value is 1153 K.

5.19 The preexponential and activation energy for the diffusion of iron in cobalt are 1.1×10^{-5} m^2/s and 253,300 J/mol, respectively. At what temperature will the diffusion coefficient have a value of 2.1×10^{-14} m^2/s?

Solution

For this problem we are given D_0 (1.1×10^{-5}) and Q_d (253,300 J/mol) for the diffusion of Fe in Co, and asked to compute the temperature at which $D = 2.1 \times 10^{-14}$ m^2/s. Solving for T from Equation 5.9a yields

$$T = \frac{Q_d}{R\left(\ln D_0 - \ln D\right)}$$

$$= \frac{253{,}300 \text{ J/mol}}{(8.31 \text{ J/mol-K})\left[\ln\left(1.1 \times 10^{-5} \text{ m}^2\text{/s}\right) - \ln\left(2.1 \times 10^{-14} \text{ m}^2\text{/s}\right)\right]}$$

$$= 1518 \text{ K} = 1245^\circ\text{C}$$

Note: this problem may also be solved using the “Diffusion” module in the VMSE software. Open the “Diffusion” module, click on the “D vs 1/T Plot” submodule, and then do the following:

1. In the left-hand window that appears, click on the “Custom1” box.

2. In the column on the right-hand side of this window enter the data for this problem. In the window under “D0” enter preexponential value—viz. “1.1e-5”. Next just below the “Qd” window enter the activation energy value—viz. “253.3”. It is next necessary to specify a temperature range over which the data is to be plotted. The temperature at which D has the stipulated value is probably between 1000ºC and 1500ºC, so enter “1000” in the “T Min” box that is beside “C”; and similarly for the maximum temperature—enter “1500” in the box below “T Max”.

3. Next, at the bottom of this window, click the “Add Curve” button.

4. A log D versus 1/T plot then appears, with a line for the temperature dependence of the diffusion coefficient for Fe in Co. At the top of this curve is a diamond-shaped cursor. Click-and-drag this cursor down the line to the point at which the entry under the “Diff Coeff (D):” label reads 2.1×10^{-14} m^2/s. The temperature at which the diffusion coefficient has this value is given under the label “Temperature (T):”. For this problem, the value is 1519 K.

5.20 The activation energy for the diffusion of carbon in chromium is 111,000 J/mol. Calculate the diffusion coefficient at 1100 K (827°C), given that D at 1400 K (1127°C) is 6.25×10^{-11} m^2/s.

Solution

To solve this problem it first becomes necessary to solve for D_0 from Equation 5.8 as

$$D_0 = D \exp\left(\frac{Q_d}{RT}\right)$$

$$= (6.25 \times 10^{-11} \text{ m}^2/\text{s}) \exp\left[\frac{111{,}000 \text{ J/mol}}{(8.31 \text{ J/mol-K})(1400 \text{ K})}\right]$$

$$= 8.7 \times 10^{-7} \text{ m}^2/\text{s}$$

Now, solving for D at 1100 K (again using Equation 5.8) gives

$$D = (8.7 \times 10^{-7} \text{ m}^2/\text{s}) \exp\left[-\frac{111{,}000 \text{ J/mol}}{(8.31 \text{ J/mol-K})(1100 \text{ K})}\right]$$

$$= 4.6 \times 10^{-12} \text{ m}^2/\text{s}$$

5.21 The diffusion coefficients for iron in nickel are given at two temperatures:

T (K)	D (m^2/s)
1273	9.4×10^{-16}
1473	2.4×10^{-14}

(a) Determine the values of D_0 and the activation energy Q_d.

(b) What is the magnitude of D at 1100ºC (1373 K)?

Solution

(a) Using Equation 5.9a, we set up two simultaneous equations with Q_d and D_0 as unknowns as follows:

$$\ln D_1 = \ln D_0 - \frac{Q_d}{R}\left(\frac{1}{T_1}\right)$$

$$\ln D_2 = \ln D_0 - \frac{Q_d}{R}\left(\frac{1}{T_2}\right)$$

Now, solving for Q_d in terms of temperatures T_1 and T_2 (1273 K and 1473 K) and D_1 and D_2 (9.4×10^{-16} and 2.4×10^{-14} m^2/s), we get

$$Q_d = -R \frac{\ln D_1 - \ln D_2}{\dfrac{1}{T_1} - \dfrac{1}{T_2}}$$

$$= -(8.31 \text{ J/mol-K}) \frac{\ln\left(9.4 \times 10^{-16}\right) - \ln\left(2.4 \times 10^{-14}\right)}{\dfrac{1}{1273 \text{ K}} - \dfrac{1}{1473 \text{ K}}}$$

$$= 252{,}400 \text{ J/mol}$$

Now, solving for D_0 from Equation 5.8 (and using the 1273 K value of D)

$$D_0 = D_1 \exp\left(\frac{Q_d}{RT_1}\right)$$

$$= \left(9.4 \times 10^{-16}\ \text{m}^2/\text{s}\right) \exp\left[\frac{252{,}400\ \text{J/mol}}{(8.31\ \text{J/mol-K})(1273\ \text{K})}\right]$$

$$= 2.2 \times 10^{-5}\ \text{m}^2/\text{s}$$

(b) Using these values of D_0 and Q_d, D at 1373 K is just

$$D = \left(2.2 \times 10^{-5}\ \text{m}^2/\text{s}\right) \exp\left[\frac{252{,}400\ \text{J/mol}}{(8.31\ \text{J/mol-K})(1373\ \text{K})}\right]$$

$$= 5.4 \times 10^{-15}\ \text{m}^2/\text{s}$$

Note: this problem may also be solved using the “Diffusion” module in the VMSE software. Open the “Diffusion” module, click on the “D_0 and Q_d from Experimental Data” submodule, and then do the following:

1. In the left-hand window that appears, enter the two temperatures from the table in the book (viz. “1273” and “1473”, in the first two boxes under the column labeled “T (K)”. Next, enter the corresponding diffusion coefficient values (viz. “9.4e-16” and “2.4e-14”).

3. Next, at the bottom of this window, click the “Plot data” button.

4. A log D versus 1/T plot then appears, with a line for the temperature dependence for this diffusion system. At the top of this window are give values for D_0 and Q_d; for this specific problem these values are 2.17×10^{-5} m^2/s and 252 kJ/mol, respectively

5. To solve the (b) part of the problem we utilize the diamond-shaped cursor that is located at the top of the line on this plot. Click-and-drag this cursor down the line to the point at which the entry under the “Temperature (T):” label reads “1373”. The value of the diffusion coefficient at this temperature is given under the label “Diff Coeff (D):”. For our problem, this value is 5.4×10^{-15} m^2/s.

5.22 The diffusion coefficients for silver in copper are given at two temperatures:

T (°C)	D (m^2/s)
650	5.5×10^{-16}
900	1.3×10^{-13}

(a) Determine the values of D_0 and Q_d.

(b) What is the magnitude of D at 875°C?

Solution

(a) Using Equation 5.9a, we set up two simultaneous equations with Q_d and D_0 as unknowns as follows:

$$\ln D_1 = \ln D_0 - \frac{Q_d}{R}\left(\frac{1}{T_1}\right)$$

$$\ln D_2 = \ln D_0 - \frac{Q_d}{R}\left(\frac{1}{T_2}\right)$$

Solving for Q_d in terms of temperatures T_1 and T_2 (923 K [650°C] and 1173 K [900°C]) and D_1 and D_2 (5.5×10^{-16} and 1.3×10^{-13} m^2/s), we get

$$Q_d = -R\,\frac{\ln D_1 - \ln D_2}{\dfrac{1}{T_1} - \dfrac{1}{T_2}}$$

$$= -\frac{(8.31\ \text{J/mol-K})\left[\ln\left(5.5 \times 10^{-16}\right) - \ln\left(1.3 \times 10^{-13}\right)\right]}{\dfrac{1}{923\ \text{K}} - \dfrac{1}{1173\ \text{K}}}$$

$$= 196{,}700\ \text{J/mol}$$

Now, solving for D_0 from Equation 5.8 (and using the 650°C value of D)

$$D_0 = D_1 \exp\left(\frac{Q_d}{RT_1}\right)$$

$$= \left(5.5 \times 10^{-16}\ \text{m}^2/\text{s}\right) \exp\left[\frac{196{,}700\ \text{J/mol}}{(8.31\ \text{J/mol-K})(923\ \text{K})}\right]$$

$$= 7.5 \times 10^{-5}\ \text{m}^2/\text{s}$$

(b) Using these values of D_0 and Q_d, D at 1148 K (875°C) is just

$$D = \left(7.5 \times 10^{-5}\ \text{m}^2/\text{s}\right) \exp\left[\frac{196{,}700\ \text{J/mol}}{(8.31\ \text{J/mol-K})(1148\ \text{K})}\right]$$

$$= 8.3 \times 10^{-14}\ \text{m}^2/\text{s}$$

Note: this problem may also be solved using the “Diffusion” module in the VMSE software. Open the “Diffusion” module, click on the “D_0 and Q_d from Experimental Data” submodule, and then do the following:

1. In the left-hand window that appears, enter the two temperatures from the table in the book (converted from degrees Celsius to Kelvins) (viz. “923” (650ºC) and “1173” (900ºC), in the first two boxes under the column labeled “T (K)”. Next, enter the corresponding diffusion coefficient values (viz. “5.5e-16” and “1.3e-13”).

3. Next, at the bottom of this window, click the “Plot data” button.

4. A log D versus 1/T plot then appears, with a line for the temperature dependence for this diffusion system. At the top of this window are give values for D_0 and Q_d; for this specific problem these values are 7.55 × 10^{-5} m^2/s and 196 kJ/mol, respectively

5. To solve the (b) part of the problem we utilize the diamond-shaped cursor that is located at the top of the line on this plot. Click-and-drag this cursor down the line to the point at which the entry under the “Temperature (T):” label reads “1148” (i.e., 875ºC). The value of the diffusion coefficient at this temperature is given under the label “Diff Coeff (D):”. For our problem, this value is 8.9 × 10^{-14} m^2/s.

5.23 Below is shown a plot of the logarithm (to the base 10) of the diffusion coefficient versus reciprocal of the absolute temperature, for the diffusion of iron in chromium. Determine values for the activation energy and preexponential.

Solution

This problem asks us to determine the values of Q_d and D_0 for the diffusion of Fe in Cr from the plot of log D versus 1/T. According to Equation 5.9b the slope of this plot is equal to $\frac{Q_d}{2.3R}$ (rather than $\frac{Q_d}{R}$ since we are using log D rather than ln D) and the intercept at 1/T = 0 gives the value of log D_0. The slope is equal to

$$\text{slope} = \frac{\Delta(\log D)}{\Delta\left(\frac{1}{T}\right)} = \frac{\log D_1 - \log D_2}{\frac{1}{T_1} - \frac{1}{T_2}}$$

Taking $1/T_1$ and $1/T_2$ as 0.65×10^{-3} and 0.60×10^{-3} K^{-1}, respectively, then the corresponding values of D_1 and D_2 are 2.81×10^{-16} and 1.82×10^{-15}, as noted in the figure below.

The values of $\log D_1$ and $\log D_2$ are –15.60 and –14.74, and therefore,

$$Q_d = -2.3\,R(\text{slope})$$

$$Q_d = -2.3\,R\left[\frac{\log D_1 - \log D_2}{\dfrac{1}{T_1} - \dfrac{1}{T_2}}\right]$$

$$= -(2.3)(8.31\ \text{J/mol-K})\left[\frac{-15.60 - (-14.74)}{\left(0.65 \times 10^{-3} - 0.60 \times 10^{-3}\right)\ \text{K}^{-1}}\right]$$

$$= 329{,}000\ \text{J/mol}$$

Rather than trying to make a graphical extrapolation to determine D_0, a more accurate value is obtained analytically using Equation 5.9b taking a specific value of both D and T (from $1/T$) from the plot given in the problem; for example, $D = 1.0 \times 10^{-15}\ \text{m}^2/\text{s}$ at $T = 1626$ K ($1/T = 0.615 \times 10^{-3}\ \text{K}^{-1}$). Therefore

$$D_0 = D \exp\left(\frac{Q_d}{RT}\right)$$

$$= \left(1.0 \times 10^{-15}\ \text{m}^2/\text{s}\right)\exp\left[\frac{329{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(1626\ \text{K})}\right]$$

$$= 3.75 \times 10^{-5}\ \text{m}^2/\text{s}$$

5.24 Carbon is allowed to diffuse through a steel plate 15 mm thick. The concentrations of carbon at the two faces are 0.65 and 0.30 kg C/m^3 Fe, which are maintained constant. If the preexponential and activation energy are 6.2×10^{-7} m^2/s and 80,000 J/mol, respectively, compute the temperature at which the diffusion flux is 1.43×10^{-9} kg/m^2-s.

Solution

Combining Equations 5.3 and 5.8 yields

$$J = -D \frac{\Delta C}{\Delta x}$$

$$= -D_0 \frac{\Delta C}{\Delta x} \exp\left(-\frac{Q_d}{RT}\right)$$

Solving for T from this expression leads to

$$T = \left(\frac{Q_d}{R}\right) \frac{1}{\ln\left(-\dfrac{D_0 \Delta C}{J \Delta x}\right)}$$

And incorporation of values provided in the problem statement yields

$$= \left(\frac{80{,}000 \text{ J/mol}}{8.31 \text{ J/mol-K}}\right) \frac{1}{\ln\left[\dfrac{(6.2 \times 10^{-7} \text{ m}^2/\text{s})(0.65 \text{ kg/m}^3 - 0.30 \text{ kg/m}^3)}{(1.43 \times 10^{-9} \text{ kg/m}^2\text{-s})(15 \times 10^{-3} \text{ m})}\right]}$$

$$= 1044 \text{ K} = 771^\circ\text{C}$$

5.25 The steady-state diffusion flux through a metal plate is 5.4×10^{-10} kg/m^2-s at a temperature of 727°C (1000 K) and when the concentration gradient is -350 kg/m^4. Calculate the diffusion flux at 1027°C (1300 K) for the same concentration gradient and assuming an activation energy for diffusion of 125,000 J/mol.

Solution

In order to solve this problem, we must first compute the value of D_0 from the data given at 727°C (1000 K); this requires the combining of both Equations 5.3 and 5.8 as

$$J = -D\frac{\Delta C}{\Delta x}$$

$$= -D_0\frac{\Delta C}{\Delta x}\exp\left(-\frac{Q_d}{RT}\right)$$

Solving for D_0 from the above expression gives

$$D_0 = -\frac{J}{\frac{\Delta C}{\Delta x}}\exp\left(\frac{Q_d}{RT}\right)$$

$$= -\left(\frac{5.4 \times 10^{-10}\ \text{kg/m}^2\text{-s}}{-350\ \text{kg/m}^4}\right)\exp\left[\frac{125{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(1000\ \text{K})}\right]$$

$$= 5.26 \times 10^{-6}\ \text{m}^2/\text{s}$$

The value of the diffusion flux at 1300 K may be computed using these same two equations as follows:

$$J = -D_0\left(\frac{\Delta C}{\Delta x}\right)\exp\left(-\frac{Q_d}{RT}\right)$$

$$= -\left(5.26 \times 10^{-6}\ \text{m}^2/\text{s}\right)\left(-350\ \text{kg/m}^4\right)\exp\left[-\frac{125{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(1300\ \text{K})}\right]$$

$$= 1.74 \times 10^{-8}\ \text{kg/m}^2\text{-s}$$

5.26 At approximately what temperature would a specimen of iron have to be carburized for 2 h to produce the same diffusion result as at 900qC for 15 h?

Solution

To solve this problem it is necessary to employ Equation 5.7

$$Dt = \text{constant}$$

Which, for this problem, takes the form

$$D_{900}t_{900} = D_T t_T$$

At 900qC, and using the data from Table 5.2, for the diffusion of carbon in J-iron—i.e.,

D_0 = 2.3 u10^{-5} m^2/s

Q_d = 148,000 J/mol

the diffusion coefficient is equal to

$$D_{900} = \left(2.3 \ \text{u}\, 10^{-5} \ \text{m}^2/\text{s}\right) \exp \left[\frac{148{,}000 \ \text{J/mol}}{(8.31 \ \text{J/mol-K})(900 \quad 273 \ \text{K})} \right]$$

$$= 5.9 \ \text{u}10^{-12} \ \text{m}^2/\text{s}$$

Thus, from the above equation

$$\left(5.9 \ \text{u}\, 10^{-12} \ \text{m}^2/\text{s}\right)(15 \ \text{h}) = D_T (2 \ \text{h})$$

And, solving for D_T

$$D_T = \frac{\left(5.9 \ \text{u}10^{-12} \ \text{m}^2/\text{s}\right)(15 \ \text{h})}{2 \ \text{h}} = 4.43 \ \text{u}\, 10^{-11} \ \text{m}^2/\text{s}$$

Now, solving for T from Equation 5.9a gives

$$T = \frac{Q_d}{R\left(\ln D_T \quad \ln D_0\right)}$$

$$= \frac{148{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})\left[\ln\left(4.43\times10^{-11}\ \text{m}^2/\text{s}\right) - \ln\left(2.3\times10^{-5}\ \text{m}^2/\text{s}\right)\right]}$$

$$= 1353\text{K} = 1080^\circ\text{C}$$

5.27 (a) Calculate the diffusion coefficient for copper in aluminum at 500ºC.

(b) What time will be required at 600ºC to produce the same diffusion result (in terms of concentration at a specific point) as for 10 h at 500ºC?

Solution

(a) We are asked to calculate the diffusion coefficient for Cu in Al at 500°C. Using the data in Table 5.2 and Equation 5.8

$$D = D_0 \exp\left(-\frac{Q_d}{RT}\right)$$

$$= \left(6.5 \times 10^{-5}\ \mathrm{m^2/s}\right) \exp\left[-\frac{136{,}000\ \mathrm{J/mol}}{(8.31\ \mathrm{J/mol\text{-}K})(500 + 273\ \mathrm{K})}\right]$$

$$= 4.15 \times 10^{-14}\ \mathrm{m^2/s}$$

(b) This portion of the problem calls for the time required at 600°C to produce the same diffusion result as for 10 h at 500°C. Equation 5.7 is employed as

$$D_{500}t_{500} = D_{600}t_{600}$$

Now, from Equation 5.8 the value of the diffusion coefficient at 600°C is calculated as

$$D_{600} = \left(6.5 \times 10^{-5}\ \mathrm{m^2/s}\right) \exp\left[-\frac{136{,}000\ \mathrm{J/mol}}{(8.31\ \mathrm{J/mol\text{-}K})(600 + 273\ \mathrm{K})}\right]$$

$$= 4.69 \times 10^{-13}\ \mathrm{m^2/s}$$

Thus,

$$t_{600} = \frac{D_{500}t_{500}}{D_{600}}$$

$$= \frac{\left(4.15 \times 10^{-14}\ \mathrm{m^2/s}\right)(10\ \mathrm{h})}{\left(4.69 \times 10^{-13}\ \mathrm{m^2/s}\right)} = 0.88\ \mathrm{h}$$

5.28 A copper-nickel diffusion couple similar to that shown in Figure 5.1a is fashioned. After a 700-h heat treatment at 1100°C (1373 K) the concentration of Cu is 2.5 wt% at the 3.0-mm position within the nickel. At what temperature must the diffusion couple need to be heated to produce this same concentration (i.e., 2.5 wt% Cu) at a 2.0-mm position after 700 h? The preexponential and activation energy for the diffusion of Cu in Ni are given in Table 5.2.

Solution

In order to determine the temperature to which the diffusion couple must be heated so as to produce a concentration of 2.5 wt% Ni at the 2.0-mm position, we must first utilize Equation 5.6b with time t being a constant. That is

$$\frac{x^2}{D} = \text{constant}$$

Or

$$\frac{x_{1100}^2}{D_{1100}} = \frac{x_T^2}{D_T}$$

Now, solving for D_T from this equation, yields

$$D_T = \frac{x_T^2 D_{1100}}{x_{1100}^2}$$

and incorporating the temperature dependence of D_{1100} utilizing Equation (5.8), realizing that for the diffusion of Cu in Ni (Table 5.2)

$D_0 = 2.7 \times 10^{-5}\ \text{m}^2/\text{s}$

$Q_d = 256{,}000\ \text{J/mol}$

then

$$D_T = \frac{x_T^2 \left[D_0 \exp\left(-\frac{Q_d}{RT}\right)\right]}{x_{1100}^2}$$

$$= \frac{(2\ \text{mm})^2 \left[(2.7 \times 10^{-5}\ \text{m}^2/\text{s}) \exp\left(-\frac{256{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(1373\ \text{K})}\right)\right]}{(3\ \text{mm})^2}$$

$$= 2.16 \times 10^{-15}\ \mathrm{m^2/s}$$

We now need to find the T at which D has this value. This is accomplished by rearranging Equation 5.9a and solving for T as

$$T = \frac{Q_d}{R\left(\ln D_0 \quad \ln D\right)}$$

$$= \frac{256{,}000\ \mathrm{J/mol}}{(8.31\ \mathrm{J/mol\text{-}K})\ \ln\left(2.7 \times 10^{-5}\ \mathrm{m^2/s}\right) \quad \ln\left(2.16 \times 10^{-15}\ \mathrm{m^2/s}\right)}$$

$$= 1325\ \mathrm{K} = 1052^\circ\mathrm{C}$$

5.29 A diffusion couple similar to that shown in Figure 5.1a is prepared using two hypothetical metals A and B. After a 30-h heat treatment at 1000 K (and subsequently cooling to room temperature) the concentration of A in B is 3.2 wt% at the 15.5-μm position within metal B. If another heat treatment is conducted on an identical diffusion couple, only at 800 K for 30 h, at what position will the composition be 3.2 wt% A? Assume that the preexponential and activation energy for the diffusion coefficient are 1.8×10^{-5} m^2/s and 152,000 J/mol, respectively.

Solution

In order to determine the position within the diffusion couple at which the concentration of A in B is 3.2 wt%, we must employ Equation 5.6b with Dt constant. That is

$$\frac{x^2}{D} = \text{constant}$$

Or

$$\frac{x_{800}^2}{D_{800}} = \frac{x_{1000}^2}{D_{1000}}$$

It is first necessary to compute values for both D_{800} and D_{1000}; this is accomplished using Equation 5.8 as follows:

$$D_{800} = \left(1.8 \times 10^{-5}\ \text{m}^2/\text{s}\right) \exp\left[-\frac{152{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(800\ \text{K})}\right]$$

$$= 2.12 \times 10^{-15}\ \text{m}^2/\text{s}$$

$$D_{1000} = \left(1.8 \times 10^{-5}\ \text{m}^2/\text{s}\right) \exp\left[-\frac{152{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(1000\ \text{K})}\right]$$

$$= 2.05 \times 10^{-13}\ \text{m}^2/\text{s}$$

Now, solving the above expression for x_{800} yields

$$x_{800} = x_{1000}\sqrt{\frac{D_{800}}{D_{1000}}}$$

$$= (15.5\ \text{mm})\sqrt{\frac{2.12 \times 10^{15}\ \text{m}^2/\text{s}}{2.05 \times 10^{13}\ \text{m}^2/\text{s}}}$$

$$= 1.6\ \text{mm}$$

5.30 The outer surface of a steel gear is to be hardened by increasing its carbon content. The carbon is to be supplied from an external carbon-rich atmosphere, which is maintained at an elevated temperature. A diffusion heat treatment at 850°C (1123 K) for 10 min increases the carbon concentration to 0.90 wt% at a position 1.0 mm below the surface. Estimate the diffusion time required at 650°C (923 K) to achieve this same concentration also at a 1.0-mm position. Assume that the surface carbon content is the same for both heat treatments, which is maintained constant. Use the diffusion data in Table 5.2 for C diffusion in γ-Fe.

Solution

In order to compute the diffusion time at 650°C to produce a carbon concentration of 0.90 wt% at a position 1.0 mm below the surface we must employ Equation 5.6b with position (x) constant; that is

$$Dt = \text{constant}$$

Or

$$D_{850}t_{850} = D_{650}t_{650}$$

In addition, it is necessary to compute values for both D_{850} and D_{650} using Equation 5.8. From Table 5.2, for the diffusion of C in γ-Fe, Q_d = 80,000 J/mol and $D_0 = 6.2 \times 10^{-7}$ m^2/s. Therefore,

$$D_{850} = \left(6.2 \times 10^{-7}\ \text{m}^2/\text{s}\right) \exp\left[-\frac{80{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(850 + 273\ \text{K})}\right]$$

$$= 1.17 \times 10^{-10}\ \text{m}^2/\text{s}$$

$$D_{650} = \left(6.2 \times 10^{-7}\ \text{m}^2/\text{s}\right) \exp\left[-\frac{80{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(650 + 273\ \text{K})}\right]$$

$$= 1.83 \times 10^{-11}\ \text{m}^2/\text{s}$$

Now, solving the original equation for t_{650} gives

$$t_{650} = \frac{D_{850}t_{850}}{D_{650}}$$

$$= \frac{\left(1.17 \times 10^{10}\ \text{m}^2/\text{s}\right)(10\ \text{min})}{1.83 \times 10^{11}\ \text{m}^2/\text{s}}$$

$$= 63.9\ \text{min}$$

5.31 An FCC iron-carbon alloy initially containing 0.20 wt% C is carburized at an elevated temperature and in an atmosphere wherein the surface carbon concentration is maintained at 1.0 wt%. If after 49.5 h the concentration of carbon is 0.35 wt% at a position 4.0 mm below the surface, determine the temperature at which the treatment was carried out.

Solution

This problem asks us to compute the temperature at which a nonsteady-state 49.5 h diffusion anneal was carried out in order to give a carbon concentration of 0.35 wt% C in FCC Fe at a position 4.0 mm below the surface. From Equation 5.5

$$\frac{C_x - C_0}{C_s - C_0} = \frac{0.35 - 0.20}{1.0 - 0.20} = 0.1875 = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

Or

$$\operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) = 0.8125$$

Now it becomes necessary, using the data in Table 5.1 and linear interpolation, to determine the value of $\frac{x}{2\sqrt{Dt}}$.

Thus

z	erf (z)
0.90	0.7970
y	0.8125
0.95	0.8209

$$\frac{y - 0.90}{0.95 - 0.90} = \frac{0.8125 - 0.7970}{0.8209 - 0.7970}$$

From which

$$y = 0.9324$$

Thus,

$$\frac{x}{2\sqrt{Dt}} = 0.9324$$

And since t = 49.5 h (178,200 s) and x = 4.0 mm (4.0×10^{-3} m), solving for D from the above equation yields

$$D = \frac{x^2}{(4t)(0.9324)^2}$$

$$= \frac{(4.0 \times 10^{-3} \text{ m})^2}{(4)(178{,}200 \text{ s})(0.869)} = 2.58 \times 10^{-11} \text{ m}^2/\text{s}$$

Now, in order to determine the temperature at which D has the above value, we must employ Equation 5.9a; solving this equation for T yields

$$T = \frac{Q_d}{R(\ln D_0 - \ln D)}$$

From Table 5.2, D_0 and Q_d for the diffusion of C in FCC Fe are 2.3×10^{-5} m^2/s and 148,000 J/mol, respectively. Therefore

$$T = \frac{148{,}000 \text{ J/mol}}{(8.31 \text{ J/mol-K})\left[\ln(2.3 \times 10^{-5} \text{ m}^2/\text{s}) - \ln(2.58 \times 10^{-11} \text{ m}^2/\text{s})\right]}$$

$$= 1300 \text{ K} = 1027°\text{C}$$

Diffusion in Semiconducting Materials

5.32 Phosphorus atoms are to be diffused into a silicon wafer using both predeposition and drive-in heat treatments; the background concentration of P in this silicon material is known to be 5×10^{19} atoms/m^3. The predeposition treatment is to be conducted at 950°C for 45 minutes; the surface concentration of P is to be maintained at a constant level of 1.5×10^{26} atoms/m^3. Drive-in diffusion will be carried out at 1200°C for a period of 2.5 h. For the diffusion of P in Si, values of Q_d and D_0 are 3.40 eV and 1.1×10^{-4} m^2/s, respectively.

(a) Calculate the value of Q_0.

(b) Determine the value of x_j for the drive-in diffusion treatment.

(c) Also for the drive-in treatment, compute the position x at which the concentration of P atoms is 10^{24} m^{-3}.

Solution

(a) For this portion of the problem we are asked to determine the value of Q_0. This is possible using Equation 5.12. However, it is first necessary to determine the value of D for the predeposition treatment [D_p at T_p = 950°C (1223 K)] using Equation 5.8. Thus

$$D_p = D_0 \exp\left(-\frac{Q_d}{kT_p}\right)$$

$$= (1.1 \times 10^{-4}\ \text{m}^2/\text{s}) \exp\left[-\frac{3.40\ \text{eV}}{(8.62 \times 10^{-5}\ \text{eV/atom-K})(1223\ \text{K})}\right]$$

$$= 1.08 \times 10^{-18}\ \text{m}^2/\text{s}$$

The value of Q_0 may be determined as follows:

$$Q_0 = 2C_s \sqrt{\frac{D_p t_p}{\pi}}$$

$$= (2)(1.5 \times 10^{26}\ \text{atoms/m}^3) \sqrt{\frac{(1.08 \times 10^{-18}\ \text{m}^2/\text{s})(45\ \text{min})(60\ \text{s/min})}{\pi}}$$

$$= 9.14 \times 10^{18}\ \text{atoms/m}^2$$

(b) Computation of the junction depth requires that we use Equation 5.13. However, before this is possible it is necessary to calculate D at the temperature of the drive-in treatment [D_d at 1200°C (1473 K)]. Thus,

$$D_d = (1.1 \times 10^{-4}\ \text{m}^2/\text{s}) \exp\left[-\frac{3.40\ \text{eV}}{(8.62 \times 10^{-5}\ \text{eV/atom-K})(1473\ \text{K})}\right]$$

$$= 2.58 \times 10^{-16}\ \text{m}^2/\text{s}$$

Now from Equation 5.13

$$x_j = \left[(4D_d t_d) \ln\left(\frac{Q_0}{C_B\sqrt{\pi D_d t_d}}\right)\right]^{1/2}$$

$$= \left\{(4)(2.58 \times 10^{-16}\ \text{m}^2/\text{s})(9000\ \text{s}) \ln\left[\frac{9.14 \times 10^{18}\ \text{atoms/m}^2}{(5 \times 10^{19}\ \text{atoms/m}^3)\sqrt{(\pi)(2.58 \times 10^{-16}\ \text{m}^2/\text{s})(9000\ \text{s})}}\right]\right\}^{1/2}$$

$$= 1.21 \times 10^{-5}\ \text{m} = 12.1\ \mu\text{m}$$

(c) For a concentration of 10^{24} P atoms/m^3 for the drive-in treatment, we compute the value of x using Equation 5.11. However, it is first necessary to manipulate Equation 5.11 so that x is the dependent variable. Taking natural logarithms of both sides leads to

$$\ln C(x,t) = \ln\left(\frac{Q_0}{\sqrt{\pi D_d t_d}}\right) - \frac{x^2}{4D_d t_d}$$

Now, rearranging and solving for x leads to

$$x = \left\{(4D_d t_d) \ln\left[\frac{Q_0}{C(x,t)\sqrt{\pi D_d t_d}}\right]\right\}^{1/2}$$

Now, incorporating values for Q_0 and D_d determined above and taking $C(x,t) = 10^{24}$ P atoms/m^3 yields

$$x = \left\{(4)(2.58 \times 10^{-16})(9000) \ln\left[\frac{9.14 \times 10^{18}}{(10^{24})\sqrt{(\pi)(2.58 \times 10^{-16})(9000)}}\right]\right\}^{1/2}$$

$$3.36 \times 10^{6} \text{ m} \qquad 3.36\ \mu\text{m}$$

5.33 Aluminum atoms are to be diffused into a silicon wafer using both predeposition and drive-in heat treatments; the background concentration of Al in this silicon material is known to be 3×10^{19} atoms/m^3. The drive-in diffusion treatment is to be carried out at 1050°C for a period of 4.0 h, which gives a junction depth x_j of 3.0 μm. Compute the predeposition diffusion time at 950°C if the surface concentration is maintained at a constant level of 2×10^{25} atoms/m^3. For the diffusion of Al in Si, values of Q_d and D_0 are 3.41 eV and 1.38×10^{-4} m^2/s, respectively.

Solution

This problem asks that we compute the time for the predeposition heat treatment for the diffusion of Al in Si. In order to do this it is necessary to determine the value of Q_0 from Equation 5.13. However, before doing this we must first calculate D_d, using Equation 5.8. Therefore

$$D_d = D_0 \exp\left(-\frac{Q_d}{kT_d}\right)$$

$$= (1.38 \times 10^{-4}\ \mathrm{m^2/s}) \exp\left[-\frac{3.41\ \mathrm{eV}}{(8.62 \times 10^{-5}\ \mathrm{eV/atom\text{-}K})(1050^\circ\mathrm{C} + 273\ \mathrm{K})}\right]$$

$$= 1.43 \times 10^{-17}\ \mathrm{m^2/s}$$

Now, solving for Q_0 in Equation 5.13 leads to

$$Q_0 = C_B \sqrt{\pi D_d t_d}\ \exp\left(\frac{x_j^2}{4D_d t_d}\right)$$

In the problem statement we are given the following values:

$C_B = 3 \times 10^{19}$ atoms/m^3

$t_d = 4$ h (14,400 s)

$x_j = 3.0\ \mu\mathrm{m} = 3.0 \times 10^{-6}$ m

Therefore, incorporating these values into the above equation yields

$$Q_0 = (3 \times 10^{19}\ \mathrm{atoms/m^3})\sqrt{(\pi)(1.43 \times 10^{-17}\ \mathrm{m^2/s})(14{,}400\ \mathrm{s})}\ \exp\left[\frac{(3.0 \times 10^{-6}\ \mathrm{m})^2}{(4)(1.43 \times 10^{-17}\ \mathrm{m^2/s})(14{,}400\ \mathrm{s})}\right]$$

$$= 1.34 \times 10^{18}\ \text{atoms/m}^2$$

We may now compute the value of t_p using Equation 5.12. However, before this is possible it is necessary to determine D_p (at 950°C) using Equation 5.8. Thus

$$D_p = (1.38 \times 10^{-4}\ \text{m}^2/\text{s})\exp\left[-\frac{3.41\ \text{eV}}{(8.62 \times 10^{-5}\ \text{eV/atom-K})(950°\text{C} + 273\ \text{K})}\right]$$

$$= 1.24 \times 10^{-18}\ \text{m}^2/\text{s}$$

Now, solving for t_p in Equation 5.12 we get

$$t_p = \frac{\pi Q_0^2}{4C_s^2 D_p}$$

And incorporating the value of C_s provided in the problem statement (2×10^{25} atoms/m^3) as well as values for Q_0 and D_p determined above, leads to

$$t_p = \frac{\pi\left(1.34 \times 10^{18}\ \text{atoms/m}^2\right)^2}{(4)\left(2 \times 10^{25}\ \text{atoms/m}^3\right)^2(1.24 \times 10^{-18}\ \text{m}^2/\text{s})}$$

$$= 2.84 \times 10^3\ \text{s} = 47.4\ \text{min}$$

DESIGN PROBLEMS

Steady-State Diffusion

5.D1 It is desired to enrich the partial pressure of hydrogen in a hydrogen-nitrogen gas mixture for which the partial pressures of both gases are 0.1013 MPa (1 atm). It has been proposed to accomplish this by passing both gases through a thin sheet of some metal at an elevated temperature; inasmuch as hydrogen diffuses through the plate at a higher rate than does nitrogen, the partial pressure of hydrogen will be higher on the exit side of the sheet. The design calls for partial pressures of 0.0709 MPa (0.7 atm) and 0.02026 MPa (0.2 atm), respectively, for hydrogen and nitrogen. The concentrations of hydrogen and nitrogen (C_H and C_N, in mol/m^3) in this metal are functions of gas partial pressures (p_{H_2} and p_{N_2}, in MPa) and absolute temperature and are given by the following expressions:

$$C_H \quad 2.5 \times 10^3 \sqrt{p_{H_2}} \exp\left(\frac{27.8 \text{ kJ/mol}}{RT}\right) \tag{5.16a}$$

$$C_N \quad 2.75 \times 10^3 \sqrt{p_{N_2}} \exp\left(\frac{37.6 \text{ kJ/mol}}{RT}\right) \tag{5.16b}$$

Furthermore, the diffusion coefficients for the diffusion of these gases in this metal are functions of the absolute temperature as follows:

$$D_H (\text{m}^2/\text{s}) \quad 1.4 \times 10^{7} \exp\left(\frac{13.4 \text{ kJ/mol}}{RT}\right) \tag{5.17a}$$

$$D_N (\text{m}^2/\text{s}) \quad 3.0 \times 10^{7} \exp\left(\frac{76.15 \text{ kJ/mol}}{RT}\right) \tag{5.17b}$$

Is it possible to purify hydrogen gas in this manner? If so, specify a temperature at which the process may be carried out, and also the thickness of metal sheet that would be required. If this procedure is not possible, then state the reason(s) why.

Solution

This problem calls for us to ascertain whether or not a hydrogen-nitrogen gas mixture may be enriched with respect to hydrogen partial pressure by allowing the gases to diffuse through a metal sheet at an elevated temperature. If this is possible, the temperature and sheet thickness are to be specified; if such is not possible, then we are to state the reasons why. Since this situation involves steady-state diffusion, we employ Fick's first law, Equation 5.3. Inasmuch as the partial pressures on the high-pressure side of the sheet are the same, and the pressure of hydrogen on the low pressure side is 3.5 times that of nitrogen, and concentrations are proportional to the square root of the partial pressure, the diffusion flux of hydrogen J_H is the square root of 3.5 times the diffusion flux of nitrogen J_N--i.e.

$$J_H = \sqrt{3.5}\, J_N$$

Thus, equating the Fick's law expressions incorporating the given equations for the diffusion coefficients and concentrations in terms of partial pressures leads to the following

$$J_H$$

$$= \frac{1}{\Delta x} \times (2.5 \times 10^{3}) \left(\sqrt{0.1013\ \mathrm{MPa}} - \sqrt{0.0709\ \mathrm{MPa}}\right) \exp\left(-\frac{27.8\ \mathrm{kJ}}{RT}\right) (1.4 \times 10^{-7}\ \mathrm{m^2/s}) \exp\left(-\frac{13.4\ \mathrm{kJ}}{RT}\right)$$

$$= \sqrt{3.5}\, J_N$$

$$= \frac{\sqrt{3.5}}{\Delta x} \times (2.75 \times 10^{3}) \left(\sqrt{0.1013\ \mathrm{MPa}} - \sqrt{0.02026\ \mathrm{MPa}}\right) \exp\left(-\frac{37.6\ \mathrm{kJ}}{RT}\right) (3.0 \times 10^{-7}\ \mathrm{m^2/s}) \exp\left(-\frac{76.15\ \mathrm{kJ}}{RT}\right)$$

The Δx's cancel out, which means that the process is independent of sheet thickness. Now solving the above expression for the absolute temperature T gives

$$T = 3237\ \mathrm{K}$$

which value is extremely high (surely above the melting point of the metal). Thus, such a diffusion process is not possible

5.D2 A gas mixture is found to contain two diatomic A and B species for which the partial pressures of both are 0.05065 MPa (0.5 atm). This mixture is to be enriched in the partial pressure of the A species by passing both gases through a thin sheet of some metal at an elevated temperature. The resulting enriched mixture is to have a partial pressure of 0.02026 MPa (0.2 atm) for gas A, and 0.01013 MPa (0.1 atm) for gas B. The concentrations of A and B (C_A and C_B, in mol/m^3) are functions of gas partial pressures (p_{A_2} and p_{B_2}, in MPa) and absolute temperature according to the following expressions:

$$C_A = 200\sqrt{p_{A_2}}\exp\left(-\frac{25.0\text{ kJ/mol}}{RT}\right) \tag{5.18a}$$

$$C_B = 1.0 \times 10^{3}\sqrt{p_{B_2}}\exp\left(-\frac{30.0\text{ kJ/mol}}{RT}\right) \tag{5.18b}$$

Furthermore, the diffusion coefficients for the diffusion of these gases in the metal are functions of the absolute temperature as follows:

$$D_A\,(\text{m}^2/\text{s}) = 4.0 \times 10^{-7}\exp\left(-\frac{15.0\text{ kJ/mol}}{RT}\right) \tag{5.19a}$$

$$D_B\,(\text{m}^2/\text{s}) = 2.5 \times 10^{-6}\exp\left(-\frac{24.0\text{ kJ/mol}}{RT}\right) \tag{5.19b}$$

Is it possible to purify the A gas in this manner? If so, specify a temperature at which the process may be carried out, and also the thickness of metal sheet that would be required. If this procedure is not possible, then state the reason(s) why.

Solution

This problem calls for us to ascertain whether or not an A_2-B_2 gas mixture may be enriched with respect to the A partial pressure by allowing the gases to diffuse through a metal sheet at an elevated temperature. If this is possible, the temperature and sheet thickness are to be specified; if such is not possible, then we are to state the reasons why. Since this situation involves steady-state diffusion, we employ Fick's first law, Equation 5.3. Inasmuch as the partial pressures on the high-pressure side of the sheet are the same, and the pressure of A_2 on the low pressure side is 2.0 times that of B_2, and concentrations are proportional to the square root of the partial pressure, the diffusion flux of A, J_A, is the square root of 2.0 times the diffusion flux of nitrogen—J_B—i.e.

$$J_A = \sqrt{2.0}\,J_B$$

Thus, equating the Fick's law expressions incorporating the given equations for the diffusion coefficients and concentrations in terms of partial pressures leads to the following

$$J_A = \frac{1}{\Delta x} \times (200)\left(\sqrt{0.05065\ \text{MPa}} - \sqrt{0.02026\ \text{MPa}}\right)\exp\left(-\frac{25.0\ \text{kJ}}{RT}\right)(4.0 \times 10^{-7}\ \text{m}^2/\text{s})\exp\left(-\frac{15.0\ \text{kJ}}{RT}\right)$$

$$\sqrt{2.0}\, J_B = \frac{\sqrt{2.0}}{\Delta x} \times (1.0 \times 10^{3})\left(\sqrt{0.05065\ \text{MPa}} - \sqrt{0.01013\ \text{MPa}}\right)\exp\left(-\frac{30.0\ \text{kJ}}{RT}\right)(2.5 \times 10^{-6}\ \text{m}^2/\text{s})\exp\left(-\frac{24.0\ \text{kJ}}{RT}\right)$$

The Δx's cancel out, which means that the process is independent of sheet thickness. Now solving the above expression for the absolute temperature T gives

$$T = 401\ \text{K}\ (128^\circ\text{C})$$

Thus, it is possible to carry out this procedure at 401 K or 128°C.

Nonsteady-State Diffusion

5.D3 The wear resistance of a steel shaft is to be improved by hardening its surface. This is to be accomplished by increasing the nitrogen content within an outer surface layer as a result of nitrogen diffusion into the steel. The nitrogen is to be supplied from an external nitrogen-rich gas at an elevated and constant temperature. The initial nitrogen content of the steel is 0.002 wt%, whereas the surface concentration is to be maintained at 0.50 wt%. For this treatment to be effective, a nitrogen content of 0.10 wt% must be established at a position 0.40 mm below the surface. Specify appropriate heat treatments in terms of temperature and time for temperatures between 475°C and 625°C. The preexponential and activation energy for the diffusion of nitrogen in iron are 3×10^{-7} m^2/s and 76,150 J/mol, respectively, over this temperature range.

Solution

This is a nonsteady-state diffusion situation; thus, it is necessary to employ Equation 5.5, utilizing the following values for the concentration parameters:

$$C_0 = 0.002 \text{ wt\% N}$$
$$C_s = 0.50 \text{ wt\% N}$$
$$C_x = 0.10 \text{ wt\% N}$$

Therefore

$$\frac{C_x - C_0}{C_s - C_0} = \frac{0.10 - 0.002}{0.50 - 0.002}$$

$$= 0.1968 = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

And thus

$$1 - 0.1968 = 0.8032 = \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

Using linear interpolation and the data presented in Table 5.1

<u>z</u>	<u>erf (z)</u>
0.9000	0.7970
y	0.8032
0.9500	0.8209

$$\frac{0.8032 - 0.7970}{0.8209 - 0.7970} = \frac{y - 0.9000}{0.9500 - 0.9000}$$

From which

$$y = \frac{x}{2\sqrt{Dt}} = 0.9130$$

The problem stipulates that x = 0.40 mm = 4.0×10^{-4} m. Therefore

$$\frac{4.0 \times 10^{-4}\ \text{m}}{2\sqrt{Dt}} = 0.9130$$

Which leads to

$$Dt = 4.80 \times 10^{-8}\ \text{m}^2$$

Furthermore, the diffusion coefficient depends on temperature according to Equation 5.8; and, as stipulated in the problem statement, $D_0 = 3 \times 10^{-7}$ m^2/s and Q_d = 76,150 J/mol. Hence

$$Dt = D_0 \exp\left(-\frac{Q_d}{RT}\right)(t) = 4.80 \times 10^{-8}\ \text{m}^2$$

$$\left(3.0 \times 10^{-7}\ \text{m}^2/\text{s}\right) \exp\left[-\frac{76{,}150\ \text{J/mol}}{(8.31\ \text{J/mol-K})(T)}\right](t) = 4.80 \times 10^{-8}\ \text{m}^2$$

And solving for the time t

$$t\ (\text{in s}) = \frac{0.160}{\exp\left(-\frac{9163.7}{T}\right)}$$

Thus, the required diffusion time may be computed for some specified temperature (in K). Below are tabulated t values for three different temperatures that lie within the range stipulated in the problem.

Temperature (°C)	Time	
	s	h
500	22,500	6.3
550	11,000	3.1
600	5800	1.6

Diffusion in Semiconducting Materials

5.D4 One integrated circuit design calls for the diffusion of arsenic into silicon wafers; the background concentration of As in Si is 2.5×10^{20} atoms/m^3. The predeposition heat treatment is to be conducted at 1000°C for 45 minutes, with a constant surface concentration of 8×10^{26} As atoms/m^3. At a drive-in treatment temperature of 1100°C, determine the diffusion time required for a junction depth of 1.2 μm. For this system, values of Q_d and D_0 are 4.10 eV and 2.29×10^{-3} m^2/s, respectively.

Solution

This problem asks that we compute the drive-in diffusion time for arsenic diffusion in silicon. It is first necessary to determine the value of Q_0 using Equation 5.12. But before this is possible, the value of D_p at 1000°C must be computed with the aid of Equation 5.8. Thus,

$$D_p = D_0 \exp\left(-\frac{Q_d}{kT_p}\right)$$

$$= (2.29 \times 10^{-3}\ \text{m}^2/\text{s}) \exp\left[-\frac{4.10\ \text{eV}}{(8.62 \times 10^{-5}\ \text{eV/atom-K})(1000^\circ\text{C} + 273\ \text{K})}\right]$$

$$= 1.36 \times 10^{-19}\ \text{m}^2/\text{s}$$

Now for the computation of Q_0 using Equation 5.12:

$$Q_0 = 2C_s \sqrt{\frac{D_p t_p}{\pi}}$$

$$= (2)(8 \times 10^{26}\ \text{atoms/m}^3) \sqrt{\frac{(1.36 \times 10^{-19}\ \text{m}^2/\text{s})(45\ \text{min})(60\ \text{s/min})}{\pi}}$$

$$= 1.73 \times 10^{19}\ \text{atoms/m}^2$$

We now desire to calculate t_d in Equation 5.13. Algebraic manipulation and rearrangement of this expression leads to

$$\exp\left(-\frac{x_j^2}{4D_d t_d}\right) = \frac{Q_0}{C_B\sqrt{\pi D_d t_d}}$$

At this point it is necessary to determine the value of D_d (at 1100°C). Thus

$$D_d = (2.29 \times 10^{-3}\ \text{m}^2/\text{s}) \exp\left[-\frac{4.10\ \text{eV}}{(8.62 \times 10^{-5}\ \text{eV/atom-K})(1100^\circ\text{C} + 273\ \text{K})}\right]$$

$$= 2.06 \times 10^{-18}\ \text{m}^2/\text{s}$$

And incorporation of values of all parameters except t_d in the above expression yields

$$\exp\left[-\frac{(1.2 \times 10^{-6}\ \text{m})^2}{(4)(2.06 \times 10^{-18}\ \text{m}^2/\text{s})t_d}\right] = \frac{1.73 \times 10^{19}\ \text{atoms/m}^2}{(2.5 \times 10^{20}\ \text{atoms/m}^3)\sqrt{(\pi)(2.06 \times 10^{-18}\ \text{m}^2/\text{s})t_d}}$$

which expression reduces to

$$\exp\left(-\frac{1.75 \times 10^{5}\ \text{s}}{t_d}\right) = \frac{2.72 \times 10^{7}\ \text{s}^{1/2}}{\sqrt{t_d}}$$

Solving for t_d is not a simple matter. One possibility is to use a graphing technique. Let us take the logarithm of both sides of the above equation, which gives

$$-\frac{1.75 \times 10^{5}\ \text{s}}{t_d} = \ln\left(\frac{2.72 \times 10^{7}\ \text{s}^{1/2}}{\sqrt{t_d}}\right)$$

Now if we plot the terms on both left and right hand sides of this equation versus t_d, the value of t_d at the point of intersection of the two resulting curves is correct answer. Below is such a plot:

As noted, the two curves intersect at about 13,900 s, which corresponds to $t_d = 3.86$ h.

$$W = \frac{V}{A}$$

For static equilibrium in the x' direction the following condition must be met:

$$¦ F_{x'} = 0$$

which means that

$$PÖ \quad P \cos T = 0$$

Or that

$$P' = P \cos T$$

Now it is possible to write an expression for the stress V' in terms of P' and A' using the above expression and the relationship between A and A' [Figure (a)]:

$$V' = \frac{PC̃}{AC̃}$$

$$= \frac{P \cos T}{\frac{A}{\cos T}} = \frac{P}{A} \cos^2 T$$

However, it is the case that P/A = V, and, after making this substitution into the above expression, we have Equation 6.4a—that is

$$V' = V\cos^2 T$$

Now, for static equilibrium in the y' direction, it is necessary that

$$¦ F_{yÕ} = 0$$

$$= VÖ + P\sin T$$

Or

$$V' = P\sin T$$

We now write an expression for W' as

$$W\tilde{O} = \frac{V\tilde{C}}{A\hat{C}}$$

And, substitution of the above equation for V' and also the expression for A' gives

$$W' = \frac{V\tilde{C}}{A\hat{C}}$$

$$= \frac{\frac{P\sin T}{A}}{\cos T}$$

$$= \frac{P}{A}\sin T\cos T$$

$$= V\sin T\cos T$$

which is just Equation 6.4b.

6.2 (a) Equations 6.4a and 6.4b are expressions for normal (1(• DQG VKHDU 2 • VWUHVVHV U
IXQFWLRQ RI WKH DSSOLHG WHQVLOH VWUHVV 1 DQG WKH LQFOLQDW
of Figure 6.4). Make a plot on which is presented the orientation parameters of these expressions (i.e., cos^2 DQG
VLQ FRV YHUVXV

(b) From this plot, at what angle of inclination is the normal stress a maximum?

(c) Also, at what inclination angle is the shear stress a maximum?

Solution

(a) Below are plotted curves of cos^{2}T (for V′) and sin T cos T (for V′) versus T.

(b) The maximum normal stress occurs at an inclination angle of 0 q.

(c) The maximum shear stress occurs at an inclination angle of 45 q.

Stress-Strain Behavior

6.3 A specimen of aluminum having a rectangular cross section 10 mm × 12.7 mm (0.4 in. × 0.5 in.) is pulled in tension with 35,500 N (8000 lbf) force, producing only elastic deformation. Calculate the resulting strain.

Solution

This problem calls for us to calculate the elastic strain that results for an aluminum specimen stressed in tension. The cross-sectional area is just (10 mm)(12.7 mm) = 127 mm^2 (= 1.27 × 10^{-4} m^2 = 0.20 in.^{2}); also, the elastic modulus for Al is given in Table 6.1 as 69 GPa (or 69 × 10^9 N/m^2). Combining Equations 6.1 and 6.5 and solving for the strain yields

$$\varepsilon = \frac{\sigma}{E} = \frac{F}{A_0 E} = \frac{35{,}500\ \text{N}}{\left(1.27 \times 10^{-4}\ \text{m}^2\right)\left(69 \times 10^{9}\ \text{N/m}^2\right)} = 4.1 \times 10^{-3}$$

6.4 A cylindrical specimen of a titanium alloy having an elastic modulus of 107 GPa (15.5×10^6 psi) and an original diameter of 3.8 mm (0.15 in.) will experience only elastic deformation when a tensile load of 2000 N (450 $\mathrm{lb_f}$) is applied. Compute the maximum length of the specimen before deformation if the maximum allowable elongation is 0.42 mm (0.0165 in.).

<u>Solution</u>

We are asked to compute the maximum length of a cylindrical titanium alloy specimen (before deformation) that is deformed elastically in tension. For a cylindrical specimen

$$A_0 = \pi \left(\frac{d_0}{2}\right)^2$$

where d_0 is the original diameter. Combining Equations 6.1, 6.2, and 6.5 and solving for l_0 leads to

$$l_0 = \frac{\Delta l}{\varepsilon} = \frac{\Delta l}{\dfrac{\sigma}{E}} = \frac{\Delta l E}{\dfrac{F}{A_0}} = \frac{\Delta l E \pi \left(\dfrac{d_0}{2}\right)^2}{F} = \frac{\Delta l E \pi d_0^2}{4F}$$

$$= \frac{(0.42 \times 10^{-3}\ \mathrm{m})(107 \times 10^9\ \mathrm{N/m^2})\,(\pi)(3.8 \times 10^{-3}\ \mathrm{m})^2}{(4)(2000\ \mathrm{N})}$$

= 0.255 m = 255 mm (10.0 in.)

6.5 A steel bar 100 mm (4.0 in.) long and having a square cross section 20 mm (0.8 in.) on an edge is pulled in tension with a load of 89,000 N (20,000 lb_f), and experiences an elongation of 0.10 mm (4.0×10^{-3} in.). Assuming that the deformation is entirely elastic, calculate the elastic modulus of the steel.

Solution

This problem asks us to compute the elastic modulus of steel. For a square cross-section, $A_0 = b_0^2$, where b_0 is the edge length. Combining Equations 6.1, 6.2, and 6.5 and solving for E leads to

$$E = \frac{\sigma}{\varepsilon} = \frac{\dfrac{F}{A_0}}{\dfrac{\Delta l}{l_0}} = \frac{F l_0}{b_0^2 \, \Delta l}$$

$$= \frac{(89{,}000\ \text{N})\left(100 \times 10^{-3}\ \text{m}\right)}{\left(20 \times 10^{-3}\ \text{m}\right)^2 \left(0.10 \times 10^{-3}\ \text{m}\right)}$$

$$= 223 \times 10^{9}\ \text{N/m}^2 = 223\ \text{GPa}\ \ (31.3 \times 10^{6}\ \text{psi})$$

6.6 Consider a cylindrical titanium wire 3.0 mm (0.12 in.) in diameter and 2.5×10^4 mm (1000 in.) long. Calculate its elongation when a load of 500 N (112 $\mathrm{lb_f}$) is applied. Assume that the deformation is totally elastic.

Solution

In order to compute the elongation of the Ti wire when the 500 N load is applied we must employ Equations 6.1, 6.2, and 6.5, solving for Δl and realizing that for Ti, E = 107 GPa (15.5×10^6 psi) (Table 6.1),

$$\Delta l = l_0 \varepsilon = l_0 \frac{\sigma}{E} = \frac{l_0 F}{E A_0} = \frac{l_0 F}{E \pi \left(\frac{d_0}{2}\right)^2} = \frac{4 l_0 F}{E \pi d_0^2}$$

$$= \frac{(4)(25\ \mathrm{m})(500\ \mathrm{N})}{\left(107 \times 10^9\ \mathrm{N/m^2}\right)(\pi)\left(3 \times 10^{-3}\ \mathrm{m}\right)^2} = 0.0165\ \mathrm{m} = 16.5\ \mathrm{mm}\ \ (0.65\ \mathrm{in.})$$

6.7 For a bronze alloy, the stress at which plastic deformation begins is 275 MPa (40,000 psi), and the modulus of elasticity is 115 GPa (16.7×10^6 psi).

(a) What is the maximum load that may be applied to a specimen with a cross-sectional area of 325 mm^2 (0.5 $\mathrm{in.}^2$) without plastic deformation?

(b) If the original specimen length is 115 mm (4.5 in.), what is the maximum length to which it may be stretched without causing plastic deformation?

Solution

(a) This portion of the problem calls for a determination of the maximum load that can be applied without plastic deformation (F_y). Taking the yield strength to be 275 MPa, and employment of Equation 6.1 leads to

$$F_y = \sigma_y A_0 = (275 \times 10^6\ \mathrm{N/m^2})(325 \times 10^{-6}\ \mathrm{m^2})$$

$$= 89{,}375\ \mathrm{N} \quad (20{,}000\ \mathrm{lb_f})$$

(b) The maximum length to which the sample may be deformed without plastic deformation is determined from Equations 6.2 and 6.5 as

$$l_i = l_0 \left(1 + \frac{\sigma}{E}\right)$$

$$= (115\ \mathrm{mm}) \left[1 + \frac{275\ \mathrm{MPa}}{115 \times 10^3\ \mathrm{MPa}}\right] = 115.28\ \mathrm{mm}\ (4.51\ \mathrm{in.})$$

6.8 A cylindrical rod of copper (E = 110 GPa, 16×10^6 psi) having a yield strength of 240 MPa (35,000 psi) is to be subjected to a load of 6660 N (1500 $\mathrm{lb_f}$). If the length of the rod is 380 mm (15.0 in.), what must be the diameter to allow an elongation of 0.50 mm (0.020 in.)?

Solution

This problem asks us to compute the diameter of a cylindrical specimen of copper in order to allow an elongation of 0.50 mm. Employing Equations 6.1, 6.2, and 6.5, assuming that deformation is entirely elastic

$$\sigma = \frac{F}{A_0} = \frac{F}{\pi\left(\dfrac{d_0^2}{4}\right)} = E\,\frac{\Delta l}{l_0}$$

Or, solving for d_0

$$d_0 = \sqrt{\frac{4\,l_0 F}{\pi E\,\Delta l}}$$

$$= \sqrt{\frac{(4)\left(380 \times 10^{-3}\ \mathrm{m}\right)(6660\ \mathrm{N})}{(\pi)\left(110 \times 10^{9}\ \mathrm{N/m^2}\right)\left(0.50 \times 10^{-3}\ \mathrm{m}\right)}}$$

$$= 7.65 \times 10^{-3}\ \mathrm{m} = 7.65\ \mathrm{mm}\ \ (0.30\ \mathrm{in.})$$

6.9 Compute the elastic moduli for the following metal alloys, whose stress-strain behaviors may be observed in the "Tensile Tests" module of Virtual Materials Science and Engineering (VMSE): (a) titanium, (b) tempered steel, (c) aluminum, and (d) carbon steel. How do these values compare with those presented in Table 6.1 for the same metals?

Solution

The elastic modulus is the slope in the linear elastic region (Equation 6.10) as

$$E = \frac{\Delta\sigma}{\Delta\varepsilon} = \frac{\sigma_2 - \sigma_1}{\varepsilon_2 - \varepsilon_1}$$

Since stress-strain curves for all of the metals/alloys pass through the origin, we make take $\sigma_1 = 0$ and $\varepsilon_1 = 0$. Determinations of σ_2 and ε_2 are possible by moving the cursor to some arbitrary point in the linear region of the curve and then reading corresponding values in the "Stress" and "Strain" windows that are located below the plot.

(a) For the titanium alloy, we selected σ_2 = 404.2 MPa with its corresponding ε_2 = 0.0038. Therefore,

$$E = \frac{\sigma_2 - \sigma_1}{\varepsilon_2 - \varepsilon_1} = \frac{404.2\ \text{MPa} - 0\ \text{MPa}}{0.0038 - 0} = 106{,}400\ \text{MPa} = 106.4\ \text{GPa}$$

The elastic modulus for titanium given in Table 6.1 is 107 GPa, which is in very good agreement with this value.

(b) For the tempered steel, we selected σ_2 = 962.2 MPa with its corresponding ε_2 = 0.0047. Therefore,

$$E = \frac{\sigma_2 - \sigma_1}{\varepsilon_2 - \varepsilon_1} = \frac{962.2\ \text{MPa} - 0\ \text{MPa}}{0.0047 - 0} = 204{,}700\ \text{MPa} = 204.7\ \text{GPa}$$

The elastic modulus for steel given in Table 6.1 is 207 GPa, which is in reasonably good agreement with this value.

(c) For the aluminum, we selected σ_2 = 145.1 MPa with its corresponding ε_2 = 0.0021. Therefore,

$$E = \frac{\sigma_2 \quad \sigma_1}{\varepsilon_2 \quad \varepsilon_1} \qquad \frac{145.1\text{ MPa} \quad 0\text{ MPa}}{0.0021 \quad 0} \qquad 69{,}100\text{ MPa} \qquad 69.1\text{ GPa}$$

The elastic modulus for aluminum given in Table 6.1 is 69 GPa, which is in excellent agreement with this value.

(d) For the carbon steel, we selected σ_2 = 129 MPa with its corresponding ε_2 = 0.0006. Therefore,

$$E = \frac{\sigma_2 \quad \sigma_1}{\varepsilon_2 \quad \varepsilon_1} \qquad \frac{129\text{ MPa} \quad 0\text{ MPa}}{0.0006 \quad 0} \qquad 215{,}000\text{ MPa} \qquad 215\text{ GPa}$$

The elastic modulus for steel given in Table 6.1 is 207 GPa, which is in reasonable agreement with this value.

6.10 Consider a cylindrical specimen of a steel alloy (Figure 6.21) 10.0 mm (0.39 in.) in diameter and 75 mm (3.0 in.) long that is pulled in tension. Determine its elongation when a load of 20,000 N (4,500 lb$_f$) is applied.

Solution

This problem asks that we calculate the elongation Δl of a specimen of steel the stress-strain behavior of which is shown in Figure 6.21. First it becomes necessary to compute the stress when a load of 20,000 N is applied using Equation 6.1 as

$$\sigma = \frac{F}{A_0} = \frac{F}{\pi\left(\frac{d_0}{2}\right)^2} = \frac{20{,}000\ \mathrm{N}}{\pi\left(\frac{10.0 \times 10^{-3}\ \mathrm{m}}{2}\right)^2} = 255\ \mathrm{MPa}\ (37{,}700\ \mathrm{psi})$$

Referring to Figure 6.21, at this stress level we are in the elastic region on the stress-strain curve, which corresponds to a strain of 0.0012. Now, utilization of Equation 6.2 to compute the value of Δl

$$\Delta l = \varepsilon l_0 = (0.0012)(75\ \mathrm{mm}) = 0.090\ \mathrm{mm}\ (0.0036\ \mathrm{in.})$$

6.11 Figure 6.22 shows, for a gray cast iron, the tensile engineering stress–strain curve in the elastic region. Determine (a) the tangent modulus at 10.3 MPa (1500 psi), and (b) the secant modulus taken to 6.9 MPa (1000 psi).

Solution

(a) This portion of the problem asks that the tangent modulus be determined for the gray cast iron, the stress-strain behavior of which is shown in Figure 6.22. In the figure below is shown a tangent draw on the curve at a stress of 10.3 MPa (1500 psi).

The slope of this line, i.e., $\Delta\sigma/\Delta\epsilon$, the tangent modulus, is computed as follows:

$$\frac{\Delta\sigma}{\Delta\epsilon} = \frac{15\text{ MPa} - 5\text{ MPa}}{0.0074 - 0.0003} = 1410\text{ MPa} = 1.41\text{ GPa} \quad (2.04 \times 10^5\text{ psi})$$

(b) The secant modulus taken from the origin is calculated by taking the slope of a secant drawn from the origin through the stress-strain curve at 6.9 MPa (1,000 psi). This secant is drawn on the curve shown below:

The slope of this line, the secant modulus, is computed as follows:

$$\frac{\Delta\sigma}{\Delta\varepsilon} = \frac{15\ \text{MPa} - 0\ \text{MPa}}{0.0047 - 0} = 3190\ \text{MPa} = 3.19\ \text{GPa} \quad (4.63 \times 10^5\ \text{psi})$$

6.12 As noted in Section 3.15, for single crystals of some substances, the physical properties are anisotropic; that is, they are dependent on crystallographic direction. One such property is the modulus of elasticity. For cubic single crystals, the modulus of elasticity in a general [uvw] direction, E_{uvw}, is described by the relationship

$$\frac{1}{E_{uvw}} = \frac{1}{E_{\langle 100\rangle}} - 3\left(\frac{1}{E_{\langle 100\rangle}} - \frac{1}{E_{\langle 111\rangle}}\right)\left(\alpha^2\beta^2 + \beta^2\gamma^2 + \gamma^2\alpha^2\right)$$

where $E_{\langle 100\rangle}$ and $E_{\langle 111\rangle}$ are the moduli of elasticity in [100] and [111] directions, respectively; α, β, and γ are th cosines of the angles between [uvw] and the respective [100], [010], and [001] directions. Verify that the $E_{\langle 110\rangle}$ values for aluminum, copper, and iron in Table 3.3 are correct.

Solution

We are asked, using the equation given in the problem statement, to verify that the modulus of elasticity values along [110] directions given in Table 3.3 for aluminum, copper, and iron are correct. The α, β, and γ parameters in the equation correspond, respectively, to the cosines of the angles between the [110] direction and [100], [010] and [001] directions. Since these angles are 45°, 45°, and 90°, the values of α, β, and γ are 0.707, 0.707, and 0, respectively. Thus, the given equation takes the form

$$\frac{1}{E_{\langle 110\rangle}}$$

$$= \frac{1}{E_{\langle 100\rangle}} - 3\left(\frac{1}{E_{\langle 100\rangle}} - \frac{1}{E_{\langle 111\rangle}}\right)\left[(0.707)^2(0.707)^2 + (0.707)^2(0)^2 + (0)^2(0.707)^2\right]$$

$$= \frac{1}{E_{\langle 100\rangle}} - (0.75)\left(\frac{1}{E_{\langle 100\rangle}} - \frac{1}{E_{\langle 111\rangle}}\right)$$

Utilizing the values of $E_{<100>}$ and $E_{<111>}$ from Table 3.3 for Al

$$\frac{1}{E_{\langle 110\rangle}} = \frac{1}{63.7\ \text{GPa}} - (0.75)\left(\frac{1}{63.7\ \text{GPa}} - \frac{1}{76.1\ \text{GPa}}\right)$$

Which leads to, $E_{<110>}$ = 72.6 GPa, the value cited in the table.

For Cu,

$$\frac{1}{E_{\langle 110\rangle}} = \frac{1}{66.7\ \text{GPa}} \quad (0.75)\left(\frac{1}{66.7\ \text{GPa}} \quad \frac{1}{191.1\ \text{GPa}}\right)$$

Thus, $E_{<110>}$ = 130.3 GPa, which is also the value cited in the table.

Similarly, for Fe

$$\frac{1}{E_{\langle 110\rangle}} = \frac{1}{125.0\ \text{GPa}} \quad (0.75)\left(\frac{1}{125.0\ \text{GPa}} \quad \frac{1}{272.7\ \text{GPa}}\right)$$

And $E_{<110>}$ = 210.5 GPa, which is also the value given in the table.

6.13 In Section 2.6 it was noted that the net bonding energy E_N between two isolated positive and negative ions is a function of interionic distance r as follows:

$$E_N = -\frac{A}{r} + \frac{B}{r^n} \qquad (6.25)$$

where A, B, and n are constants for the particular ion pair. Equation 6.25 is also valid for the bonding energy between adjacent ions in solid materials. The modulus of elasticity E is proportional to the slope of the interionic force–separation curve at the equilibrium interionic separation; that is,

$$E \propto \left(\frac{dF}{dr}\right)_{r_0}$$

Derive an expression for the dependence of the modulus of elasticity on these A, B, and n parameters (for the two-ion system) using the following procedure:

1. Establish a relationship for the force F as a function of r, realizing that

$$F = \frac{dE_N}{dr}$$

2. Now take the derivative dF/dr.
3. Develop an expression for r_0, the equilibrium separation. Since r_0 corresponds to the value of r at the minimum of the E_N-versus-r curve (Figure 2.8b), take the derivative dE_N/dr, set it equal to zero, and solve for r, which corresponds to r_0.
4. Finally, substitute this expression for r_0 into the relationship obtained by taking dF/dr.

Solution

This problem asks that we derive an expression for the dependence of the modulus of elasticity, E, on the parameters A, B, and n in Equation 6.25. It is first necessary to take dE_N/dr in order to obtain an expression for the force F; this is accomplished as follows:

$$F = \frac{dE_N}{dr} = \frac{d\left(-\dfrac{A}{r}\right)}{dr} + \frac{d\left(\dfrac{B}{r^n}\right)}{dr}$$

$$= \frac{A}{r^2} - \frac{nB}{r^{(n+1)}}$$

The second step is to set this dE_N/dr expression equal to zero and then solve for r $(= r_0)$. The algebra for this procedure is carried out in Problem 2.14, with the result that

$$r_0 = \left(\frac{A}{nB}\right)^{1/(1-n)}$$

Next it becomes necessary to take the derivative of the force (dF/dr), which is accomplished as follows:

$$\frac{dF}{dr} = \frac{d\left(\frac{A}{r^2}\right)}{dr} + \frac{d\left(\frac{-nB}{r^{(n+1)}}\right)}{dr}$$

$$= \frac{-2A}{r^3} + \frac{(n)(n+1)B}{r^{(n+2)}}$$

Now, substitution of the above expression for r_0 into this equation yields

$$\left(\frac{dF}{dr}\right)_{r_0} = \frac{-2A}{\left(\frac{A}{nB}\right)^{3/(1-n)}} + \frac{(n)(n+1)B}{\left(\frac{A}{nB}\right)^{(n+2)/(1-n)}}$$

which is the expression to which the modulus of elasticity is proportional.

6.14 Using the solution to Problem 6.13, rank the magnitudes of the moduli of elasticity for the following hypothetical X, Y, and Z materials from the greatest to the least. The appropriate A, B, and n parameters (Equation 6.25) for these three materials are tabulated below; they yield E_N in units of electron volts and r in nanometers:

Material	A	B	n
X	2.5	2.0×10^{-5}	8
Y	2.3	8.0×10^{-6}	10.5
Z	3.0	1.5×10^{-5}	9

Solution

This problem asks that we rank the magnitudes of the moduli of elasticity of the three hypothetical metals X, Y, and Z. From Problem 6.13, it was shown for materials in which the bonding energy is dependent on the interatomic distance r according to Equation 6.25, that the modulus of elasticity E is proportional to

$$E \propto -\frac{2A}{\left(\frac{A}{nB}\right)^{3/(1-n)}} + \frac{(n)(n+1)B}{\left(\frac{A}{nB}\right)^{(n+2)/(1-n)}}$$

For metal X, A = 2.5, B = 2.0 × 10^{-5}, and n = 8. Therefore,

$$E \propto -\frac{(2)(2.5)}{\left[\frac{2.5}{(8)(2\times10^{-5})}\right]^{3/(1-8)}} + \frac{(8)(8+1)(2\times10^{-5})}{\left[\frac{2.5}{(8)(2\times10^{-5})}\right]^{(8+2)/(1-8)}}$$

$$= 1097$$

For metal Y, A = 2.3, B = 8 × 10^{-6}, and n = 10.5. Hence

$$E \propto -\frac{(2)(2.3)}{\left[\frac{2.3}{(10.5)(8\times10^{-6})}\right]^{3/(1-10.5)}} + \frac{(10.5)(10.5+1)(8\times10^{-6})}{\left[\frac{2.3}{(10.5)(8\times10^{-6})}\right]^{(10.5+2)/(1-10.5)}}$$

$$= 551$$

And, for metal Z, A = 3.0, B = 1.5 × 10^{-5}, and n = 9. Thus

$$E \propto -\frac{(2)(3.0)}{\left[\frac{3.0}{(9)\left(1.5\times10^{-5}\right)}\right]^{3/(1-9)}} + \frac{(9)(9+1)\left(1.5\times10^{-5}\right)}{\left[\frac{3.0}{(9)\left(1.5\times10^{-5}\right)}\right]^{(9+2)/(1-9)}}$$

$$= 1024$$

Therefore, metal X has the highest modulus of elasticity.

Elastic Properties of Materials

6.15 A cylindrical specimen of aluminum having a diameter of 19 mm (0.75 in.) and length of 200 mm (8.0 in.) is deformed elastically in tension with a force of 48,800 N (11,000 lbf). Using the data contained in Table 6.1, determine the following:

(a) The amount by which this specimen will elongate in the direction of the applied stress.

(b) The change in diameter of the specimen. Will the diameter increase or decrease?

Solution

(a) We are asked, in this portion of the problem, to determine the elongation of a cylindrical specimen of aluminum. Combining Equations 6.1, 6.2, and 6.5, leads to

$$V = E ł$$

$$\frac{F}{S\left(\frac{d_0}{2}\right)^2} = E\,\frac{' l}{l_0}$$

Or, solving for ' l (and realizing that E = 69 GPa, Table 6.1), yields

$$' l = \frac{4F l_0}{S d_0^2 E}$$

$$= \frac{(4)(48{,}800\ \mathrm{N})\left(200\ \mathrm{u}10^{\ 3}\,\mathrm{m}\right)}{(S)\left(19\ \mathrm{u}10^{\ 3}\,\mathrm{m}\right)^2\left(69\ \mathrm{u}10^{9}\,\mathrm{N/m^2}\right)} \quad 5\ \mathrm{u}\,10^{-4}\ \mathrm{m}\ =\ 0.50\ \mathrm{mm}\ \ (0.02\ \mathrm{in.})$$

(b) We are now called upon to determine the change in diameter, 'd. Using Equation 6.8

$$Q = \ \frac{H_x}{H_z} = \ \frac{'d / d_0}{' l / l_0}$$

From Table 6.1, for aluminum, Q 1 R Z V R O Y L Q J W K H D E R Y H H [S U H V V L R Q I R U 'd yields

$$'d \ = \ \frac{Q' l\ d_0}{l_0} = \ \frac{(0.33)(0.50\ \mathrm{mm})(19\ \mathrm{mm})}{200\ \mathrm{mm}}$$

$$= -1.6\ \mathrm{u}10^{-2}\ \mathrm{mm}\ \ (-6.2\ \mathrm{u}10^{-4}\ \mathrm{in.})$$

The diameter will decrease.

6.16 A cylindrical bar of steel 10 mm (0.4 in.) in diameter is to be deformed elastically by application of a force along the bar axis. Using the data in Table 6.1, determine the force that will produce an elastic reduction of 3×10^{-3} mm (1.2×10^{-4} in.) in the diameter.

Solution

This problem asks that we calculate the force necessary to produce a reduction in diameter of 3×10^{-3} mm for a cylindrical bar of steel. For a cylindrical specimen, the cross-sectional area is equal to

$$A_0 = \frac{\pi d_0^2}{4}$$

Now, combining Equations 6.1 and 6.5 leads to

$$\sigma = \frac{F}{A_0} = \frac{F}{\dfrac{\pi d_0^2}{4}} = E\varepsilon_z$$

And, since from Equation 6.8

$$\varepsilon_z = -\frac{\varepsilon_x}{\nu} = -\frac{\dfrac{\Delta d}{d_0}}{\nu} = -\frac{\Delta d}{\nu d_0}$$

Substitution of this equation into the above expression gives

$$\frac{F}{\dfrac{\pi d_0^2}{4}} = E\left(-\frac{\Delta d}{\nu d_0}\right)$$

And, solving for F leads to

$$F = \frac{d_0 \Delta d \, \pi E}{4\nu}$$

From Table 6.1, for steel, $\nu = 0.30$ and $E = 207$ GPa. Thus,

$$F = \frac{\left(10 \times 10^{-3}\,\text{m}\right)\left(3.0 \times 10^{-6}\,\text{m}\right)(\pi)\left(207 \times 10^{9}\,\text{N/m}^2\right)}{(4)(0.30)}$$

$$= 16{,}250\ \text{N}\ \left(3770\ \text{lb}_\text{f}\right)$$

6.17 A cylindrical specimen of some alloy 8 mm (0.31 in.) in diameter is stressed elastically in tension. A force of 15,700 N (3530 lb_f) produces a reduction in specimen diameter of 5×10^{-3} mm (2×10^{-4} in.). Compute Poisson's ratio for this material if its modulus of elasticity is 140 GPa (20.3×10^6 psi).

Solution

This problem asks that we compute Poisson's ratio for the metal alloy. From Equations 6.5 and 6.1

$$\epsilon_z = \frac{\sigma}{E} = \frac{F}{A_0 E} = \frac{F}{\pi\left(\frac{d_0}{2}\right)^2 E} = \frac{4F}{\pi d_0^2 E}$$

Since the transverse strain ϵ_x is just

$$\epsilon_x = \frac{\Delta d}{d_0}$$

and Poisson's ratio is defined by Equation 6.8, then

$$\nu = -\frac{\epsilon_x}{\epsilon_z} = -\frac{\Delta d / d_0}{\left(\frac{4F}{\pi d_0^2 E}\right)} = -\frac{d_0 \Delta d \pi E}{4F}$$

$$= -\frac{(8 \times 10^{-3}\ \text{m})(-5 \times 10^{-6}\ \text{m})(\pi)(140 \times 10^9\ \text{N/m}^2)}{(4)(15{,}700\ \text{N})} = 0.280$$

6.18 A cylindrical specimen of a hypothetical metal alloy is stressed in compression. If its original and final diameters are 20.000 and 20.025 mm, respectively, and its final length is 74.96 mm, compute its original length if the deformation is totally elastic. The elastic and shear moduli for this alloy are 105 GPa and 39.7 GPa, respectively.

Solution

This problem asks that we compute the original length of a cylindrical specimen that is stressed in compression. It is first convenient to compute the lateral strain ε_x as

$$\varepsilon_x = \frac{\Delta d}{d_0} = \frac{20.025\ \text{mm} - 20.000\ \text{mm}}{20.000\ \text{mm}} = 1.25 \times 10^{-3}$$

In order to determine the longitudinal strain ε_z we need Poisson's ratio, which may be computed using Equation 6.9; solving for ν yields

$$\nu = \frac{E}{2G} - 1 = \frac{105 \times 10^3\ \text{MPa}}{(2)\left(39.7 \times 10^3\ \text{MPa}\right)} - 1 = 0.322$$

Now ε_z may be computed from Equation 6.8 as

$$\varepsilon_z = -\frac{\varepsilon_x}{\nu} = -\frac{1.25 \times 10^{-3}}{0.322} = -3.88 \times 10^{-3}$$

Now solving for l_0 using Equation 6.2

$$l_0 = \frac{l_i}{1 + \varepsilon_z}$$

$$= \frac{74.96\ \text{mm}}{1 - 3.88 \times 10^{-3}} = 75.25\ \text{mm}$$

6.19 Consider a cylindrical specimen of some hypothetical metal alloy that has a diameter of 8.0 mm (0.31 in.). A tensile force of 1000 N (225 lb_f) produces an elastic reduction in diameter of 2.8×10^{-4} mm (1.10×10^{-5} in.). Compute the modulus of elasticity for this alloy, given that Poisson's ratio is 0.30.

Solution

This problem asks that we calculate the modulus of elasticity of a metal that is stressed in tension. Combining Equations 6.5 and 6.1 leads to

$$E = \frac{\sigma}{\varepsilon_z} = \frac{F}{A_0 \varepsilon_z} = \frac{F}{\varepsilon_z \pi \left(\frac{d_0}{2}\right)^2} = \frac{4F}{\varepsilon_z \pi d_0^2}$$

From the definition of Poisson's ratio, (Equation 6.8) and realizing that for the transverse strain, $\varepsilon_x = \frac{\Delta d}{d_0}$

$$\varepsilon_z = -\frac{\varepsilon_x}{\nu} = -\frac{\Delta d}{d_0 \nu}$$

Therefore, substitution of this expression for ε_z into the above equation yields

$$E = \frac{4F}{\varepsilon_z \pi d_0^2} = \frac{4F\nu}{\pi d_0 \Delta d}$$

$$= \frac{(4)(1000\ \text{N})(0.30)}{\pi(8 \times 10^{-3}\ \text{m})(2.8 \times 10^{-7}\ \text{m})} = 1.705 \times 10^{11}\ \text{Pa} = 170.5\ \text{GPa} \quad (24.7 \times 10^{6}\ \text{psi})$$

6.20 A brass alloy is known to have a yield strength of 275 MPa (40,000 psi), a tensile strength of 380 MPa (55,000 psi), and an elastic modulus of 103 GPa (15×10^6 psi). A cylindrical specimen of this alloy 12.7 mm (0.50 in.) in diameter and 250 mm (10.0 in.) long is stressed in tension and found to elongate 7.6 mm (0.30 in.). On the basis of the information given, is it possible to compute the magnitude of the load that is necessary to produce this change in length? If so, calculate the load. If not, explain why.

Solution

We are asked to ascertain whether or not it is possible to compute, for brass, the magnitude of the load necessary to produce an elongation of 7.6 mm (0.30 in.). It is first necessary to compute the strain at yielding from the yield strength and the elastic modulus, and then the strain experienced by the test specimen. Then, if

$$\varepsilon(\text{test}) < \varepsilon(\text{yield})$$

deformation is elastic, and the load may be computed using Equations 6.1 and 6.5. However, if

$$\varepsilon(\text{test}) > \varepsilon(\text{yield})$$

computation of the load is not possible inasmuch as deformation is plastic and we have neither a stress-strain plot nor a mathematical expression relating plastic stress and strain. We compute these two strain values as

$$\varepsilon(\text{test}) = \frac{\Delta l}{l_0} = \frac{7.6 \text{ mm}}{250 \text{ mm}} = 0.03$$

and

$$\varepsilon(\text{yield}) = \frac{\sigma_y}{E} = \frac{275 \text{ MPa}}{103 \times 10^3 \text{ MPa}} = 0.0027$$

Therefore, computation of the load is not possible since $\varepsilon(\text{test}) > \varepsilon(\text{yield})$.

6.21 A cylindrical metal specimen 12.7 mm (0.5 in.) in diameter and 250 mm (10 in.) long is to be subjected to a tensile stress of 28 MPa (4000 psi); at this stress level the resulting deformation will be totally elastic.

(a) If the elongation must be less than 0.080 mm (3.2 u 10^{-3} in.), which of the metals in Table 6.1 are suitable candidates? Why?

(b) If, in addition, the maximum permissible diameter decrease is 1.2 u 10^{-3} mm (4.7 u 10^{-5} in.) when the tensile stress of 28 MPa is applied, which of the metals that satisfy the criterion in part (a) are suitable candidates? Why?

Solution

(a) This part of the problem asks that we ascertain which of the metals in Table 6.1 experience an elongation of less than 0.080 mm when subjected to a tensile stress of 28 MPa. The maximum strain that may be sustained (using Equation 6.2) is just

$$H = \frac{'l}{l_0} = \frac{0.080 \text{ mm}}{250 \text{ mm}} = 3.2 \text{ u } 10^{-4}$$

Since the stress level is given (50 MPa), using Equation 6.5 it is possible to compute the minimum modulus of elasticity which is required to yield this minimum strain. Hence

$$E = \frac{V}{H} = \frac{28 \text{ MPa}}{3.2 \text{ u} 10^{-4}} = 87.5 \text{ GPa}$$

Which means that those metals with moduli of elasticity greater than this value are acceptable candidates—namely, brass, Cu, Ni, steel, Ti and W.

(b) This portion of the problem further stipulates that the maximum permissible diameter decrease is 1.2 u 10^{-3} mm when the tensile stress of 28 MPa is applied. This translates into a maximum lateral strain $H_x(\text{max})$ as

$$H_{x(\text{max})} = \frac{'d}{d_0} = \frac{1.2 \text{ u} 10^{-3} \text{ mm}}{12.7 \text{ mm}} = 9.45 \text{ u } 10^{-5}$$

But, since the specimen contracts in this lateral direction, and we are concerned that this strain be less than 9.45 u 10^{-5}, then the criterion for this part of the problem may be stipulated as $\frac{'d}{d_0}$ 9.45 u 10^{-5}.

Now, Poisson’s ratio is defined by Equation 6.8 as

$$\nu = -\frac{\varepsilon_x}{\varepsilon_z}$$

For each of the metal alloys let us consider a possible lateral strain, $\varepsilon_x = \frac{\Delta d}{d_0}$. Furthermore, since the deformation is elastic, then, from Equation 6.5, the longitudinal strain, ε_z, is equal to

$$\varepsilon_z = \frac{\sigma}{E}$$

Substituting these expressions for ε_x and ε_z into the definition of Poisson's ratio we have

$$\nu = -\frac{\varepsilon_x}{\varepsilon_z} = -\frac{\dfrac{\Delta d}{d_0}}{\dfrac{\sigma}{E}}$$

which leads to the following:

$$\frac{\Delta d}{d_0} = \frac{\nu\sigma}{E}$$

Using values for ν and E found in Table 6.1 for the six metal alloys that satisfy the criterion for part (a), and for σ = 28 MPa, we are able to compute a $\frac{\Delta d}{d_0}$ for each alloy as follows:

$$\frac{\Delta d}{d_0}(\text{brass}) = \frac{(0.34)(28 \times 10^6\ \text{N/m}^2)}{97 \times 10^9\ \text{N/m}^2} = 9.81 \times 10^{-5}$$

$$\frac{\Delta d}{d_0}(\text{copper}) = \frac{(0.34)(28 \times 10^6\ \text{N/m}^2)}{110 \times 10^9\ \text{N/m}^2} = 8.65 \times 10^{-5}$$

$$\frac{\Delta d}{d_0}(\text{titanium}) = \frac{(0.34)(28 \times 10^6\ \text{N/m}^2)}{107 \times 10^9\ \text{N/m}^2} = 8.90 \times 10^{-5}$$

$$\frac{\Delta d}{d_0}(\text{nickel}) = \frac{(0.31)(28 \times 10^6\ \text{N/m}^2)}{207 \times 10^9\ \text{N/m}^2} = 4.19 \times 10^{-5}$$

$$\frac{\Delta d}{d_0}(\text{steel}) = \frac{(0.30)(28 \times 10^6\ \text{N/m}^2)}{207 \times 10^9\ \text{N/m}^2} = 4.06 \times 10^{-5}$$

$$\frac{\Delta d}{d_0}(\text{tungsten}) = -\frac{(0.28)(28 \times 10^6\ \text{N/m}^2)}{407 \times 10^9\ \text{N/m}^2} = -1.93 \times 10^{-5}$$

Thus, of the above six alloys, only brass will have a negative transverse strain that is greater than -9.45×10^{-5}. This means that the following alloys satisfy the criteria for both parts (a) and (b) of the problem: copper, titanium, nickel, steel, and tungsten.

6.22 Consider the brass alloy for which the stress-strain behavior is shown in Figure 6.12. A cylindrical specimen of this material 6 mm (0.24 in.) in diameter and 50 mm (2 in.) long is pulled in tension with a force of 5000 N (1125 lbf). If it is known that this alloy has a Poisson's ratio of 0.30, compute: (a) the specimen elongation, and (b) the reduction in specimen diameter.

Solution

(a) This portion of the problem asks that we compute the elongation of the brass specimen. The first calculation necessary is that of the applied stress using Equation 6.1, as

$$\sigma = \frac{F}{A_0} = \frac{F}{\pi\left(\frac{d_0}{2}\right)^2} = \frac{5000\ \text{N}}{\pi\left(\frac{6 \times 10^{-3}\ \text{m}}{2}\right)^2} = 177 \times 10^6\ \text{N/m}^2 = 177\ \text{MPa}\ (25{,}000\ \text{psi})$$

From the stress-strain plot in Figure 6.12, this stress corresponds to a strain of about 2.0×10^{-3}. From the definition of strain, Equation 6.2

$$\Delta l = \epsilon l_0 = \left(2.0 \times 10^{-3}\right)(50\ \text{mm}) = 0.10\ \text{mm}\ \left(4 \times 10^{-3}\ \text{in.}\right)$$

(b) In order to determine the reduction in diameter, it is necessary to use Equation 6.8 and the definition of lateral strain (i.e., $\epsilon_x = \Delta d/d_0$) as follows

$$\Delta d = d_0 \epsilon_x = -d_0 \nu \epsilon_z = -(6\ \text{mm})(0.30)\left(2.0 \times 10^{-3}\right)$$

$$= -3.6 \times 10^{-3}\ \text{mm}\ \left(-1.4 \times 10^{-4}\ \text{in.}\right)$$

6.23 A cylindrical rod 100 mm long and having a diameter of 10.0 mm is to be deformed using a tensile load of 27,500 N. It must not experience either plastic deformation or a diameter reduction of more than 7.5×10^{-3} mm. Of the materials listed as follows, which are possible candidates? Justify your choice(s).

Material	Modulus of Elasticity (GPa)	Yield Strength (MPa)	Poisson's Ratio
Aluminum alloy	70	200	0.33
Brass alloy	101	300	0.34
Steel alloy	207	400	0.30
Titanium alloy	107	650	0.34

Solution

This problem asks that we assess the four alloys relative to the two criteria presented. The first criterion is that the material not experience plastic deformation when the tensile load of 27,500 N is applied; this means that the stress corresponding to this load not exceed the yield strength of the material. Upon computing the stress

$$\sigma = \frac{F}{A_0} = \frac{F}{\pi\left(\frac{d_0}{2}\right)^2} = \frac{27{,}500\ \text{N}}{\pi\left(\frac{10 \times 10^{-3}\ \text{m}}{2}\right)^2} = 350 \times 10^6\ \text{N/m}^2 = 350\ \text{MPa}$$

Of the alloys listed, the Ti and steel alloys have yield strengths greater than 350 MPa.

Relative to the second criterion (i.e., that Δd be less than 7.5×10^{-3} mm), it is necessary to calculate the change in diameter Δd for these three alloys. From Equation 6.8

$$\nu = \frac{\varepsilon_x}{\varepsilon_z} = \frac{\frac{\Delta d}{d_0}}{\frac{\sigma}{E}} = \frac{E\,\Delta d}{\sigma d_0}$$

Now, solving for Δd from this expression,

$$\Delta d = \frac{\nu \sigma d_0}{E}$$

For the steel alloy

$$\Delta d = \frac{(0.30)(350\ \text{MPa})(10\ \text{mm})}{207 \times 10^{3}\ \text{MPa}} = 5.1 \times 10^{-3}\ \text{mm}$$

Therefore, the steel is a candidate.

For the Ti alloy

$$\Delta d = \frac{(0.34)(350\ \text{MPa})(10\ \text{mm})}{107 \times 10^{3}\ \text{MPa}} = 11.1 \times 10^{-3}\ \text{mm}$$

Hence, the titanium alloy is not a candidate.

6.24 A cylindrical rod 380 mm (15.0 in.) long, having a diameter of 10.0 mm (0.40 in.), is to be subjected to a tensile load. If the rod is to experience neither plastic deformation nor an elongation of more than 0.9 mm (0.035 in.) when the applied load is 24,500 N (5500 lbf), which of the four metals or alloys listed below are possible candidates? Justify your choice(s).

Material	Modulus of Elasticity (GPa)	Yield Strength (MPa)	Tensile Strength (MPa)
Aluminum alloy	70	255	420
Brass alloy	100	345	420
Copper	110	250	290
Steel alloy	207	450	550

Solution

This problem asks that we ascertain which of four metal alloys will not (1) experience plastic deformation, and (2) elongate more than 0.9 mm when a tensile load of 24,500 N is applied. It is first necessary to compute the stress using Equation 6.1; a material to be used for this application must necessarily have a yield strength greater than this value. Thus,

$$\sigma = \frac{F}{A_0} = \frac{24{,}500 \text{ N}}{\pi\left(\dfrac{10.0 \times 10^{-3}\text{ m}}{2}\right)^2} = 312 \text{ MPa}$$

Of the metal alloys listed, only brass and steel have yield strengths greater than this stress.

Next, we must compute the elongation produced in both brass and steel using Equations 6.2 and 6.5 in order to determine whether or not this elongation is less than 0.9 mm. For brass

$$\Delta l = \frac{\sigma l_0}{E} = \frac{(312 \text{ MPa})(380 \text{ mm})}{100 \times 10^3 \text{ MPa}} = 1.19 \text{ mm}$$

Thus, brass is not a candidate. However, for steel

$$\Delta l = \frac{\sigma l_0}{E} = \frac{(312 \text{ MPa})(380 \text{ mm})}{207 \times 10^3 \text{ MPa}} = 0.57 \text{ mm}$$

Therefore, of these four alloys, only steel satisfies the stipulated criteria.

Tensile Properties

6.25 Figure 6.21 shows the tensile engineering stress–strain behavior for a steel alloy.

(a) What is the modulus of elasticity?

(b) What is the proportional limit?

(c) What is the yield strength at a strain offset of 0.002?

(d) What is the tensile strength?

Solution

Using the stress–strain plot for a steel alloy (Figure 6.21), we are asked to determine several of its mechanical characteristics.

(a) The elastic modulus is just the slope of the initial linear portion of the curve; or, from the inset and using Equation 6.10

$$E = \frac{\sigma_2 - \sigma_1}{\epsilon_2 - \epsilon_1} = \frac{(200 - 0)\ \text{MPa}}{(0.0010 - 0)} = 200 \times 10^3\ \text{MPa} = 200\ \text{GPa}\ (29 \times 10^6\ \text{psi})$$

The value given in Table 6.1 is 207 GPa.

(b) The proportional limit is the stress level at which linearity of the stress–strain curve ends, which is approximately 300 MPa (43,500 psi).

(c) The 0.002 strain offset line intersects the stress–strain curve at approximately 400 MPa (58,000 psi).

(d) The tensile strength (the maximum on the curve) is approximately 515 MPa (74,700 psi).

6.26 A cylindrical specimen of a brass alloy having a length of 60 mm (2.36 in.) must elongate only 10.8 mm (0.425 in.) when a tensile load of 50,000 N (11,240 lb_f) is applied. Under these circumstances, what must be the radius of the specimen? Consider this brass alloy to have the stress-strain behavior shown in Figure 6.12.

Solution

We are asked to calculate the radius of a cylindrical brass specimen in order to produce an elongation of 10.8 mm when a load of 50,000 N is applied. It first becomes necessary to compute the strain corresponding to this elongation using Equation 6.2 as

$$\epsilon = \frac{\Delta l}{l_0} = \frac{10.8\ \text{mm}}{60\ \text{mm}} = 0.18$$

From Figure 6.12, a stress of 420 MPa (61,000 psi) corresponds to this strain. Since for a cylindrical specimen, stress, force, and initial radius r_0 are related as

$$\sigma = \frac{F}{\pi r_0^2}$$

then

$$r_0 = \sqrt{\frac{F}{\pi\sigma}} = \sqrt{\frac{50{,}000\ \text{N}}{\pi\left(420 \times 10^6\ \text{N/m}^2\right)}} = 0.0062\ \text{m} = 6.2\ \text{mm} \quad (0.24\ \text{in.})$$

6.27 A load of 85,000 N (19,100 lb_f) is applied to a cylindrical specimen of a steel alloy (displaying the stress–strain behavior shown in Figure 6.21) that has a cross-sectional diameter of 15 mm (0.59 in.).

(a) Will the specimen experience elastic and/or plastic deformation? Why?

(b) If the original specimen length is 250 mm (10 in.), how much will it increase in length when this load is applied?

Solution

This problem asks us to determine the deformation characteristics of a steel specimen, the stress-strain behavior for which is shown in Figure 6.21.

(a) In order to ascertain whether the deformation is elastic or plastic, we must first compute the stress, then locate it on the stress-strain curve, and, finally, note whether this point is on the elastic or plastic region. Thus, from Equation 6.1

$$\sigma = \frac{F}{A_0} = \frac{85{,}000\ \text{N}}{\pi\left(\dfrac{15 \times 10^{-3}\ \text{m}}{2}\right)^2} = 481 \times 10^6\ \text{N/m}^2 = 481\ \text{MPa}\ (69{,}900\ \text{psi})$$

The 481 MPa point is beyond the linear portion of the curve, and, therefore, the deformation will be both elastic and plastic.

(b) This portion of the problem asks us to compute the increase in specimen length. From the stress-strain curve, the strain at 481 MPa is approximately 0.0135. Thus, from Equation 6.2

$$\Delta l = \varepsilon l_0 = (0.0135)(250\ \text{mm}) = 3.4\ \text{mm}\ \ (0.135\ \text{in.})$$

6.28 A bar of a steel alloy that exhibits the stress-strain behavior shown in Figure 6.21 is subjected to a tensile load; the specimen is 300 mm (12 in.) long, and of square cross section 4.5 mm (0.175 in.) on a side.

(a) Compute the magnitude of the load necessary to produce an elongation of 0.45 mm (0.018 in.).

(b) What will be the deformation after the load has been released?

Solution

(a) We are asked to compute the magnitude of the load necessary to produce an elongation of 0.45 mm for the steel displaying the stress-strain behavior shown in Figure 6.21. First, calculate the strain, and then the corresponding stress from the plot.

$$\epsilon = \frac{\Delta l}{l_0} = \frac{0.45 \text{ mm}}{300 \text{ mm}} = 1.5 \times 10^{-3}$$

This is near the end of the elastic region; from the inset of Figure 6.21, this corresponds to a stress of about 300 MPa (43,500 psi). Now, from Equation 6.1

$$F = \sigma A_0 = \sigma b^2$$

in which b is the cross-section side length. Thus,

$$F = \left(300 \times 10^6 \text{ N/m}^2\right)\left(4.5 \times 10^{-3} \text{ m}\right)^2 = 6075 \text{ N} \ \ (1366 \text{ lb}_f)$$

(b) After the load is released there will be no deformation since the material was strained only elastically.

6.29 A cylindrical specimen of aluminum having a diameter of 0.505 in. (12.8 mm) and a gauge length of 2.000 in. (50.800 mm) is pulled in tension. Use the load–elongation characteristics tabulated below to complete parts (a) through (f)

Load		Length	
N	lb_f	mm	in.
0	0	50.800	2.000
7,330	1,650	50.851	2.002
15,100	3,400	50.902	2.004
23,100	5,200	50.952	2.006
30,400	6,850	51.003	2.008
34,400	7,750	51.054	2.010
38,400	8,650	51.308	2.020
41,300	9,300	51.816	2.040
44,800	10,100	52.832	2.080
46,200	10,400	53.848	2.120
47,300	10,650	54.864	2.160
47,500	10,700	55.880	2.200
46,100	10,400	56.896	2.240
44,800	10,100	57.658	2.270
42,600	9,600	58.420	2.300
36,400	8,200	59.182	2.330
Fracture			

(a) Plot the data as engineering stress versus engineering strain.

(b) Compute the modulus of elasticity.

(c) Determine the yield strength at a strain offset of 0.002.

(d) Determine the tensile strength of this alloy.

(e) What is the approximate ductility, in percent elongation?

(f) Compute the modulus of resilience.

Solution

This problem calls for us to make a stress–strain plot for aluminum, given its tensile load–length data, and then to determine some of its mechanical characteristics.

(a) The data are plotted below on two plots: the first corresponds to the entire stress-strain curve, while for the second, the curve extends to just beyond the elastic region of deformation.

(b) The elastic modulus is the slope in the linear elastic region (Equation 6.10) as

$$E = \frac{\Delta \sigma}{\Delta \varepsilon} = \frac{200 \text{ MPa} - 0 \text{ MPa}}{0.0032 - 0} = 62.5 \times 10^3 \text{ MPa} = 62.5 \text{ GPa} \quad (9.1 \times 10^6 \text{ psi})$$

(c) For the yield strength, the 0.002 strain offset line is drawn dashed. It intersects the stress-strain curve at approximately 285 MPa (41,000 psi).

(d) The tensile strength is approximately 370 MPa (54,000 psi), corresponding to the maximum stress on the complete stress-strain plot.

(e) The ductility, in percent elongation, is just the plastic strain at fracture, multiplied by one-hundred. The total fracture strain at fracture is 0.165; subtracting out the elastic strain (which is about 0.005) leaves a plastic strain of 0.160. Thus, the ductility is about 16%EL.

(f) From Equation 6.14, the modulus of resilience is just

$$U_r = \frac{\sigma_y^2}{2E}$$

which, using data computed above gives a value of

$$U_r = \frac{(285\ \text{MPa})^2}{(2)\left(62.5 \times 10^3\ \text{MPa}\right)} = 0.65\ \text{MN/m}^2 = 0.65 \times 10^6\ \text{N/m}^2 = 6.5 \times 10^5\ \text{J/m}^3 \quad \left(93.8\ \text{in.-lb}_f/\text{in.}^3\right)$$

6.30 A specimen of ductile cast iron having a rectangular cross section of dimensions 4.8 mm × 15.9 mm (3/16 in. × 5/8 in.) is deformed in tension. Using the load-elongation data tabulated below, complete problems (a) through (f).

Load		Length	
N	$\mathrm{lb_f}$	mm	in.
0	0	75.000	2.953
4,740	1,065	75.025	2.954
9,140	2,055	75.050	2.955
12,920	2,900	75.075	2.956
16,540	3,720	75.113	2.957
18,300	4,110	75.150	2.959
20,170	4,530	75.225	2.962
22,900	5,145	75.375	2.968
25,070	5,635	75.525	2.973
26,800	6,025	75.750	2.982
28,640	6,440	76.500	3.012
30,240	6,800	78.000	3.071
31,100	7,000	79.500	3.130
31,280	7,030	81.000	3.189
30,820	6,930	82.500	3.248
29,180	6,560	84.000	3.307
27,190	6,110	85.500	3.366
24,140	5,430	87.000	3.425
18,970	4,265	88.725	3.493
Fracture			

(a) Plot the data as engineering stress versus engineering strain.

(b) Compute the modulus of elasticity.

(c) Determine the yield strength at a strain offset of 0.002.

(d) Determine the tensile strength of this alloy.

(e) Compute the modulus of resilience.

(f) What is the ductility, in percent elongation?

Solution

This problem calls for us to make a stress-strain plot for a ductile cast iron, given its tensile load-length data, and then to determine some of its mechanical characteristics.

(a) The data are plotted below on two plots: the first corresponds to the entire stress-strain curve, while for the second, the curve extends just beyond the elastic region of deformation.

(b) The elastic modulus is the slope in the linear elastic region (Equation 6.10) as

$$E = \frac{\Delta\sigma}{\Delta\epsilon} = \frac{100\ \text{MPa} - 0\ \text{MPa}}{0.0005 - 0} = 200 \times 10^{3}\ \text{MPa} = 200\ \text{GPa} \quad (29 \times 10^{6}\ \text{psi})$$

(c) For the yield strength, the 0.002 strain offset line is drawn dashed. It intersects the stress-strain curve at approximately 280 MPa (40,500 psi).

(d) The tensile strength is approximately 410 MPa (59,500 psi), corresponding to the maximum stress on the complete stress-strain plot.

(e) From Equation 6.14, the modulus of resilience is just

$$U_r = \frac{\sigma_y^2}{2E}$$

which, using data computed above, yields a value of

$$U_r = \frac{(280 \times 10^{6}\ \text{N/m}^2)^2}{(2)(200 \times 10^{9}\ \text{N/m}^2)} = 1.96 \times 10^{5}\ \text{J/m}^3 \quad (28.3\ \text{in.-lb}_f/\text{in.}^3)$$

(f) The ductility, in percent elongation, is just the plastic strain at fracture, multiplied by one hundred. The total fracture strain at fracture is 0.185; subtracting out the elastic strain (which is about 0.001) leaves a plastic strain of 0.184. Thus, the ductility is about 18.4%EL.

6.31 For the titanium alloy, whose stress strain behavior may be observed in the “Tensile Tests” module of Virtual Materials Science and Engineering (VMSE), determine the following:

(a) the approximate yield strength (0.002 strain offset),

(b) the tensile strength, and

(c) the approximate ductility, in percent elongation.

How do these values compare with those for the two Ti-6Al-4V alloys presented in Table B.4 of Appendix B?

Solution

(a) It is possible to do a screen capture and then print out the entire stress-strain curve for the Ti alloy. The intersection of a straight line parallel to the initial linear region of the curve and offset at a strain of 0.002 with this curve is at approximately 720 MPa.

(b) The maximum reading in the stress window located below the plot as the curser point is dragged along the stress-strain curve is 1000 MPa, the value of the tensile strength.

(c) The approximate percent elongation corresponds to the strain at fracture multiplied by 100 (i.e., 12%) minus the maximum elastic strain (i.e., value of strain at which the linearity of the curve ends multiplied by 100—in this case about 0.5%); this gives a value of about 11.5%EL.

From Table B.4 in Appendix B, yield strength, tensile strength, and percent elongation values for the anneal Ti-6Al-4V are 830 MPa, 900 MPa, and 14%EL, while for the solution heat treated and aged alloy, the corresponding values are 1103 MPa, 1172 MPa, and 10%EL. Thus, tensile strength and percent elongation values for the VMSE alloy are slightly lower than for the annealed material in Table B.4 (720 vs 830 MPa, and 11.5 vs. 14 %EL), whereas the tensile strength is slightly higher (1000 vs. 900 MPa).

6.32 For the tempered steel alloy, whose stress strain behavior may be observed in the “Tensile Tests” module of Virtual Materials Science and Engineering (VMSE), determine the following:

(a) the approximate yield strength (0.002 strain offset),

(b) the tensile strength, and

(c) the approximate ductility, in percent elongation.

How do these values compare with those for the oil-quenched and tempered 4140 and 4340 steel alloys presented in Table B.4 of Appendix B?

Solution

(a) It is possible to do a screen capture and then print out the entire stress-strain curve for the tempered steel alloy. The intersection of a straight line parallel to the initial linear region of the curve and offset at a strain of 0.002 with this curve is at approximately 1430 MPa.

(b) The maximum reading in the stress window located below the plot as the curser point is dragged along the stress-strain curve is 1656 MPa, the value of the tensile strength.

(c) The approximate percent elongation corresponds to the strain at fracture multiplied by 100 (i.e., 14.8%) minus the maximum elastic strain (i.e., value of strain at which the linearity of the curve ends multiplied by 100—in this case about 0.8%); this gives a value of about 14.0%EL.

For the oil-quenched and tempered 4140 and 4340 steel alloys, yield strength values presented in Table B.4 of Appendix B are 1570 MPa and 1620 MPa, respectively; these values are somewhat larger than the 1430 MPa for the tempered steel alloy of VMSE. Tensile strength values for these 4140 and 4340 alloys are, respectively 1720 MPa and 1760 MPa (compared to 1656 MPa for the VMSE steel). And, finally, the respective ductilities for the 4140 and 4340 alloys are 11.5%EL and 12%EL, which are slightly lower than the 14%EL value for the VMSE steel.

6.33 For the aluminum alloy, whose stress strain behavior may be observed in the “Tensile Tests” module of Virtual Materials Science and Engineering (VMSE), determine the following:

(a) the approximate yield strength (0.002 strain offset),

(b) the tensile strength, and

(c) the approximate ductility, in percent elongation.

How do these values compare with those for the 2024 aluminum alloy (T351 temper) presented in Table B.4 of Appendix B?

Solution

(a) It is possible to do a screen capture and then print out the entire stress-strain curve for the aluminum alloy. The intersection of a straight line parallel to the initial linear region of the curve and offset at a strain of 0.002 with this curve is at approximately 300 MPa.

(b) The maximum reading in the stress window located below the plot as the curser point is dragged along the stress-strain curve is 484 MPa, the value of the tensile strength.

(c) The approximate percent elongation corresponds to the strain at fracture multiplied by 100 (i.e., 22.4%) minus the maximum elastic strain (i.e., value of strain at which the linearity of the curve ends multiplied by 100—in this case about 0.5%); this gives a value of about 21.9%EL.

For the 2024 aluminum alloy (T351 temper), the yield strength value presented in Table B.4 of Appendix B is 325, which is slightly larger than the 300 MPa for the aluminum alloy of VMSE. The tensile strength value for the 2024-T351 is 470 MPa (compared to 484 MPa for the VMSE alloy). And, finally, the ductility for 2024-T351 is 20%EL, which is about the same as for the VMSE aluminum (21.9%EL).

6.34 For the (plain) carbon steel alloy, whose stress strain behavior may be observed in the "Tensile Tests" module of Virtual Materials Science and Engineering (VMSE), determine the following:

(a) the approximate yield strength,

(b) the tensile strength, and

(c) the approximate ductility, in percent elongation.

Solution

(a) It is possible to do a screen capture and then print out the entire stress-strain curve for the plain carbon steel alloy. Inasmuch as the stress-strain curve displays the yield point phenomenon, we take the yield strength as the lower yield point, which, for this steel, is about 225 MPa.

(b) The maximum reading in the stress window located below the plot as the curser is dragged along the stress-strain curve is 274 MPa, the value of the tensile strength.

(c) The approximate percent elongation corresponds to the strain at fracture multiplied by 100 (i.e., 43.0%) minus the maximum elastic strain (i.e., value of strain at which the linearity of the curve ends multiplied by 100—in this case about 0.6%); this gives a value of about 42.4%EL.

6.35 A cylindrical metal specimen having an original diameter of 12.8 mm (0.505 in.) and gauge length of 50.80 mm (2.000 in.) is pulled in tension until fracture occurs. The diameter at the point of fracture is 6.60 mm (0.260 in.), and the fractured gauge length is 72.14 mm (2.840 in.). Calculate the ductility in terms of percent reduction in area and percent elongation.

Solution

This problem calls for the computation of ductility in both percent reduction in area and percent elongation. Percent reduction in area is computed using Equation 6.12 as

$$\%RA = \frac{\pi\left(\frac{d_0}{2}\right)^2 - \pi\left(\frac{d_f}{2}\right)^2}{\pi\left(\frac{d_0}{2}\right)^2} \times 100$$

in which d_0 and d_f are, respectively, the original and fracture cross-sectional areas. Thus,

$$\%RA = \frac{\pi\left(\frac{12.8\text{ mm}}{2}\right)^2 - \pi\left(\frac{6.60\text{ mm}}{2}\right)^2}{\pi\left(\frac{12.8\text{ mm}}{2}\right)^2} \times 100 = 73.4\%$$

While, for percent elongation, we use Equation 6.11 as

$$\%EL = \left(\frac{l_f - l_0}{l_0}\right) \times 100$$

$$= \frac{72.14\text{ mm} - 50.80\text{ mm}}{50.80\text{ mm}} \times 100 = 42\%$$

6.36 Calculate the moduli of resilience for the materials having the stress-strain behaviors shown in Figures 6.12 and 6.21.

Solution

This problem asks us to calculate the moduli of resilience for the materials having the stress-strain behaviors shown in Figures 6.12 and 6.21. According to Equation 6.14, the modulus of resilience U_r is a function of the yield strength and the modulus of elasticity as

$$U_r = \frac{\sigma_y^2}{2E}$$

The values for σ_y and E for the brass in Figure 6.12 are determined in Example Problem 6.3 as 250 MPa (36,000 psi) and 93.8 GPa (13.6×10^6 psi), respectively. Thus

$$U_r = \frac{(250\ \text{MPa})^2}{(2)\left(93.8 \times 10^3\ \text{MPa}\right)} = 3.32 \times 10^5\ \text{J/m}^3 \quad \left(48.2\ \text{in.-lb}_f/\text{in.}^3\right)$$

Values of the corresponding parameters for the steel alloy (Figure 6.21) are determined in Problem 6.25 as 400 MPa (58,000 psi) and 200 GPa (29×10^6 psi), respectively, and therefore

$$U_r = \frac{(400\ \text{MPa})^2}{(2)\left(200 \times 10^3\ \text{MPa}\right)} = 4.0 \times 10^5\ \text{J/m}^3 \quad \left(58\ \text{in.-lb}_f/\text{in.}^3\right)$$

6.37 Determine the modulus of resilience for each of the following alloys:

	Yield Strength	
Material	MPa	psi
Steel alloy	550	80,000
Brass alloy	350	50,750
Aluminum alloy	250	36,250
Titanium alloy	800	116,000

Use modulus of elasticity values in Table 6.1.

Solution

The moduli of resilience of the alloys listed in the table may be determined using Equation 6.14. Yiel strength values are provided in this table, whereas the elastic moduli are tabulated in Table 6.1.

For steel

$$U_r = \frac{\sigma_y^2}{2E}$$

$$= \frac{(550 \times 10^6\ \mathrm{N/m^2})^2}{(2)(207 \times 10^9\ \mathrm{N/m^2})} = 7.31 \times 10^5\ \mathrm{J/m^3}\ \ (107\ \mathrm{in.\text{-}lb_f/in.^3})$$

For the brass

$$U_r = \frac{(350 \times 10^6\ \mathrm{N/m^2})^2}{(2)(97 \times 10^9\ \mathrm{N/m^2})} = 6.31 \times 10^5\ \mathrm{J/m^3}\ \ (92.0\ \mathrm{in.\text{-}lb_f/in.^3})$$

For the aluminum alloy

$$U_r = \frac{(250 \times 10^6\ \mathrm{N/m^2})^2}{(2)(69 \times 10^9\ \mathrm{N/m^2})} = 4.53 \times 10^5\ \mathrm{J/m^3}\ \ (65.7\ \mathrm{in.\text{-}lb_f/in.^3})$$

And, for the titanium alloy

$$U_r = \frac{(800 \times 10^6\ \mathrm{N/m^2})^2}{(2)(107 \times 10^9\ \mathrm{N/m^2})} = 30.0 \times 10^5\ \mathrm{J/m^3}\ \ (434\ \mathrm{in.\text{-}lb_f/in.^3})$$

6.38 A brass alloy to be used for a spring application must have a modulus of resilience of at least 0.75 MPa (110 psi). What must be its minimum yield strength?

Solution

The modulus of resilience, yield strength, and elastic modulus of elasticity are related to one another through Equation 6.14; the value of E for brass given in Table 6.1 is 97 GPa. Solving for V_y from this expression yields

$$V_y = \sqrt{2U_r E} = \sqrt{(2)(0.75 \text{ MPa})(97 \text{ u} 10^3 \text{ MPa})}$$

$$= 381 \text{ MPa} \ \ (55{,}500 \text{ psi})$$

True Stress and Strain

6.39 Show that Equations 6.18a and 6.18b are valid when there is no volume change during deformation.

Solution

To show that Equation 6.18a is valid, we must first rearrange Equation 6.17 as

$$A_i = \frac{A_0 l_0}{l_i}$$

Substituting this expression into Equation 6.15 yields

$$\sigma_T = \frac{F}{A_i} = \frac{F}{A_0}\left(\frac{l_i}{l_0}\right) = \sigma\left(\frac{l_i}{l_0}\right)$$

But, from Equation 6.2

$$\varepsilon = \frac{l_i}{l_0} - 1$$

Or

$$\frac{l_i}{l_0} = \varepsilon + 1$$

Thus,

$$\sigma_T = \sigma\left(\frac{l_i}{l_0}\right) = \sigma(\varepsilon + 1)$$

For Equation 6.18b

$$\varepsilon_T = \ln(1 + \varepsilon)$$

is valid since, from Equation 6.16

$$H_T = \ln\left(\frac{I_i}{I_0}\right)$$

and

$$\frac{I_i}{I_0} = H + 1$$

from above.

6.40 Demonstrate that Equation 6.16, the expression defining true strain, may also be represented by

$$\epsilon_T = \ln\left(\frac{A_0}{A_i}\right)$$

when specimen volume remains constant during deformation. Which of these two expressions is more valid during necking? Why?

Solution

This problem asks us to demonstrate that true strain may also be represented by

$$\epsilon_T = \ln\left(\frac{A_0}{A_i}\right)$$

Rearrangement of Equation 6.17 leads to

$$\frac{l_i}{l_0} = \frac{A_0}{A_i}$$

Thus, Equation 6.16 takes the form

$$\epsilon_T = \ln\left(\frac{l_i}{l_0}\right) = \ln\left(\frac{A_0}{A_i}\right)$$

The expression $\epsilon_T = \ln\left(\frac{A_0}{A_i}\right)$ is more valid during necking because A_i is taken as the area of the neck.

6.41 Using the data in Problem 6.28 and Equations 6.15, 6.16, and 6.18a, generate a true stress–strain plot for aluminum. Equation 6.18a becomes invalid past the point at which necking begins; therefore, measured diameters are given below for the last four data points, which should be used in true stress computations.

Load		Length		Diameter	
N	lb_f	mm	in.	mm	in.
46,100	10,400	56.896	2.240	11.71	0.461
42,400	10,100	57.658	2.270	10.95	0.431
42,600	9,600	58.420	2.300	10.62	0.418
36,400	8,200	59.182	2.330	9.40	0.370

Solution

These true stress–strain data are plotted below.

6.42 A tensile test is performed on a metal specimen, and it is found that a true plastic strain of 0.20 is produced when a true stress of 575 MPa (83,500 psi) is applied; for the same metal, the value of K in Equation 6.19 is 860 MPa (125,000 psi). Calculate the true strain that results from the application of a true stress of 600 MPa (87,000 psi).

Solution

It first becomes necessary to solve for n in Equation 6.19. Taking logarithms of this expression and after rearrangement we have

$$n = \frac{\log \sigma_T - \log K}{\log \varepsilon_T}$$

And, incorporating values of the parameters provided in the problem statement leads to

$$n = \frac{\log (575\text{ MPa}) - \log (860\text{ MPa})}{\log (0.20)} = 0.250$$

Expressing ε_T as the dependent variable (Equation 6.19), and then solving for its value from the data stipulated in the problem statement, leads to

$$\varepsilon_T = \left(\frac{\sigma_T}{K}\right)^{1/n} = \left(\frac{600\text{ MPa}}{860\text{ MPa}}\right)^{1/0.250} = 0.237$$

6.43 For some metal alloy, a true stress of 415 MPa (60,175 psi) produces a plastic true strain of 0.475. How much will a specimen of this material elongate when a true stress of 325 MPa (46,125 psi) is applied if the original length is 300 mm (11.8 in.)? Assume a value of 0.25 for the strain-hardening exponent n.

Solution

Solution of this problem requires that we utilize Equation 6.19. It is first necessary to solve for *K* from the given true stress and strain. Rearrangement of this equation yields

$$K = \frac{\sigma_T}{(\varepsilon_T)^n} = \frac{415\ \text{MPa}}{(0.475)^{0.25}} = 500\ \text{MPa} \quad (72{,}500\ \text{psi})$$

Next we must solve for the true strain produced when a true stress of 325 MPa is applied, also using Equation 6.19. Thus

$$\varepsilon_T = \left(\frac{\sigma_T}{K}\right)^{1/n} = \left(\frac{325\ \text{MPa}}{500\ \text{MPa}}\right)^{1/0.25} = 0.179 = \ln\left(\frac{l_i}{l_0}\right)$$

Now, solving for l_i gives

$$l_i = l_0 e^{0.179} = (300\ \text{mm})e^{0.179} = 358.8\ \text{mm} \quad (14.11\ \text{in.})$$

And finally, the elongation is just

$$\Delta l = l_i - l_0 = 358.8\ \text{mm} - 300\ \text{mm} = 58.8\ \text{mm} \quad (2.31\ \text{in.})$$

6.44 The following true stresses produce the corresponding true plastic strains for a brass alloy:

True Stress (psi)	True Strain
50,000	0.10
60,000	0.20

What true stress is necessary to produce a true plastic strain of 0.25?

Solution

For this problem, we are given two values of ε_T and σ_T, from which we are asked to calculate the true stress which produces a true plastic strain of 0.25. Employing Equation 6.19, we may set up two simultaneous equations with two unknowns (the unknowns being K and n), as

$$\log (50{,}000 \text{ psi}) = \log K + n \log (0.10)$$

$$\log (60{,}000 \text{ psi}) = \log K + n \log (0.20)$$

Solving for n from these two expressions yields

$$n = \frac{\log (50{,}000) - \log (60{,}000)}{\log (0.10) - \log (0.20)} = 0.263$$

and for K

$$\log K = 4.96 \text{ or } K = 10^{4.96} = 91{,}623 \text{ psi}$$

Thus, for $\varepsilon_T = 0.25$

$$\sigma_T = K (\varepsilon_T)^n = (91{,}623 \text{ psi})(0.25)^{0.263} = 63{,}700 \text{ psi} \quad (440 \text{ MPa})$$

6.45 For a brass alloy, the following engineering stresses produce the corresponding plastic engineering strains, prior to necking:

Engineering Stress (MPa)	Engineering Strain
235	0.194
250	0.296

On the basis of this information, compute the engineering stress necessary to produce an engineering strain of 0.25.

Solution

For this problem we first need to convert engineering stresses and strains to true stresses and strains so that the constants K and n in Equation 6.19 may be determined. Since $V_T = V(1 + H)$ then

$$V_{T1} = (235 \text{ MPa})(1 + 0.194) = 280 \text{ MPa}$$

$$V_{T2} = (250 \text{ MPa})(1 + 0.296) = 324 \text{ MPa}$$

Similarly for strains, since $H_T = \ln(1 + H)$ then

$$H_{T1} = \ln(1 + 0.194) = 0.177$$

$$H_{T2} = \ln(1 + 0.296) = 0.259$$

Taking logarithms of Equation 6.19, we get

$$\log V_T = \log K + n \log H_T$$

which allows us to set up two simultaneous equations for the above pairs of true stresses and true strains, with K and n as unknowns. Thus

$$\log(280) = \log K + n \log(0.177)$$

$$\log(324) = \log K + n \log(0.259)$$

Solving for these two expressions yields K = 543 MPa and n = 0.383.

Now, converting $\epsilon = 0.25$ to true strain

$$\epsilon_T = \ln(1 + 0.25) = 0.223$$

The corresponding σ_T to give this value of ϵ_T (using Equation 6.19) is just

$$\sigma_T = K\epsilon_T^n = (543 \text{ MPa})(0.223)^{0.383} = 306 \text{ MPa}$$

Now converting this value of σ_T to an engineering stress using Equation 6.18a gives

$$\sigma = \frac{\sigma_T}{1 + \epsilon} = \frac{306 \text{ MPa}}{1 + 0.25} = 245 \text{ MPa}$$

6.46 Find the toughness (or energy to cause fracture) for a metal that experiences both elastic and plastic deformation. Assume Equation 6.5 for elastic deformation, that the modulus of elasticity is 172 GPa (25×10^6 psi), and that elastic deformation terminates at a strain of 0.01. For plastic deformation, assume that the relationship between stress and strain is described by Equation 6.19, in which the values for K and n are 6900 MPa (1×10^6 psi) and 0.30, respectively. Furthermore, plastic deformation occurs between strain values of 0.01 and 0.75, at which point fracture occurs.

<u>Solution</u>

This problem calls for us to compute the toughness (or energy to cause fracture). The easiest way to do this is to integrate both elastic and plastic regions, and then add them together.

$$\text{Toughness} = \int \sigma \, d\varepsilon$$

$$= \int_0^{0.01} E\varepsilon \, d\varepsilon + \int_{0.01}^{0.75} K\varepsilon^n \, d\varepsilon$$

$$= \left.\frac{E\varepsilon^2}{2}\right|_0^{0.01} + \left.\frac{K}{(n+1)}\,\varepsilon^{(n+1)}\right|_{0.01}^{0.75}$$

$$= \frac{172 \times 10^9 \text{ N/m}^2}{2}(0.01)^2 + \frac{6900 \times 10^6 \text{ N/m}^2}{(1.0 + 0.3)}\left[(0.75)^{1.3} - (0.01)^{1.3}\right]$$

$$= 3.65 \times 10^9 \text{ J/m}^3 \;\left(5.29 \times 10^5 \text{ in.-lb}_f/\text{in.}^3\right)$$

6.47 For a tensile test, it can be demonstrated that necking begins when

$$\frac{d\sigma_T}{d\epsilon_T} = \sigma_T \qquad (6.26)$$

Using Equation 6.19, determine the value of the true strain at this onset of necking.

Solution

Let us take the derivative of Equation 6.19, set it equal to σ_T, and then solve for ϵ_T from the resulting expression. Thus

$$\frac{d\left[K(\epsilon_T)^n\right]}{d\epsilon_T} = Kn(\epsilon_T)^{(n-1)} = \sigma_T$$

However, from Equation 6.19, $\sigma_T = K(\epsilon_T)^n$, which, when substituted into the above expression, yields

$$Kn(\epsilon_T)^{(n-1)} = K(\epsilon_T)^n$$

Now solving for ϵ_T from this equation leads to

$$\epsilon_T = n$$

as the value of the true strain at the onset of necking.

6.48 Taking the logarithm of both sides of Equation 6.19 yields

$$\log \sigma_T = \log K + n \log \varepsilon_T \qquad (6.27)$$

Thus, a plot of $\log \sigma_T$ versus $\log \varepsilon_T$ in the plastic region to the point of necking should yield a straight line having a slope of n and an intercept (at $\log \varepsilon_T = 0$) of log K.

Using the appropriate data tabulated in Problem 6.29, make a plot of $\log \sigma_T$ versus $\log \varepsilon_T$ and determine the values of n and K. It will be necessary to convert engineering stresses and strains to true stresses and strains using Equations 6.18a and 6.18b.

Solution

This problem calls for us to utilize the appropriate data from Problem 6.29 in order to determine the values of n and K for this material. From Equation 6.27 the slope and intercept of a $\log \sigma_T$ versus $\log \varepsilon_T$ plot will yield n and log K, respectively. However, Equation 6.19 is only valid in the region of plastic deformation to the point of necking; thus, only the 7th, 8th, 9th, and 10th data points may be utilized. The log-log plot with these data points is given below.

The slope yields a value of 0.136 for n, whereas the intercept gives a value of 2.7497 for log K, and thus $K = 10^{2.7497} = 562$ MPa.

Elastic Recovery After Plastic Deformation

6.49 A cylindrical specimen of a brass alloy 7.5 mm (0.30 in.) in diameter and 90.0 mm (3.54 in.) long is pulled in tension with a force of 6000 N (1350 lb_f); the force is subsequently released.

(a) Compute the final length of the specimen at this time. The tensile stress–strain behavior for this alloy is shown in Figure 6.12.

(b) Compute the final specimen length when the load is increased to 16,500 N (3700 lb_f) and then released.

Solution

(a) In order to determine the final length of the brass specimen when the load is released, it first becomes necessary to compute the applied stress using Equation 6.1; thus

$$\sigma = \frac{F}{A_0} = \frac{F}{\pi\left(\frac{d_0}{2}\right)^2} = \frac{6000\ \text{N}}{\pi\left(\frac{7.5\times10^{-3}\ \text{m}}{2}\right)^2} = 136\ \text{MPa}\ \ (19{,}000\ \text{psi})$$

Upon locating this point on the stress–strain curve (Figure 6.12), we note that it is in the linear, elastic region; therefore, when the load is released the specimen will return to its original length of 90 mm (3.54 in.).

(b) In this portion of the problem we are asked to calculate the final length, after load release, when the load is increased to 16,500 N (3700 lb_f). Again, computing the stress

$$\sigma = \frac{16{,}500\ \text{N}}{\pi\left(\frac{7.5\times10^{-3}\ \text{m}}{2}\right)^2} = 373\ \text{MPa}\ \ (52{,}300\ \text{psi})$$

The point on the stress–strain curve corresponding to this stress is in the plastic region. We are able to estimate the amount of permanent strain by drawing a straight line parallel to the linear elastic region; this line intersects the strain axis at a strain of about 0.08 which is the amount of plastic strain. The final specimen length l_i may be determined from a rearranged form of Equation 6.2 as

$$l_i = l_0(1 + \varepsilon) = (90\ \text{mm})(1 + 0.08) = 97.20\ \text{mm}\ (3.82\ \text{in.})$$

6.50 A steel alloy specimen having a rectangular cross section of dimensions 12.7 mm × 6.4 mm (0.5 in. × 0.25 in.) has the stress–strain behavior shown in Figure 6.21. If this specimen is subjected to a tensile force of 38,000 N (8540 $\mathrm{lb_f}$) then

(a) Determine the elastic and plastic strain values.

(b) If its original length is 460 mm (18.0 in.), what will be its final length after the load in part (a) is applied and then released?

<u>Solution</u>

(a) We are asked to determine both the elastic and plastic strain values when a tensile force of 38,000 N (8540 $\mathrm{lb_f}$) is applied to the steel specimen and then released. First it becomes necessary to determine the applied stress using Equation 6.1; thus

$$\sigma = \frac{F}{A_0} = \frac{F}{b_0 d_0}$$

where b_0 and d_0 are cross-sectional width and depth (12.7 mm and 6.4 mm, respectively). Thus

$$\sigma = \frac{38{,}000\ \mathrm{N}}{\left(12.7 \times 10^{-3}\ \mathrm{m}\right)\left(6.4 \times 10^{-3}\ \mathrm{m}\right)} = 468 \times 10^{6}\ \mathrm{N/m^2} = 468\ \mathrm{MPa}\ (68{,}300\ \mathrm{psi})$$

From Figure 6.21, this point is in the plastic region so the specimen will be both elastic and plastic strains. The total strain at this point, ε_t, is about 0.010. We are able to estimate the amount of permanent strain recovery ε_e from Hooke's law, Equation 6.5 as

$$\varepsilon_e = \frac{\sigma}{E}$$

And, since E = 207 GPa for steel (Table 6.1)

$$\varepsilon_e = \frac{468\ \mathrm{MPa}}{207 \times 10^{3}\ \mathrm{MPa}} = 0.00226$$

The value of the plastic strain, ε_p is just the difference between the total and elastic strains; that is

$$\varepsilon_p = \varepsilon_t - \varepsilon_e = 0.010 - 0.00226 = 0.00774$$

(b) If the initial length is 460 mm (18.0 in.) then the final specimen length l_i may be determined from a rearranged form of Equation 6.2 using the plastic strain value as

$$l_i = l_0(1 + H_p) = (460 \text{ mm})(1 + 0.00774) = 463.6 \text{ mm } (18.14 \text{ in.})$$

Hardness

6.51 (a) A 10-mm-diameter Brinell hardness indenter produced an indentation 1.62 mm in diameter in a steel alloy when a load of 500 kg was used. Compute the HB of this material.

(b) What will be the diameter of an indentation to yield a hardness of 450 HB when a 500 kg load is used?

<u>Solution</u>

(a) We are asked to compute the Brinell hardness for the given indentation. It is necessary to use the equation in Table 6.5 for HB, where $P = 500$ kg, $d = 1.62$ mm, and $D = 10$ mm. Thus, the Brinell hardness is computed as

$$\text{HB} = \frac{2P}{\pi D\left[D - \sqrt{D^2 - d^2}\right]}$$

$$= \frac{(2)(500\text{ kg})}{(\pi)(10\text{ mm})\left[10\text{ mm} - \sqrt{(10\text{ mm})^2 - (1.62\text{ mm})^2}\right]} = 241$$

(b) This part of the problem calls for us to determine the indentation diameter d which will yield a 450 HB when $P = 500$ kg. Solving for d from the equation in Table 6.5 gives

$$d = \sqrt{D^2 - \left[D - \frac{2P}{(\text{HB})\pi D}\right]^2}$$

$$= \sqrt{(10\text{ mm})^2 - \left[10\text{ mm} - \frac{(2)(500\text{ kg})}{(450)(\pi)(10\text{ mm})}\right]^2} = 1.19\text{ mm}$$

6.52 Estimate the Brinell and Rockwell hardnesses for the following:

(a) The naval brass for which the stress-strain behavior is shown in Figure 6.12.

(b) The steel alloy for which the stress-strain behavior is shown in Figure 6.21.

Solution

This problem calls for estimations of Brinell and Rockwell hardnesses.

(a) For the brass specimen, the stress-strain behavior for which is shown in Figure 6.12, the tensile strength is 450 MPa (65,000 psi). From Figure 6.19, the hardness for brass corresponding to this tensile strength is about 125 HB or 70 HRB.

(b) The steel alloy (Figure 6.21) has a tensile strength of about 515 MPa (74,700 psi) [Problem 6.25(d)]. This corresponds to a hardness of about 160 HB or ~90 HRB from the line for steels in Figure 6.19. Alternately, using Equation 6.20a

$$\mathrm{HB} = \frac{\mathrm{TS(MPa)}}{3.45} = \frac{515\ \mathrm{MPa}}{3.45} = 149$$

6.53 Using the data represented in Figure 6.19, specify equations relating tensile strength and Brinell hardness for brass and nodular cast iron, similar to Equations 6.20a and 6.20b for steels.

Solution

These equations, for a straight line, are of the form

$$TS = C + (E)(HB)$$

where TS is the tensile strength, HB is the Brinell hardness, and C and E are constants, which need to be determined.

One way to solve for C and E is analytically—establishing two equations using TS and HB data points on the plot, as

$$(TS)_1 = C + (E)(BH)_1$$
$$(TS)_2 = C + (E)(BH)_2$$

Solving for E from these two expressions yields

$$E = \frac{(TS)_1 \quad (TS)_2}{(HB)_2 \quad (HB)_1}$$

For nodular cast iron, if we make the arbitrary choice of $(HB)_1$ and $(HB)_2$ as 200 and 300, respectively, then, from Figure 6.19, $(TS)_1$ and $(TS)_2$ take on values of 600 MPa (87,000 psi) and 1100 MPa (160,000 psi), respectively. Substituting these values into the above expression and solving for E gives

$$E = \frac{600\ \text{MPa} \quad 1100\ \text{MPa}}{200\ \text{HB} \quad 300\ \text{HB}} = 5.0\ \text{MPa/HB}\ \ (730\ \text{psi/HB})$$

Now, solving for C yields

$$C = (TS)_1 - (E)(BH)_1$$

$$= 600\ \text{MPa} - (5.0\ \text{MPa/HB})(200\ \text{HB}) = -400\ \text{MPa}\ (-59{,}000\ \text{psi})$$

Thus, for nodular cast iron, these two equations take the form

$$TS(\text{MPa}) = -400 + 5.0 \times HB$$

$$TS(\text{psi}) = -59{,}000 + 730 \times HB$$

Now for brass, we take $(HB)_1$ and $(HB)_2$ as 100 and 200, respectively, then, from Figure 7.31, $(TS)_1$ and $(TS)_2$ take on values of 370 MPa (54,000 psi) and 660 MPa (95,000 psi), respectively. Substituting these values into the above expression and solving for E gives

$$E = \frac{370\ \text{MPa} - 660\ \text{MPa}}{100\ HB - 200\ HB} = 2.9\ \text{MPa/HB}\ \ (410\ \text{psi/HB})$$

Now, solving for C yields

$$C = (TS)_1 - (E)(BH)_1$$

$$= 370\ \text{MPa} - (2.9\ \text{MPa/HB})(100\ \text{HB}) = 80\ \text{MPa}\ (13{,}000\ \text{psi})$$

Thus, for brass these two equations take the form

$$TS(\text{MPa}) = 80 + 2.9 \times HB$$

$$TS(\text{psi}) = 13{,}000 + 410 \times HB$$

Variability of Material Properties

6.54 Cite five factors that lead to scatter in measured material properties.

Solution

The five factors that lead to scatter in measured material properties are the following: (1) test method; (2) variation in specimen fabrication procedure; (3) operator bias; (4) apparatus calibration; and (5) material inhomogeneities and/or compositional differences.

6.55 Below are tabulated a number of Rockwell B hardness values that were measured on a single steel specimen. Compute average and standard deviation hardness values.

83.3	80.7	86.4
88.3	84.7	85.2
82.8	87.8	86.9
86.2	83.5	84.4
87.2	85.5	86.3

Solution

The average of the given hardness values is calculated using Equation 6.21 as

$$\overline{HRB} = \frac{\sum_{i=1}^{15} HRB_i}{15}$$

$$= \frac{83.3 + 88.3 + 82.8 + \ldots + 86.3}{15} = 85.3$$

And we compute the standard deviation using Equation 6.22 as follows:

$$s = \sqrt{\frac{\sum_{i=1}^{15} \left(HRB_i - \overline{HRB}\right)^2}{15 - 1}}$$

$$= \left[\frac{(83.3 - 85.3)^2 + (88.3 - 85.3)^2 + \ldots + (86.3 - 85.3)^2}{14}\right]^{1/2}$$

$$= \sqrt{\frac{60.31}{14}} = 2.08$$

Design/Safety Factors

6.56 Upon what three criteria are factors of safety based?

Solution

The criteria upon which factors of safety are based are (1) consequences of failure, (2) previous experience, (3) accuracy of measurement of mechanical forces and/or material properties, and (4) economics.

6.57 Determine working stresses for the two alloys that have the stress–strain behaviors shown in Figures 6.12 and 6.21.

Solution

The working stresses for the two alloys the stress–strain behaviors of which are shown in Figures 6.12 and 6.21 are calculated by dividing the yield strength by a factor of safety, which we will take to be 2. For the brass alloy (Figure 6.12), since $\sigma_y \cong 250$ MPa (36,000 psi), the working stress is 125 MPa (18,000 psi), whereas for the steel alloy (Figure 6.21), σ_y = 400 MPa (58,000 psi), and, therefore, σ_w = 200 MPa (29,000 psi).

DESIGN PROBLEMS

6.D1 A large tower is to be supported by a series of steel wires. It is estimated that the load on each wire will be 11,100 N (2500 lbf). Determine the minimum required wire diameter assuming a factor of safety of 2 and a yield strength of 1030 MPa (150,000 psi).

Solution

For this problem the working stress is computed using Equation 6.24 with N = 2, as

$$\sigma_w = \frac{\sigma_y}{2} = \frac{1030\,\text{MPa}}{2} = 515\ \text{MPa (75,000 psi)}$$

Since the force is given, the area may be determined from Equation 6.1, and subsequently the original diameter d_0 may be calculated as

$$A_0 = \frac{F}{\sigma_w} = \pi\left(\frac{d_0}{2}\right)^2$$

And

$$d_0 = \sqrt{\frac{4F}{\pi\sigma_w}} = \sqrt{\frac{(4)(11{,}100\ \text{N})}{\pi\left(515\times10^6\ \text{N/m}^2\right)}}$$

$$= 5.23\times10^{-3}\ \text{m} = 5.23\ \text{mm (0.206 in.)}$$

6.D2 (a) Gaseous hydrogen at a constant pressure of 1.013 MPa (10 atm) is to flow within the inside of a thin-walled cylindrical tube of nickel that has a radius of 0.1 m. The temperature of the tube is to be 300°C and the pressure of hydrogen outside of the tube will be maintained at 0.01013 MPa (0.1 atm). Calculate the minimum wall thickness if the diffusion flux is to be no greater than 1×10^{-7} mol/m^2-s. The concentration of hydrogen in the nickel, C_H (in moles hydrogen per m^3 of Ni) is a function of hydrogen pressure, p_{H_2} (in MPa) and absolute temperature (T) according to

$$C_H = 30.8\sqrt{p_{H_2}}\exp\left(-\frac{12.3\ \text{kJ/mol}}{RT}\right) \qquad (6.28)$$

Furthermore, the diffusion coefficient for the diffusion of H in Ni depends on temperature as

$$D_H = 4.76 \times 10^{-7}\exp\left(-\frac{39.56\ \text{kJ/mol}}{RT}\right) \qquad (6.29)$$

(b) For thin-walled cylindrical tubes that are pressurized, the circumferential stress is a function of the pressure difference across the wall Δp cylinder radius r

$$\sigma = \frac{r\,\Delta p}{4\,\Delta x} \qquad (6.30)$$

Compute the circumferential stress to which the walls of this pressurized cylinder are exposed.

(c) The room-temperature yield strength of Ni is 100 MPa (15,000 psi) and, furthermore, σ_y diminishes about 5 MPa for every 50°C rise in temperature. Would you expect the wall thickness computed in part (b) to be suitable for this Ni cylinder at 300°C? Why or why not?

(d) If this thickness is found to be suitable, compute the minimum thickness that could be used without any deformation of the tube walls. How much would the diffusion flux increase with this reduction in thickness? On the other hand, if the thickness determined in part (c) is found to be unsuitable, then specify a minimum thickness that you would use. In this case, how much of a diminishment in diffusion flux would result?

Solution

(a) This portion of the problem asks for us to compute the wall thickness of a thin-walled cylindrical Ni tube at 300°C through which hydrogen gas diffuses. The inside and outside pressures are, respectively, 1.1013 and 0.01013 MPa, and the diffusion flux is to be no greater than 1×10^{-7} mol/m^2-s. This is a steady-state diffusion problem, which necessitates that we employ Equation 5.3. The concentrations at the inside and outside wall faces may be determined using Equation 6.28, and, furthermore, the diffusion coefficient is computed using Equation 6.29. Solving for Δx (using Equation 5.3)

$$\Delta x = -\frac{D\,\Delta C}{J}$$

$$= \frac{1}{1 \times 10^{7}\ \text{mol/m}^2\ \text{s}} \times$$

$$(4.76 \times 10^{-7}) \exp\left(\frac{39{,}560\ \text{J/mol}}{(8.31\ \text{J/mol-K})(300 \quad 273\ \text{K})}\right) \times$$

$$(30.8)\exp\left(\frac{12{,}300\ \text{J/mol}}{(8.31\ \text{J/mol-K})(300 \quad 273\ \text{K})}\right)\sqrt{0.01013\ \text{MPa}} \quad \sqrt{1.1013\ \text{MPa}}$$

$$= 0.0025\ \text{m} = 2.5\ \text{mm}$$

(b) Now we are asked to determine the circumferential stress:

$$\sigma = \frac{r\,\Delta p}{4\,\Delta x}$$

$$= \frac{(0.10\ \text{m})(1.013\ \text{MPa} \quad 0.01013\ \text{MPa})}{(4)(0.0025\ \text{m})}$$

$$= 10.0\ \text{MPa}$$

(c) Now we are to compare this value of stress to the yield strength of Ni at 300°C, from which it is possible to determine whether or not the 2.5 mm wall thickness is suitable. From the information given in the problem, we may write an equation for the dependence of yield strength (σ_y) on temperature (T) as follows:

$$\sigma_y = 100\ \text{MPa} \quad \frac{5\ \text{MPa}}{50^\circ\text{C}}\left(T \quad T_r\right)$$

where T_r is room temperature and for temperature in degrees Celsius. Thus, at 300°C

$$\sigma_y = 100\ \text{MPa} \quad (0.1\ \text{MPa}/^\circ\text{C})(300^\circ\text{C} \quad 20^\circ\text{C}) = 72\ \text{MPa}$$

Inasmuch as the circumferential stress (10 MPa) is much less than the yield strength (72 MPa), this thickness is entirely suitable.

(d) And, finally, this part of the problem asks that we specify how much this thickness may be reduced and still retain a safe design. Let us use a working stress by dividing the yield stress by a factor of safety, according to Equation 6.24. On the basis of our experience, let us use a value of 2.0 for N. Thus

$$\sigma_w = \frac{\sigma_y}{N} = \frac{72\ \text{MPa}}{2} = 36\ \text{MPa}$$

Using this value for σ_w and Equation 6.30, we now compute the tube thickness as

$$\Delta x = \frac{r\,\Delta p}{4\,\sigma_w}$$

$$= \frac{(0.10\ \text{m})(1.013\ \text{MPa} - 0.01013\ \text{MPa})}{4(36\ \text{MPa})}$$

$$= 0.00070\ \text{m} = 0.70\ \text{mm}$$

Substitution of this value into Fick's first law we calculate the diffusion flux as follows:

$$J = -D\frac{\Delta C}{\Delta x}$$

$$= -\left(4.76 \times 10^{-7}\right)\exp\left[-\frac{39{,}560\ \text{J/mol}}{(8.31\ \text{J/mol-K})(300 + 273\ \text{K})}\right] \times$$

$$\frac{(30.8)\exp\left[-\frac{12{,}300\ \text{J/mol}}{(8.31\ \text{J/mol-K})(300 + 273\ \text{K})}\right]\left(\sqrt{0.01013\ \text{MPa}} - \sqrt{1.013\ \text{MPa}}\right)}{0.0007\ \text{m}}$$

$$= 3.53 \times 10^{-7}\ \text{mol/m}^2\text{-s}$$

Thus, the flux increases by approximately a factor of 3.5, from 1×10^{-7} to 3.53×10^{-7} mol/m^2-s with this reduction in thickness.

6.D3 Consider the steady-state diffusion of hydrogen through the walls of a cylindrical nickel tube as described in Problem 6.D2. One design calls for a diffusion flux of 5×10^{-8} mol/m^2-s, a tube radius of 0.125 m, and inside and outside pressures of 2.026 MPa (20 atm) and 0.0203 MPa (0.2 atm), respectively; the maximum allowable temperature is 450°C. Specify a suitable temperature and wall thickness to give this diffusion flux and yet ensure that the tube walls will not experience any permanent deformation.

Solution

This problem calls for the specification of a temperature and cylindrical tube wall thickness that will give a diffusion flux of 5×10^{-8} mol/m^2-s for the diffusion of hydrogen in nickel; the tube radius is 0.125 m and the inside and outside pressures are 2.026 and 0.0203 MPa, respectively. There are probably several different approaches that may be used; and, of course, there is not one unique solution. Let us employ the following procedure to solve this problem: (1) assume some wall thickness, and, then, using Fick's first law for diffusion (which also employs Equations 5.3 and 6.29), compute the temperature at which the diffusion flux is that required; (2) compute the yield strength of the nickel at this temperature using the dependence of yield strength on temperature as stated in Problem 6.D2; (3) calculate the circumferential stress on the tube walls using Equation 6.30; and (4) compare the yield strength and circumferential stress values—the yield strength should probably be at least twice the stress in order to make certain that no permanent deformation occurs. If this condition is not met then another iteration of the procedure should be conducted with a more educated choice of wall thickness.

As a starting point, let us arbitrarily choose a wall thickness of 2 mm (2×10^{-3} m). The steady-state diffusion equation, Equation 5.3, takes the form

$$J = D\frac{\Delta C}{\Delta x}$$

$$= 5 \times 10^{-8}\ \text{mol/m}^2\text{-s}$$

$$= \left(4.76 \times 10^{-7}\right)\exp\left[\frac{39{,}560\ \text{J/mol}}{(8.31\ \text{J/mol-K})(T)}\right] \times$$

$$\frac{(30.8)\exp\left[\frac{12{,}300\ \text{J/mol}}{(8.31\ \text{J/mol-K})(T)}\right]\left(\sqrt{0.0203\ \text{MPa}} \quad \sqrt{2.026\ \text{MPa}}\right)}{0.002\ \text{m}}$$

Solving this expression for the temperature T gives T = 514 K = 241°C; this value is satisfactory inasmuch as it is less than the maximum allowable value (450°C).

The next step is to compute the stress on the wall using Equation 6.30; thus

$$V = \frac{r\ 'p}{4\ 'x}$$

$$= \frac{(0.125\text{ m})(2.026\text{ MPa} \quad 0.0203\text{ MPa})}{(4)\left(2\ \text{u}10^{3}\text{ m}\right)}$$

$$= 31.3\text{ MPa}$$

Now, the yield strength (V_y) of Ni at this temperature may be computed using the expression

$$V_y = 100\text{ MPa} \quad \frac{5\text{ MPa}}{50\ q\text{C}}\ T \quad T_r$$

where T_r is room temperature. Thus,

$$V_y = 100\text{ MPa} - (0.1\text{ MPa}/q\text{C})(241\ q\text{C} - 20\ q\text{C}) = 77.9\text{ MPa}$$

Inasmuch as this yield strength is greater than twice the circumferential stress, wall thickness and temperature values of 2 mm and 241qC are satisfactory design parameters.

7.2 Consider two edge dislocations of opposite sign and having slip planes that are separated by several atomic distances as indicated in the diagram. Briefly describe the defect that results when these two dislocations become aligned with each other.

Solution

When the two edge dislocations become aligned, a planar region of vacancies will exist between the dislocations as:

7.3 Is it possible for two screw dislocations of opposite sign to annihilate each other? Explain your answer.

Solution

It is possible for two screw dislocations of opposite sign to annihilate one another if their dislocation lines are parallel. This is demonstrated in the figure below.

7.4 For each of edge, screw, and mixed dislocations, cite the relationship between the direction of the applied shear stress and the direction of dislocation line motion.

Solution

For the various dislocation types, the relationships between the direction of the applied shear stress and the direction of dislocation line motion are as follows:

edge dislocation--parallel
screw dislocation--perpendicular
mixed dislocation--neither parallel nor perpendicular

Slip Systems

7.5 (a) Define a slip system.

(b) Do all metals have the same slip system? Why or why not?

Solution

(a) A slip system is a crystallographic plane, and, within that plane, a direction along which dislocation motion (or slip) occurs.

(b) All metals do not have the same slip system. The reason for this is that for most metals, the slip system will consist of the most densely packed crystallographic plane, and within that plane the most closely packed direction. This plane and direction will vary from crystal structure to crystal structure.

7.6 (a) Compare planar densities (Section 3.11 and Problem 3.54) for the (100), (110), and (111) planes for FCC.

(b) Compare planar densities (Problem 3.55) for the (100), (110), and (111) planes for BCC.

Solution

(a) For the FCC crystal structure, the planar density for the (110) plane is given in Equation 3.11 as

$$\mathrm{PD}_{110}(\mathrm{FCC}) \quad \frac{1}{4R^2\sqrt{2}} \quad \frac{0.177}{R^2}$$

Furthermore, the planar densities of the (100) and (111) planes are calculated in Homework Problem 3.54, which are as follows:

$$\mathrm{PD}_{100}(\mathrm{FCC}) = \frac{1}{4R^2} \quad \frac{0.25}{R^2}$$

$$\mathrm{PD}_{111}(\mathrm{FCC}) \quad \frac{1}{2R^2\sqrt{3}} \quad \frac{0.29}{R^2}$$

(b) For the BCC crystal structure, the planar densities of the (100) and (110) planes were determined in Homework Problem 3.55, which are as follows:

$$\mathrm{PD}_{100}(\mathrm{BCC}) = \frac{3}{16R^2} \quad \frac{0.19}{R^2}$$

$$\mathrm{PD}_{110}(\mathrm{BCC}) \quad \frac{3}{8R^2\sqrt{2}} \quad \frac{0.27}{R^2}$$

Below is a BCC unit cell, within which is shown a (111) plane.

(a)

The centers of the three corner atoms, denoted by A, B, and C lie on this plane. Furthermore, the (111) plane does not pass through the center of atom D, which is located at the unit cell center. The atomic packing of this plane is presented in the following figure; the corresponding atom positions from the Figure (a) are also noted.

(b)

Inasmuch as this plane does not pass through the center of atom D, it is not included in the atom count. One sixth of each of the three atoms labeled A, B, and C is associated with this plane, which gives an equivalence of one-half of one atom.

In Figure (b) the triangle with A, B, and C at its corners is an equilateral triangle. And, from Figure (b), the area of this triangle is $\frac{xy}{2}$. The triangle edge length, x, is equal to the length of a face diagonal, as indicated in Figure (a). And its length is related to the unit cell edge length, a, as

$$x^2 = a^2 + a^2 = 2a^2$$

or

$$x = a\sqrt{2}$$

For BCC, $a = \dfrac{4R}{\sqrt{3}}$ (Equation 3.3), and, therefore,

$$x = \frac{4R\sqrt{2}}{\sqrt{3}}$$

Also, from Figure (b), with respect to the length y we may write

$$y^2 + \left(\frac{x}{2}\right)^2 = x^2$$

which leads to $y = \dfrac{x\sqrt{3}}{2}$. And, substitution for the above expression for x yields

$$y = \frac{x\sqrt{3}}{2} = \left(\frac{4R\sqrt{2}}{\sqrt{3}}\right)\left(\frac{\sqrt{3}}{2}\right) = \frac{4R\sqrt{2}}{2}$$

Thus, the area of this triangle is equal to

$$\text{AREA} = \frac{1}{2}\,x\,y = \left(\frac{1}{2}\right)\left(\frac{4R\sqrt{2}}{\sqrt{3}}\right)\left(\frac{4R\sqrt{2}}{2}\right) = \frac{8R^2}{\sqrt{3}}$$

And, finally, the planar density for this (111) plane is

$$\text{PD}_{111}(\text{BCC}) = \frac{0.5\,\text{atom}}{\dfrac{8R^2}{\sqrt{3}}} = \frac{\sqrt{3}}{16R^2} = \frac{0.11}{R^2}$$

7.7 One slip system for the BCC crystal structure is $\{110\}\langle 111\rangle$. In a manner similar to Figure 7.6b, sketch a $\{110\}$-type plane for the BCC structure, representing atom positions with circles. Now, using arrows, indicate two different $\langle 111\rangle$ slip directions within this plane.

Solution

Below is shown the atomic packing for a BCC $\{110\}$-type plane. The arrows indicate two different $\langle 111\rangle$-type directions.

7.8 One slip system for the HCP crystal structure is $\{0001\}\langle 11\bar{2}0\rangle$. In a manner similar to Figure 7.6b, sketch a $\{0001\}$-type plane for the HCP structure and, using arrows, indicate three different $\langle 11\bar{2}0\rangle$ slip directions within this plane. You might find Figure 3.8 helpful.

Solution

Below is shown the atomic packing for an HCP $\{0001\}$-type plane. The arrows indicate three different $\langle 11\bar{2}0\rangle$-type directions.

7.9 Equations 7.1a and 7.1b, expressions for Burgers vectors for FCC and BCC crystal structures, are of the form

$$b \quad \frac{a}{2}\langle uvw\rangle$$

where a is the unit cell edge length. Also, since the magnitudes of these Burgers vectors may be determined from the following equation:

$$|b| \quad \frac{a}{2}\, u^2 \quad v^2 \quad w^2\, {}^{1/2} \tag{7.10}$$

determine values of |b| for aluminum and chromium. You may want to consult Table 3.1.

Solution

For Al, which has an FCC crystal structure, R = 0.1431 nm (Table 3.1) and $a = 2R\sqrt{2}$ = 0.4047 nm (Equation 3.1); also, from Equation 7.1a, the Burgers vector for FCC metals is

$$b \quad \frac{a}{2}\langle 110\rangle$$

Therefore, the values for u, v, and w in Equation 7.10 are 1, 1, and 0, respectively. Hence, the magnitude of the Burgers vector for Al is

$$|b| = \frac{a}{2}\sqrt{u^2 \quad v^2 \quad w^2}$$

$$= \frac{0.4047\text{nm}}{2}\sqrt{(1)^2 \quad (1)^2 \quad (0)^2} = 0.2862 \text{ nm}$$

For Cr which has a BCC crystal structure, R = 0.1249 nm (Table 3.1) and $a = \frac{4R}{\sqrt{3}}$ = 0.2884 nm (Equation 3.3); also, from Equation 7.1b, the Burgers vector for BCC metals is

$$b \quad \frac{a}{2}\langle 111\rangle$$

Therefore, the values for u, v, and w in Equation 7.10 are 1, 1, and 1, respectively. Hence, the magnitude of the Burgers vector for Cr is

$$|b| = \frac{0.2884\text{nm}}{2}\sqrt{(1)^2 \quad (1)^2 \quad (1)^2} = 0.2498 \text{ nm}$$

7.10 (a) In the manner of Equations 7.1a, 7.1b, and 7.1c, specify the Burgers vector for the simple cubic crystal structure. Its unit cell is shown in Figure 3.24. Also, simple cubic is the crystal structure for the edge dislocation of Figure 4.3, and for its motion as presented in Figure 7.1. You may also want to consult the answer to Concept Check 7.1.

(b) On the basis of Equation 7.10, formulate an expression for the magnitude of the Burgers vector, $|b|$, for simple cubic.

Solution

(a) This part of the problem asks that we specify the Burgers vector for the simple cubic crystal structure (and suggests that we consult the answer to Concept Check 7.1). This Concept Check asks that we select the slip system for simple cubic from four possibilities. The correct answer is $\{100\}\langle 010\rangle$. Thus, the Burgers vector will lie in a $\langle 010\rangle$-type direction. Also, the unit slip distance is a (i.e., the unit cell edge length, Figures 4.3 and 7.1). Therefore, the Burgers vector for simple cubic is

$$b = a\langle 010\rangle$$

Or, equivalently

$$b = a\langle 100\rangle$$

(b) The magnitude of the Burgers vector, $|b|$, for simple cubic is

$$|b| = a(1^2 + 0^2 + 0^2)^{1/2} = a$$

Slip in Single Crystals

7.11 Sometimes $\cos\phi\cos\lambda$ in Equation 7.2 is termed the Schmid factor. Determine the magnitude of the Schmid factor for an FCC single crystal oriented with its [100] direction parallel to the loading axis.

Solution

We are asked to compute the Schmid factor for an FCC crystal oriented with its [100] direction parallel to the loading axis. With this scheme, slip may occur on the (111) plane and in the $[1\bar{1}0]$ direction as noted in the figure below.

The angle between the [100] and $[1\bar{1}0]$ directions, λ, may be determined using Equation 7.6

$$\lambda = \cos^{-1}\left[\frac{u_1u_2 + v_1v_2 + w_1w_2}{\sqrt{\left(u_1^2 + v_1^2 + w_1^2\right)\left(u_2^2 + v_2^2 + w_2^2\right)}}\right]$$

where (for [100]) $u_1 = 1$, $v_1 = 0$, $w_1 = 0$, and (for $[1\bar{1}0]$) $u_2 = 1$, $v_2 = -1$, $w_2 = 0$. Therefore, λ is equal to

$$\lambda = \cos^{-1}\left[\frac{(1)(1) + (0)(-1) + (0)(0)}{\sqrt{\left[(1)^2 + (0)^2 + (0)^2\right]\left[(1)^2 + (-1)^2 + (0)^2\right]}}\right]$$

$$= \cos^{-1}\left(\frac{1}{\sqrt{2}}\right) = 45°$$

Now, the angle λ is equal to the angle between the normal to the (111) plane (which is the [111] direction), and the [100] direction. Again from Equation 7.6, and for $u_1 = 1$, $v_1 = 1$, $w_1 = 1$, and $u_2 = 1$, $v_2 = 0$, and $w_2 = 0$, we have

$$\lambda = \cos^{-1}\left[\frac{(1)(1) + (1)(0) + (1)(0)}{\sqrt{\left[(1)^2 + (1)^2 + (1)^2\right]\left[(1)^2 + (0)^2 + (0)^2\right]}}\right]$$

$$= \cos^{-1}\left(\frac{1}{\sqrt{3}}\right) = 54.7^\circ$$

Therefore, the Schmid factor is equal to

$$\cos\phi\cos\lambda = \cos(45^\circ)\cos(54.7^\circ) = \left(\frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{3}}\right) = 0.408$$

7.12 Consider a metal single crystal oriented such that the normal to the slip plane and the slip direction are at angles of 43.1° and 47.9°, respectively, with the tensile axis. If the critical resolved shear stress is 20.7 MPa (3000 psi), will an applied stress of 45 MPa (6500 psi) cause the single crystal to yield? If not, what stress will be necessary?

<u>Solution</u>

This problem calls for us to determine whether or not a metal single crystal having a specific orientation and of given critical resolved shear stress will yield. We are given that $\phi = 43.1°$, $\lambda = 47.9°$, and that the values of the critical resolved shear stress and applied tensile stress are 20.7 MPa (3000 psi) and 45 MPa (6500 psi), respectively. From Equation 7.2

$$\tau_R = \sigma \cos\phi \cos\lambda = (45\text{ MPa})(\cos 43.1°)(\cos 47.9°) = 22.0\text{ MPa (3181 psi}$$

Since the resolved shear stress (22 MPa) is greater than the critical resolved shear stress (20.7 MPa), the single crystal will yield.

7.13 A single crystal of aluminum is oriented for a tensile test such that its slip plane normal makes an angle of 28.1° with the tensile axis. Three possible slip directions make angles of 62.4°, 72.0°, and 81.1° with the same tensile axis.

(a) Which of these three slip directions is most favored?

(b) If plastic deformation begins at a tensile stress of 1.95 MPa (280 psi), determine the critical resolved shear stress for aluminum.

Solution

We are asked to compute the critical resolved shear stress for Al. As stipulated in the problem, $\phi = 28.1^\circ$, while possible values for λ are 62.4°, 72.0°, and 81.1°.

(a) Slip will occur along that direction for which $(\cos\phi\cos\lambda)$ is a maximum, or, in this case, for the largest $\cos\lambda$. Cosines for the possible λ values are given below.

$$\cos(62.4^\circ) = 0.46$$

$$\cos(72.0^\circ) = 0.31$$

$$\cos(81.1^\circ) = 0.15$$

Thus, the slip direction is at an angle of 62.4° with the tensile axis.

(b) From Equation 7.4, the critical resolved shear stress is just

$$\tau_{crss} = \sigma_y(\cos\phi\cos\lambda)_{max}$$

$$= (1.95\text{ MPa})\left[\cos(28.1^\circ)\cos(\quad)^\circ\right] \cong 0.80\text{ MPa }(114\text{ psi})$$

7.14 Consider a single crystal of silver oriented such that a tensile stress is applied along a [001] direction. If slip occurs on a (111) plane and in a $[\bar{1}01]$ direction, and is initiated at an applied tensile stress of 1.1 MPa (160 psi), compute the critical resolved shear stress.

Solution

This problem asks that we compute the critical resolved shear stress for silver. In order to do this, we must employ Equation 7.4, but first it is necessary to solve for the angles λ and φ which are shown in the sketch below.

The angle λ is the angle between the tensile axis—i.e., along the [001] direction—and the slip direction—i.e., $[\bar{1}01]$. The angle λ may be determined using Equation 7.6 as

$$\lambda = \cos^{-1}\left[\frac{u_1u_2 + v_1v_2 + w_1w_2}{\sqrt{(u_1^2 + v_1^2 + w_1^2)(u_2^2 + v_2^2 + w_2^2)}}\right]$$

where (for [001]) $u_1 = 0$, $v_1 = 0$, $w_1 = 1$, and (for $[\bar{1}01]$) $u_2 = -1$, $v_2 = 0$, $w_2 = 1$. Therefore, λ is equal to

$$\lambda = \cos^{-1}\left[\frac{(0)(-1) + (0)(0) + (1)(1)}{\sqrt{\left[(0)^2 + (0)^2 + (1)^2\right]\left[(-1)^2 + (0)^2 + (1)^2\right]}}\right]$$

$$= \cos^{-1}\left(\frac{1}{\sqrt{2}}\right) = 45°$$

Furthermore, ϕ is the angle between the tensile axis—the [001] direction—and the normal to the slip plane—i.e., the (111) plane; for this case this normal is along a [111] direction. Therefore, again using Equation 7.6

$$\phi = \cos^{-1}\left[\frac{(0)(1) + (0)(1) + (1)(1)}{\sqrt{\left[(0)^2 + (0)^2 + (1)^2\right]\left[(1)^2 + (1)^2 + (1)^2\right]}}\right]$$

$$= \cos^{-1}\left(\frac{1}{\sqrt{3}}\right) = 54.7^\circ$$

And, finally, using Equation 7.4, the critical resolved shear stress is equal to

$$\tau_{crss} = \sigma_y(\cos\phi\cos\lambda)$$

$$= (1.1\ \text{MPa})\left[\cos(54.7^\circ)\cos(45^\circ)\right] = (1.1\ \text{MPa})\left(\frac{1}{\sqrt{3}}\right)\left(\frac{1}{\sqrt{2}}\right) = 0.45\ \text{MPa}\ (65.1\ \text{psi})$$

7.15 A single crystal of a metal that has the FCC crystal structure is oriented such that a tensile stress is applied parallel to the [110] direction. If the critical resolved shear stress for this material is 1.75 MPa, calculate the magnitude(s) of applied stress(es) necessary to cause slip to occur on the (111) plane in each of the $[1\bar{1}0]$, $[10\bar{1}]$ and $[01\bar{1}]$ directions.

Solution

In order to solve this problem it is necessary to employ Equation 7.4, but first we need to solve for the for ϕ and λ angles for the three slip systems.

For each of these three slip systems, the λ will be the same—i.e., the angle between the direction of the applied stress, [110] and the normal to the (111) plane, that is, the [111] direction. The angle λ may be determined using Equation 7.6 as

$$\lambda = \cos^{-1}\left[\frac{u_1u_2 + v_1v_2 + w_1w_2}{\sqrt{\left(u_1^2 + v_1^2 + w_1^2\right)\left(u_2^2 + v_2^2 + w_2^2\right)}}\right]$$

where (for [110]) $u_1 = 1, v_1 = 1, w_1 = 0$, and (for [111]) $u_2 = 1, v_2 = 1, w_2 = 1$. Therefore, λ is equal to

$$\lambda = \cos^{-1}\left[\frac{(1)(1) + (1)(1) + (0)(1)}{\sqrt{\left[(1)^2 + (1)^2 + (0)^2\right]\left[(1)^2 + (1)^2 + (1)^2\right]}}\right]$$

$$= \cos^{-1}\left(\frac{2}{\sqrt{6}}\right) = 35.3°$$

Let us now determine ϕ for the $[1\bar{1}0]$ slip direction. Again, using Equation 7.6 where $u_1 = 1$, $v_1 = 1$, $w_1 = 0$ (for [110]), and $u_2 = 1, v_2 = -1, w_2 = 0$ (for $[1\bar{1}0]$). Therefore, ϕ is determined as

$$\phi_{[110]-[1\bar{1}0]} = \cos^{-1}\left[\frac{(1)(1) + (1)(-1) + (0)(0)}{\sqrt{\left[(1)^2 + (1)^2 + (0)^2\right]\left[(1)^2 + (-1)^2 + (0)^2\right]}}\right]$$

$$= \cos^{-1} 0 = 90°$$

Now, we solve for the yield strength for this $(111)-[1\bar{1}0]$ slip system using Equation 7.4 as

$$\sigma_y = \frac{\tau_{crss}}{(\cos\phi\cos\lambda)}$$

$$= \frac{1.75\ \text{MPa}}{\cos(35.3^\circ)\cos(90^\circ)} = \frac{1.75\ \text{MPa}}{(0.816)(0)} = \infty$$

which means that slip will not occur on this (111)–$[1\bar{1}0]$ slip system.

Now, we must determine the value of λ for the (111)–$[10\bar{1}]$ slip system—that is, the angle between the [110] and $[10\bar{1}]$ directions. Again using Equation 7.6

$$\lambda_{[110]-[10\bar{1}]} = \cos^{-1}\left[\frac{(1)(1) + (1)(0) + (0)(-1)}{\sqrt{\left[(1)^2 + (1)^2 + (0)^2\right]\left[(1)^2 + (0)^2 + (-1)^2\right]}}\right]$$

$$= \cos^{-1}\left(\frac{1}{2}\right) = 60^\circ$$

Now, we solve for the yield strength for this (111)–$[10\bar{1}]$ slip system using Equation 7.4 as

$$\sigma_y = \frac{\tau_{crss}}{(\cos\phi\cos\lambda)}$$

$$= \frac{1.75\ \text{MPa}}{\cos(35.3^\circ)\cos(60^\circ)} = \frac{1.75\ \text{MPa}}{(0.816)(0.500)} = 4.29\ \text{MPa}$$

And, finally, for the (111)–$[01\bar{1}]$ slip system, λ is computed using Equation 7.6 as follows:

$$\lambda_{[110]-[01\bar{1}]} = \cos^{-1}\left[\frac{(1)(0) + (1)(1) + (0)(-1)}{\sqrt{\left[(1)^2 + (1)^2 + (0)^2\right]\left[(0)^2 + (1)^2 + (-1)^2\right]}}\right]$$

$$= \cos^{-1}\left(\frac{1}{2}\right) = 60^\circ$$

Thus, since the values of ϕ and λ for this (110)–$[01\bar{1}]$ slip system are the same as for (111)–$[10\bar{1}]$, so also will σ_y be the same—viz 4.29 MPa.

7.16 (a) A single crystal of a metal that has the BCC crystal structure is oriented such that a tensile stress is applied in the [010] direction. If the magnitude of this stress is 2.75 MPa, compute the resolved shear stress in the $[\bar{1}11]$ direction on each of the (110) and (101) planes.

(b) On the basis of these resolved shear stress values, which slip system(s) is (are) most favorably oriented?

Solution

(a) This part of the problem asks, for a BCC metal, that we compute the resolved shear stress in the $[\bar{1}11]$ direction on each of the (110) and (101) planes. In order to solve this problem it is necessary to employ Equation 7.2, which means that we first need to solve for the angles ϕ and λ for the three slip systems.

For each of these three slip systems, the ϕ will be the same—i.e., the angle between the direction of the applied stress, [010] and the slip direction, $[\bar{1}11]$. This angle ϕ may be determined using Equation 7.6

$$\phi = \cos^{-1}\left[\frac{u_1u_2 + v_1v_2 + w_1w_2}{\sqrt{(u_1^2 + v_1^2 + w_1^2)(u_2^2 + v_2^2 + w_2^2)}}\right]$$

where (for [010]) $u_1 = 0$, $v_1 = 1$, $w_1 = 0$, and (for $[\bar{1}11]$) $u_2 = -1$, $v_2 = 1$, $w_2 = 1$. Therefore, ϕ is determined as

$$\phi = \cos^{-1}\left[\frac{(0)(-1) + (1)(1) + (0)(1)}{\sqrt{\left[(0)^2 + (1)^2 + (0)^2\right]\left[(-1)^2 + (1)^2 + (1)^2\right]}}\right]$$

$$= \cos^{-1}\left(\frac{1}{\sqrt{3}}\right) = 54.7°$$

Let us now determine λ for the angle between the direction of the applied tensile stress—i.e., the [010] direction—and the normal to the (110) slip plane—i.e., the [110] direction. Again, using Equation 7.6 where $u_1 = 0$, $v_1 = 1$, $w_1 = 0$ (for [010]), and $u_2 = 1$, $v_2 = 1$, $w_2 = 0$ (for [110]), λ is equal to

$$\lambda_{[010]-[110]} = \cos^{-1}\left[\frac{(0)(1) + (1)(1) + (0)(0)}{\sqrt{\left[(0)^2 + (1)^2 + (0)^2\right]\left[(1)^2 + (1)^2 + (0)^2\right]}}\right]$$

$$= \cos^{-1}\left(\frac{1}{\sqrt{2}}\right) = 45°$$

Now, using Equation 7.2

$$\tau_R = \sigma \cos\phi \cos\lambda$$

we solve for the resolved shear stress for this slip system as

$$\tau_{R(110)-[\bar{1}11]} = (2.75\ \text{MPa})\left[\cos(54.7^\circ)\right]\left[\cos(45^\circ)\right] = (2.75\ \text{MPa})(0.578)(0.707) = 1.12\ \text{MPa}$$

Now, we must determine the value of ϕ for the $(101)-[\bar{1}11]$ slip system—that is, the angle between the direction of the applied stress, [010], and the normal to the (101) plane, i.e., the [101] direction. Again using Equation 7.6

$$\lambda_{[010]-[101]} = \cos^{-1}\left[\frac{(0)(1) + (1)(0) + (0)(1)}{\sqrt{\left[(0)^2 + (1)^2 + (0)^2\right]\left[(1)^2 + (0)^2 + (1)^2\right]}}\right]$$

$$= \cos^{-1}(0) = 90^\circ$$

Thus, the resolved shear stress for this $(101)-[\bar{1}11]$ slip system is

$$\tau_{R(101)-[\bar{1}11]} = (2.75\ \text{MPa})\left[\cos(54.7^\circ)\right]\left[\cos(90^\circ)\right] = (2.75\ \text{MPa})(0.578)(0) = 0\ \text{MPa}$$

(b) The most favored slip system(s) is (are) the one(s) that has (have) the largest τ_R value. Therefore, the $(110)-[\bar{1}11]$ is the most favored since its τ_R (1.12 MPa) is greater than the τ_R value for $(101)-[\bar{1}11]$ (viz., 0 MPa).

7.17 Consider a single crystal of some hypothetical metal that has the FCC crystal structure and is oriented such that a tensile stress is applied along a $[\bar{1}02]$ direction. If slip occurs on a (111) plane and in a $[\bar{1}01]$ direction, compute the stress at which the crystal yields if its critical resolved shear stress is 3.42 MPa.

Solution

This problem asks for us to determine the tensile stress at which a FCC metal yields when the stress is applied along a $[\bar{1}02]$ direction such that slip occurs on a (111) plane and in a $[\bar{1}01]$ direction; the critical resolved shear stress for this metal is 3.42 MPa. To solve this problem we use Equation 7.4; however it is first necessary to determine the values of ϕ and λ. These determinations are possible using Equation 7.6. Now, λ is the angle between $[\bar{1}02]$ and $[\bar{1}01]$ directions. Therefore, relative to Equation 7.6 let us take $u_1 = -1$, $v_1 = 0$, and $w_1 = 2$, as well as $u_2 = -1$, $v_2 = 0$, and $w_2 = 1$. This leads to

$$\lambda = \cos^{-1}\left[\frac{u_1u_2 + v_1v_2 + w_1w_2}{\sqrt{\left(u_1^2 + v_1^2 + w_1^2\right)\left(u_2^2 + v_2^2 + w_2^2\right)}}\right]$$

$$= \cos^{-1}\left\{\frac{(-1)(-1) + (0)(0) + (2)(1)}{\sqrt{\left[(-1)^2 + (0)^2 + (2)^2\right]\left[(-1)^2 + (0)^2 + (1)^2\right]}}\right\}$$

$$= \cos^{-1}\left(\frac{3}{\sqrt{10}}\right) = 18.4°$$

Now for the determination of ϕ, the normal to the (111) slip plane is the [111] direction. Again using Equation 7.6, where we now take $u_1 = -1$, $v_1 = 0$, $w_1 = 2$ (for $[\bar{1}02]$), and $u_2 = 1$, $v_2 = 1$, $w_2 = 1$ (for [111]). Thus,

$$\phi = \cos^{-1}\left\{\frac{(-1)(1) + (0)(1) + (2)(1)}{\sqrt{\left[(-1)^2 + (0)^2 + (2)^2\right]\left[(1)^2 + (1)^2 + (1)^2\right]}}\right\}$$

$$= \cos^{-1}\left(\frac{3}{\sqrt{15}}\right) = 39.2°$$

It is now possible to compute the yield stress (using Equation 7.4) as

$$\sigma_y = \frac{\tau_{crss}}{\cos\phi\cos\lambda} = \frac{3.42\ \text{MPa}}{\left(\frac{3}{\sqrt{10}}\right)\left(\frac{3}{\sqrt{15}}\right)} = 4.65\ \text{MPa}$$

7.18 The critical resolved shear stress for iron is 27 MPa (4000 psi). Determine the maximum possible yield strength for a single crystal of Fe pulled in tension.

Solution

In order to determine the maximum possible yield strength for a single crystal of Fe pulled in tension, we simply employ Equation 7.5 as

$$V_y = 2\,W_{crss} = (2)(27\text{ MPa}) = 54\text{ MPa} \quad (8000\text{ psi})$$

Deformation by Twinning

7.19 List four major differences between deformation by twinning and deformation by slip relative to mechanism, conditions of occurrence, and final result.

Solution

Four major differences between deformation by twinning and deformation by slip are as follows: (1) with slip deformation there is no crystallographic reorientation, whereas with twinning there is a reorientation; (2) for slip, the atomic displacements occur in atomic spacing multiples, whereas for twinning, displacements may be other than by atomic spacing multiples; (3) slip occurs in metals having many slip systems, whereas twinning occurs in metals having relatively few slip systems; and (4) normally slip results in relatively large deformations, whereas only small deformations result for twinning.

Strengthening by Grain Size Reduction

7.20 Briefly explain why small-angle grain boundaries are not as effective in interfering with the slip process as are high-angle grain boundaries.

Solution

Small-angle grain boundaries are not as effective in interfering with the slip process as are high-angle grain boundaries because there is not as much crystallographic misalignment in the grain boundary region for small-angle, and therefore not as much change in slip direction.

7.21 Briefly explain why HCP metals are typically more brittle than FCC and BCC metals.

Solution

Hexagonal close packed metals are typically more brittle than FCC and BCC metals because there are fewer slip systems in HCP.

7.22 Describe in your own words the three strengthening mechanisms discussed in this chapter (i.e., grain size reduction, solid-solution strengthening, and strain hardening). Be sure to explain how dislocations are involved in each of the strengthening techniques.

These three strengthening mechanisms are described in Sections 7.8, 7.9, and 7.10.

7.23 (a) From the plot of yield strength versus (grain diameter)$^{-1/2}$ for a 70 Cu–30 Zn cartridge brass, Figure determine values for the constants σ_0 and k_y in Equation 7.7.

(b) Now predict the yield strength of this alloy when the average grain diameter is 1.0×10^{-3} mm.

Solution

(a) Perhaps the easiest way to solve for σ_0 and k_y in Equation 7.7 is to pick two values each of σ_y and $d^{-1/2}$ from Figure 7.15, and then solve two simultaneous equations, which may be created. For example

$d^{-1/2}$ (mm)$^{-1/2}$	σ_y (MPa)
4	75
12	175

The two equations are thus

$$75 = \sigma_0 + 4k_y$$

$$175 = \sigma_0 + 12k_y$$

Solution of these equations yield the values of

$$k_y = 12.5 \text{ MPa(mm)}^{1/2} \quad (1810 \text{ psi(mm)}^{1/2})$$

$$\sigma_0 = 25 \text{ MPa} \quad (3630 \text{ psi})$$

(b) When $d = 1.0 \times 10^{-3}$ mm, $d^{-1/2} = 31.6$ mm$^{-1/2}$, and, using Equation 7.7,

$$\sigma_y = \sigma_0 + k_y d^{-1/2}$$

$$= (25 \text{ MPa}) + \left[12.5 \text{ MPa(mm)}^{1/2}\right]\left(31.6 \text{ mm}^{-1/2}\right) = 420 \text{ MPa} \quad (61{,}000 \text{ psi})$$

7.24 The lower yield point for an iron that has an average grain diameter of 5×10^{-2} mm is 135 MPa (19,500 psi). At a grain diameter of 8×10^{-3} mm, the yield point increases to 260 MPa (37,500 psi). At what grain diameter will the lower yield point be 205 MPa (30,000 psi)?

Solution

The best way to solve this problem is to first establish two simultaneous expressions of Equation 7.7, solve for σ_0 and k_y, and finally determine the value of **d** when σ_y = 205 MPa. The data pertaining to this problem may be tabulated as follows:

σ_y	d (mm)	$d^{-1/2}$ $(\mathrm{mm})^{-1/2}$
135 MPa	5×10^{-2}	4.47
260 MPa	8×10^{-3}	11.18

The two equations thus become

$$135\ \mathrm{MPa} = \sigma_0 + (4.47)\,k_y$$

$$260\ \mathrm{MPa} = \sigma_0 + (11.18)\,k_y$$

Which yield the values, σ_0 = 51.7 MPa and k_y = 18.63 MPa$(\mathrm{mm})^{1/2}$. At a yield strength of 205 MPa

$$205\ \mathrm{MPa} = 51.7\ \mathrm{MPa} + \left[18.63\ \mathrm{MPa}(\mathrm{mm})^{1/2}\right] d^{-1/2}$$

or $d^{-1/2}$ = 8.23 $(\mathrm{mm})^{-1/2}$, which gives **d** = 1.48×10^{-2} mm.

7.25 If it is assumed that the plot in Figure 7.15 is for noncold-worked brass, determine the grain size of the alloy in Figure 7.19; assume its composition is the same as the alloy in Figure 7.15.

Solution

This problem asks that we determine the grain size of the brass for which is the subject of Figure 7.19. From Figure 7.19a, the yield strength of brass at 0%CW is approximately 175 MPa (26,000 psi). This yield strength from Figure 7.15 corresponds to a $d^{-1/2}$ value of approximately 12.0 $(\text{mm})^{-1/2}$. Thus, $d = 6.9 \times 10^{-3}$ mm.

Solid-Solution Strengthening

7.26 In the manner of Figures 7.17b and 7.18b, indicate the location in the vicinity of an edge dislocation at which an interstitial impurity atom would be expected to be situated. Now briefly explain in terms of lattice strains why it would be situated at this position.

Solution

Below is shown an edge dislocation and where an interstitial impurity atom would be located. Compressive lattice strains are introduced by the impurity atom. There will be a net reduction in lattice strain energy when these lattice strains partially cancel tensile strains associated with the edge dislocation; such tensile strains exist just below the bottom of the extra-half-plane of atoms (Figure 7.4).

Strain Hardening

7.27 (a) Show, for a tensile test, that

$$\%CW = \left(\frac{\epsilon}{\epsilon + 1}\right) \times 100$$

if there is no change in specimen volume during the deformation process (i.e., $A_0 l_0 = A_d l_d$).

(b) Using the result of part (a), compute the percent cold work experienced by naval brass (the stress–strain behavior of which is shown in Figure 6.12) when a stress of 400 MPa (58,000 psi) is applied.

Solution

(a) From Equation 7.8

$$\%CW = \left(\frac{A_0 - A_d}{A_0}\right) \times 100 = \left(1 - \frac{A_d}{A_0}\right) \times 100$$

Which is also equal to

$$\left(1 - \frac{l_0}{l_d}\right) \times 100$$

since $A_d/A_0 = l_0/l_d$, the conservation of volume stipulation given in the problem statement. Now, from the definition of engineering strain (Equation 6.2)

$$\epsilon = \frac{l_d - l_0}{l_0} = \frac{l_d}{l_0} - 1$$

Or,

$$\frac{l_0}{l_d} = \frac{1}{\epsilon + 1}$$

Substitution for l_0/l_d into the %CW expression above gives

$$\%CW = \left(1 - \frac{l_0}{l_d}\right) \times 100 = \left(1 - \frac{1}{\epsilon + 1}\right) \times 100 = \left(\frac{\epsilon}{\epsilon + 1}\right) \times 100$$

(b) From Figure 6.12, a stress of 400 MPa (58,000 psi) corresponds to a strain of 0.13. Using the above expression

$$\%CW = \left(\frac{\varepsilon}{\varepsilon + 1}\right) \times 100 = \left(\frac{0.13}{0.13 + 1.00}\right) \times 100 = 11.5\%CW$$

7.28 Two previously undeformed cylindrical specimens of an alloy are to be strain hardened by reducing their cross-sectional areas (while maintaining their circular cross sections). For one specimen, the initial and deformed radii are 16 mm and 11 mm, respectively. The second specimen, with an initial radius of 12 mm, must have the same deformed hardness as the first specimen; compute the second specimen's radius after deformation.

Solution

In order for these two cylindrical specimens to have the same deformed hardness, they must be deformed to the same percent cold work. For the first specimen

$$\%\mathrm{CW} = \frac{A_0 - A_d}{A_0} \times 100 = \frac{\pi r_0^2 - \pi r_d^2}{\pi r_0^2} \times 100$$

$$= \frac{\pi (16\ \mathrm{mm})^2 - \pi (11\ \mathrm{mm})^2}{\pi (16\ \mathrm{mm})^2} \times 100 = 52.7\%\mathrm{CW}$$

For the second specimen, the deformed radius is computed using the above equation and solving for r_d as

$$r_d = r_0 \sqrt{1 - \frac{\%\mathrm{CW}}{100}}$$

$$= (12\ \mathrm{mm}) \sqrt{1 - \frac{52.7\%\mathrm{CW}}{100}} = 8.25\ \mathrm{mm}$$

7.29 Two previously undeformed specimens of the same metal are to be plastically deformed by reducing their cross-sectional areas. One has a circular cross section, and the other is rectangular; during deformation the circular cross section is to remain circular, and the rectangular is to remain as such. Their original and deformed dimensions are as follows:

	Circular (diameter, mm)	Rectangular (mm)
Original dimensions	15.2	125 × 175
Deformed dimensions	11.4	75 × 200

Which of these specimens will be the hardest after plastic deformation, and why?

Solution

The hardest specimen will be the one that has experienced the greatest degree of cold work. Therefore, all we need do is to compute the %CW for each specimen using Equation 7.8. For the circular one

$$\%CW = \left[\frac{A_0 - A_d}{A_0}\right] \times 100$$

$$= \left[\frac{\pi r_0^2 - \pi r_d^2}{\pi r_0^2}\right] \times 100$$

$$= \left[\frac{\pi\left(\frac{15.2\text{ mm}}{2}\right)^2 - \pi\left(\frac{11.4\text{ mm}}{2}\right)^2}{\pi\left(\frac{15.2\text{ mm}}{2}\right)^2}\right] \times 100 = 43.8\%CW$$

For the rectangular one

$$\%CW = \left[\frac{(125\text{ mm})(175\text{ mm}) - (75\text{ mm})(200\text{ mm})}{(125\text{ mm})(175\text{ mm})}\right] \times 100 = 31.4\%CW$$

Therefore, the deformed circular specimen will be harder.

7.30 A cylindrical specimen of cold-worked copper has a ductility (%EL) of 25%. If its cold-worked radius is 10 mm (0.40 in.), what was its radius before deformation?

Solution

This problem calls for us to calculate the precold-worked radius of a cylindrical specimen of copper that has a cold-worked ductility of 25%EL. From Figure 7.19c, copper that has a ductility of 25%EL will have experienced a deformation of about 11%CW. For a cylindrical specimen, Equation 7.8 becomes

$$\%CW = \left[\frac{\pi r_0^2 - \pi r_d^2}{\pi r_0^2}\right] \times 100$$

Since r_d = 10 mm (0.40 in.), solving for r_0 yields

$$r_0 = \frac{r_d}{\sqrt{1 - \frac{\%CW}{100}}} = \frac{10 \text{ mm}}{\sqrt{1 - \frac{11.0}{100}}} = 10.6 \text{ mm} \quad (0.424 \text{ in.})$$

7.31 (a) What is the approximate ductility (%EL) of a brass that has a yield strength of 275 MPa (40,000 psi)?

(b) What is the approximate Brinell hardness of a 1040 steel having a yield strength of 690 MPa (100,000 psi)?

Solution

(a) In order to solve this problem, it is necessary to consult Figures 7.19a and 7.19c. From Figure 7.19a, a yield strength of 275 MPa for brass corresponds to 10%CW. A brass that has been cold-worked 10% will have a ductility of about 43%EL [Figure 7.19c].

(b) This portion of the problem asks for the Brinell hardness of a 1040 steel having a yield strength of 690 MPa (100,000 psi). From Figure 7.19a, a yield strength of 690 MPa for a 1040 steel corresponds to about 10%CW. A 1040 steel that has been cold worked 10% will have a tensile strength of about 780 MPa [Figure 7.19b]. Finally, using Equation 6.20a

$$\mathrm{HB} = \frac{\mathrm{TS(MPa)}}{3.45} = \frac{780\ \mathrm{MPa}}{3.45} = 226$$

7.32 Experimentally, it has been observed for single crystals of a number of metals that the critical resolved shear stress 2_{crss} L V D I X Q F W L R Q R I W K H $_{D}$ as G L V O R F D W L R Q G H Q V L W \ !

$$W_{crss} \quad W_0 \quad A\sqrt{U_D}$$

Z K H U_0 and 2A are constants. For copper, the critical resolved shear stress is 2.10 MPa (305 psi) at a dislocation density of 10^5 mm^{-2}. If it is known that the value of A for copper is 6.35 *u* 10^{-3} MPa-mm (0.92 psi-mm), compute the W_{crss} at a dislocation density of 10^7 mm^{-2}.

Solution

We are asked in this problem to compute the critical resolved shear stress at a dislocation density of 10^7 mm^{-2}. It is first necessary to compute the value of the constant W_0 (in the equation provided in the problem statement) from the one set of data as

$$W_0 \quad W_{crss} \quad A\sqrt{U_D}$$

$$2.10\,\text{MPa} \quad \left(6.35 \text{ u } 10^{3}\ \text{MPa-mm}\right)\sqrt{10^5\ \text{mm}^{2}} \quad 0.092\,\text{MPa}\ (13.3\,\text{psi})$$

Now, the critical resolved shear stress may be determined at a dislocation density of 10^7 mm^{-2} as

$$W_{crss} = W_0 + A\sqrt{U_D}$$

$$= (0.092\,\text{MPa}) + \left(6.35 \text{ u } 10^{-3}\ \text{MPa-mm}\right)\sqrt{10^7\ \text{mm}^{2}} = 20.2\,\text{MPa}\ (2920\,\text{psi})$$

Recovery
Recrystallization
Grain Growth

7.33 Briefly cite the differences between recovery and recrystallization processes.

Solution

For recovery, there is some relief of internal strain energy by dislocation motion; however, there are virtually no changes in either the grain structure or mechanical characteristics. During recrystallization, on the other hand, a new set of strain-free grains forms, and the material becomes softer and more ductile.

7.34 Estimate the fraction of recrystallization from the photomicrograph in Figure 7.21c.

Solution

Below is shown a square grid onto which is superimposed the recrystallized regions from the micrograph. Approximately 400 squares lie within the recrystallized areas, and since there are 672 total squares, the specimen is about 60% recrystallized.

7.35 Explain the differences in grain structure for a metal that has been cold worked and one that has been cold worked and then recrystallized.

Solution

During cold-working, the grain structure of the metal has been distorted to accommodate the deformation. Recrystallization produces grains that are equiaxed and smaller than the parent grains.

7.36 (a) What is the driving force for recrystallization?

(b) For grain growth?

Solution

(a) The driving force for recrystallization is the difference in internal energy between the strained and unstrained material.

(b) The driving force for grain growth is the reduction in grain boundary energy as the total grain boundary area decreases.

7.37 (a) From Figure 7.25, compute the length of time required for the average grain diameter to increase from 0.01 to 0.1 mm at 500°C for this brass material.

(b) Repeat the calculation at 600°C.

Solution

(a) At 500°C, the time necessary for the average grain diameter to grow to increase from 0.01 to 0.1 mm is approximately 3500 min.

(b) At 600°C the time required for this same grain size increase is approximately 150 min.

7.38 The average grain diameter for a brass material was measured as a function of time at 650°C, which is tabulated below at two different times:

Time (min)	Grain Diameter (mm)
30	3.9×10^{-2}
90	6.6×10^{-2}

(a) What was the original grain diameter?

(b) What grain diameter would you predict after 150 min at 650°C?

Solution

(a) Using the data given and Equation 7.9 (taking $n = 2$), we may set up two simultaneous equations with d_0 and K as unknowns; thus

$$\left(3.9 \times 10^{-2}\ \text{mm}\right)^2 - d_0^2 = (30\ \text{min})K$$

$$\left(6.6 \times 10^{-2}\ \text{mm}\right)^2 - d_0^2 = (90\ \text{min})K$$

Solution of these expressions yields a value of d_0, the original grain diameter, of

$$d_0 = 0.01\ \text{mm},$$

and a value for K of $4.73 \times 10^{-5}\ \text{mm}^2/\text{min}$

(b) At 150 min, the diameter d is computed using a rearranged form of Equation 7.9 as

$$d = \sqrt{d_0^2 + Kt}$$

$$= \sqrt{(0.01\ \text{mm})^2 + \left(4.73 \times 10^{-5}\ \text{mm}^2/\text{min}\right)(150\ \text{min})} = 0.085\ \text{mm}$$

7.39 An undeformed specimen of some alloy has an average grain diameter of 0.040 mm. You are asked to reduce its average grain diameter to 0.010 mm. Is this possible? If so, explain the procedures you would use and name the processes involved. If it is not possible, explain why.

Solution

Yes, it is possible to reduce the average grain diameter of an undeformed alloy specimen from 0.040 mm to 0.010 mm. In order to do this, plastically deform the material at room temperature (i.e., cold work it), and then anneal at an elevated temperature in order to allow recrystallization and some grain growth to occur until the average grain diameter is 0.010 mm.

7.40 Grain growth is strongly dependent on temperature (i.e., rate of grain growth increases with increasing temperature), yet temperature is not explicitly given as a part of Equation 7.9.

(a) Into which of the parameters in this expression would you expect temperature to be included?

(b) On the basis of your intuition, cite an explicit expression for this temperature dependence.

Solution

(a) The temperature dependence of grain growth is incorporated into the constant K in Equation 7.9.

(b) The explicit expression for this temperature dependence is of the form

$$K = K_0 \exp\left(\frac{Q}{RT}\right)$$

in which K_0 is a temperature-independent constant, the parameter Q is an activation energy, and R and T are the gas constant and absolute temperature, respectively.

7.41 An uncold-worked brass specimen of average grain size 0.008 mm has a yield strength of 160 MPa (23,500 psi). Estimate the yield strength of this alloy after it has been heated to 600°C for 1000 s, if it is known that the value of k_y is 12.0 MPa-mm$^{1/2}$ (1740 psi-mm$^{1/2}$).

Solution

In order to solve this problem, it is first necessary to calculate the constant σ_0 in Equation 7.7 as

$$\sigma_0 = \sigma_y \quad k_y d^{-1/2}$$

$$= 160\,\text{MPa} \quad \left(12.0\,\text{MPa} \quad \text{mm}^{1/2}\right)(0.008\,\text{mm})^{\;1/2} \quad 25.8\,\text{MPa}\ (4046\,\text{psi})$$

Next, we must determine the average grain size after the heat treatment. From Figure 7.25 at 600°C after 1000 s (16.7 min) the average grain size of a brass material is about 0.20 mm. Therefore, calculating σ_y at this new grain size using Equation 7.7 we get

$$\sigma_y = \sigma_0 \quad k_y d^{-1/2}$$

$$= 25.8\,\text{MPa} \quad \left(12.0\ \text{MPa-}\,\text{mm}^{1/2}\right)(0.20\,\text{mm})^{-1/2} = 52.6\,\text{MPa}\ (7940\,\text{psi})$$

DESIGN PROBLEMS

Strain Hardening
Recrystallization

7.D1 Determine whether or not it is possible to cold work steel so as to give a minimum Brinell hardness of 225, and at the same time have a ductility of at least 12%EL. Justify your decision.

Solution

The tensile strength corresponding to a Brinell hardness of 225 may be determined using Equation 6.20a as

$$\mathrm{TS(MPa)} = 3.45 \times \mathrm{HB} = (3.45)(225) = 776\ \mathrm{MPa}$$

Furthermore, from Figure 7.19b, in order to achieve a tensile strength of 776 MPa, deformation of at least 9%CW is necessary. Finally, if we cold work the steel to 9%CW, then the ductility is 17%EL from Figure 7.19c. Therefore, it is possible to meet both of these criteria by plastically deforming the steel.

7.D2 Determine whether or not it is possible to cold work brass so as to give a minimum Brinell hardness of 120 and at the same time have a ductility of at least 20%EL. Justify your decision.

Solution

According to Figure 6.19, a Brinell hardness of 120 corresponds to a tensile strength of 440 MPa (63,500 psi.) Furthermore, from Figure 7.19, in order to achieve a tensile strength of 440 MPa, deformation of at least 26%CW is necessary. Finally, if we are to achieve a ductility of at least 20%EL, then a maximum deformation of 23%CW is possible from Figure 7.19c. Therefore, it is not possible to meet both of these criteria by plastically deforming brass.

7.D3 A cylindrical specimen of cold-worked steel has a Brinell hardness of 250.

(a) Estimate its ductility in percent elongation.

(b) If the specimen remained cylindrical during deformation and its original radius was 5 mm (0.20 in.), determine its radius after deformation.

Solution

(a) From Figure 6.19, a Brinell hardness of 250 corresponds to a tensile strength of 860 MPa (125,000 psi), which, from Figure 7.19b, requires a deformation of 25%CW. Furthermore, 25%CW yields a ductility of about 11%EL for steel, Figure 7.19c

(b) We are now asked to determine the radius after deformation if the undeformed radius is 5 mm (0.20 in.). From Equation 7.8 and for a cylindrical specimen

$$\%\text{CW} = \left[\frac{\pi r_0^2 - \pi r_d^2}{\pi r_0^2}\right] \times 100$$

Now, solving for r_d from this expression, we get

$$r_d = r_0\sqrt{1 - \frac{\%\text{CW}}{100}}$$

$$= (5\ \text{mm})\sqrt{1 - \frac{25}{100}} = 4.33\ \text{mm}\ \ (0.173\ \text{in.})$$

7.D4 It is necessary to select a metal alloy for an application that requires a yield strength of at least 345 MPa (50,000 psi) while maintaining a minimum ductility (%EL) of 20%. If the metal may be cold worked, decide which of the following are candidates: copper, brass, and a 1040 steel. Why?

Solution

For each of these alloys, the minimum cold work necessary to achieve the yield strength may be determined from Figure 7.19a, while the maximum possible cold work for the ductility is found in Figure 7.19c. These data are tabulated below.

	Yield Strength (> 345 MPa)	Ductility (> 20%EL)
Steel	Any %CW	< 5%CW
Brass	> 20%CW	< 23%CW
Copper	> 54%CW	< 15%CW

Thus, both the 1040 steel and brass are possible candidates since for these alloys there is an overlap of percents coldwork to give the required minimum yield strength and ductility values.

7.D5 A cylindrical rod of 1040 steel originally 15.2 mm (0.60 in.) in diameter is to be cold worked by drawing; the circular cross section will be maintained during deformation. A cold-worked tensile strength in excess of 840 MPa (122,000 psi) and a ductility of at least 12%EL are desired. Furthermore, the final diameter must be 10 mm (0.40 in.). Explain how this may be accomplished.

Solution

First let us calculate the percent cold work and attendant tensile strength and ductility if the drawing is carried out without interruption. From Equation 7.8

$$\%\text{CW} = \frac{\pi\left(\frac{d_0}{2}\right)^2 - \pi\left(\frac{d_d}{2}\right)^2}{\pi\left(\frac{d_0}{2}\right)^2} \times 100$$

$$= \frac{\pi\left(\frac{15.2\ \text{mm}}{2}\right)^2 - \pi\left(\frac{10\ \text{mm}}{2}\right)^2}{\pi\left(\frac{15.2\ \text{mm}}{2}\right)^2} \times 100 = 56\%\text{CW}$$

At 56%CW, the steel will have a tensile strength on the order of 920 MPa (133,000 psi) [Figure 7.19(b)], which is adequate; however, the ductility will be less than 10%EL [Figure 7.19(c)], which is insufficient.

Instead of performing the drawing in a single operation, let us initially draw some fraction of the total deformation, then anneal to recrystallize, and, finally, cold work the material a second time in order to achieve the final diameter, tensile strength, and ductility.

Reference to Figure 7.19(b) indicates that 20%CW is necessary to yield a tensile strength of 840 MPa (122,000 psi). Similarly, a maximum of 21%CW is possible for 12%EL [Figure 7.19(c)]. The average of these extremes is 20.5%CW. Again using Equation 7.8, if the final diameter after the first drawing is d_0', then

$$20.5\%\text{CW} = \frac{\pi\left(\frac{d_0'}{2}\right)^2 - \pi\left(\frac{10\ \text{mm}}{2}\right)^2}{\pi\left(\frac{d_0'}{2}\right)^2} \times 100$$

And, solving the above expression for d_0', yields

$$d_0' = \frac{10 \text{ mm}}{\sqrt{1 \quad \frac{20.5\%\text{CW}}{100}}} = 11.2 \text{ mm} \ \ (0.45 \text{ in}$$

7.D6 A cylindrical rod of copper originally 16.0 mm (0.625 in.) in diameter is to be cold worked by drawing; the circular cross section will be maintained during deformation. A cold-worked yield strength in excess of 250 MPa (36,250 psi) and a ductility of at least 12%EL are desired. Furthermore, the final diameter must be 11.3 mm (0.445 in.). Explain how this may be accomplished.

Solution

Let us first calculate the percent cold work and attendant yield strength and ductility if the drawing is carried out without interruption. From Equation 7.8

$$\%\text{CW} = \frac{\pi\left(\frac{d_0}{2}\right)^2 - \pi\left(\frac{d_d}{2}\right)^2}{\pi\left(\frac{d_0}{2}\right)^2} \times 100$$

$$= \frac{\pi\left(\frac{16.0\text{ mm}}{2}\right)^2 - \pi\left(\frac{11.3\text{ mm}}{2}\right)^2}{\pi\left(\frac{16.0\text{ mm}}{2}\right)^2} \times 100 = 50\%\text{CW}$$

At 50%CW, the copper will have a yield strength on the order of 330 MPa (48,000 psi), Figure 7.19a, which is adequate; however, the ductility will be about 4%EL, Figure 7.19c, which is insufficient.

Instead of performing the drawing in a single operation, let us initially draw some fraction of the total deformation, then anneal to recrystallize, and, finally, cold work the material a second time in order to achieve the final diameter, yield strength, and ductility.

Reference to Figure 7.19a indicates that 21%CW is necessary to give a yield strength of 250 MPa. Similarly, a maximum of 23%CW is possible for 12%EL [Figure 7.19c]. The average of these two values is 22%CW, which we will use in the calculations. Thus, to achieve both the specified yield strength and ductility, the copper must be deformed to 22%CW. If the final diameter after the first drawing is d'_0, then, using Equation 7.8

$$22\%\text{CW} = \frac{\pi\left(\frac{d'_0}{2}\right)^2 - \pi\left(\frac{11.3\text{ mm}}{2}\right)^2}{\pi\left(\frac{d'_0}{2}\right)^2} \times 100$$

And, solving for d'_0 from the above expression yields

$$d_0' = \frac{11.3\ \text{mm}}{\sqrt{1 \quad \frac{22\%\text{CW}}{100}}} = 12.8\ \text{mm}\ \ (0.50\ \text{in.})$$

7.D7 A cylindrical 1040 steel rod having a minimum tensile strength of 865 MPa (125,000 psi), a ductility of at least 10%EL, and a final diameter of 6.0 mm (0.25 in.) is desired. Some 7.94 mm (0.313 in.) diameter 1040 steel stock, which has been cold worked 20% is available. Describe the procedure you would follow to obtain this material. Assume that 1040 steel experiences cracking at 40%CW.

Solution

This problem calls for us to cold work some 1040 steel stock that has been previously cold worked in order to achieve minimum tensile strength and ductility values of 865 MPa (125,000 psi) and 10%EL, respectively, while the final diameter must be 6.0 mm (0.25 in.). Furthermore, the material may not be deformed beyond 40%CW. Let us start by deciding what percent coldwork is necessary for the minimum tensile strength and ductility values, assuming that a recrystallization heat treatment is possible. From Figure 7.19b, at least 25%CW is required for a tensile strength of 865 MPa. Furthermore, according to Figure 7.19c, 10%EL corresponds a maximum of 30%CW. Let us take the average of these two values (i.e., 27.5%CW), and determine what previous specimen diameter is required to yield a final diameter of 6.0 mm. For cylindrical specimens, Equation 7.8 takes the form

$$\%CW = \frac{\pi\left(\frac{d_0}{2}\right)^2 - \pi\left(\frac{d_d}{2}\right)^2}{\pi\left(\frac{d_0}{2}\right)^2} \times 100$$

Solving for the original diameter d_0 yields

$$d_0 = \frac{d_d}{\sqrt{1 - \frac{\%CW}{100}}} = \frac{6.0 \text{ mm}}{\sqrt{1 - \frac{27.5\%CW}{100}}} = 7.05 \text{ mm} \quad (0.278 \text{ in.})$$

Now, let us determine its undeformed diameter realizing that a diameter of 7.94 mm corresponds to 20%CW. Again solving for d_0 using the above equation and assuming d_d = 7.94 mm yields

$$d_0 = \frac{d_d}{\sqrt{1 - \frac{\%CW}{100}}} = \frac{7.94 \text{ mm}}{\sqrt{1 - \frac{20\%CW}{100}}} = 8.88 \text{ mm} \quad (0.350 \text{ in.})$$

At this point let us see if it is possible to deform the material from 8.88 mm to 7.05 mm without exceeding the 40%CW limit. Again employing Equation 7.8

$$\%\text{CW} = \frac{\pi\left(\frac{8.88\ \text{mm}}{2}\right)^2 - \pi\left(\frac{7.05\ \text{mm}}{2}\right)^2}{\pi\left(\frac{8.88\ \text{mm}}{2}\right)^2} \times 100 = 37\%\text{CW}$$

In summary, the procedure which can be used to produce the desired material would be as follows: cold work the as-received stock to 7.05 mm (0.278 in.), heat treat it to achieve complete recrystallization, and then cold work the material again to 6.0 mm (0.25 in.), which will give the desired tensile strength and ductility.

8.2 Estimate the theoretical fracture strength of a brittle material if it is known that fracture occurs by the propagation of an elliptically shaped surface crack of length 0.25 mm (0.01 in.) and having a tip radius of curvature of 1.2×10^{-3} mm (4.7×10^{-5} in.) when a stress of 1200 MPa (174,000 psi) is applied.

Solution

In order to estimate the theoretical fracture strength of this material it is necessary to calculate σ_m using Equation 8.1 given that σ_0 = 1200 MPa, a = 0.25 mm, and $\rho_t = 1.2 \times 10^{-3}$ mm. Thus,

$$\sigma_m = 2\sigma_0 \left(\frac{a}{\rho_t}\right)^{1/2}$$

$$= (2)(1200\ \text{MPa})\left[\frac{0.25\ \text{mm}}{1.2 \times 10^{-3}\ \text{mm}}\right]^{1/2} = 3.5 \times 10^4\ \text{MPa} = 35\ \text{GPa}\ \left(5.1 \times 10^6\ \text{psi}\right)$$

8.3 If the specific surface energy for soda-lime glass is 0.30 J/m^2, using data contained in Table 12.5, compute the critical stress required for the propagation of a surface crack of length 0.05 mm.

Solution

We may determine the critical stress required for the propagation of an surface crack in soda-lime glass using Equation 8.3; taking the value of 69 GPa (Table 12.5) as the modulus of elasticity, we get

$$\sigma_c = \left[\frac{2E\gamma_s}{\pi a}\right]^{1/2}$$

$$= \left[\frac{(2)\left(69 \times 10^9 \text{ N/m}^2\right)(0.30 \text{ N/m})}{(\pi)\left(0.05 \times 10^{-3} \text{ m}\right)}\right]^{1/2} = 16.2 \times 10^6 \text{ N/m}^2 = 16.2 \text{ MPa}$$

8.4 A polystyrene component must not fail when a tensile stress of 1.25 MPa (180 psi) is applied. Determine the maximum allowable surface crack length if the surface energy of polystyrene is 0.50 J/m^2 (2.86 $\times 10^{-3}$ in.-lb$_f$/in.^{2}). Assume a modulus of elasticity of 3.0 GPa (0.435 $\times 10^6$ psi).

Solution

The maximum allowable surface crack length for polystyrene may be determined using Equation 8.3; taking 3.0 GPa as the modulus of elasticity, and solving for a, leads to

$$a = \frac{2E\gamma_s}{\pi\sigma_c^2} = \frac{(2)\left(3 \times 10^9 \text{ N/m}^2\right)(0.50 \text{ N/m})}{(\pi)\left(1.25 \times 10^6 \text{ N/m}^2\right)^2}$$

$$= 6.1 \times 10^{-4} \text{ m} = 0.61 \text{ mm} \ \ (0.024 \text{ in.})$$

8.5 A specimen of a 4340 steel alloy having a plane strain fracture toughness of $45\ \text{MPa}\sqrt{\text{m}}$ $(41\ \text{ksi}\sqrt{\text{in.}})$ is exposed to a stress of 1000 MPa (145,000 psi). Will this specimen experience fracture if it is known that the largest surface crack is 0.75 mm (0.03 in.) long? Why or why not? Assume that the parameter Y has a value of 1.0.

Solution

This problem asks us to determine whether or not the 4340 steel alloy specimen will fracture when exposed to a stress of 1000 MPa, given the values of K_{Ic}, Y, and the largest value of a in the material. This requires that we solve for σ_c from Equation 8.6. Thus

$$\sigma_c = \frac{K_{Ic}}{Y\sqrt{\pi a}} = \frac{45\ \text{MPa}\sqrt{\text{m}}}{(1.0)\sqrt{(\pi)\left(0.75\times10^{-3}\ \text{m}\right)}} = 927\ \text{MPa}\quad(133{,}500\ \text{psi})$$

Therefore, fracture will most likely occur because this specimen will tolerate a stress of 927 MPa (133,500 psi) before fracture, which is less than the applied stress of 1000 MPa (145,000 psi).

8.6 Some aircraft component is fabricated from an aluminum alloy that has a plane strain fracture toughness of $35 \text{ MPa}\sqrt{\text{m}}$ $(31.9 \text{ ksi}\sqrt{\text{in.}})$. It has been determined that fracture results at a stress of 250 MPa (36,250 psi) when the maximum (or critical) internal crack length is 2.0 mm (0.08 in.). For this same component and alloy, will fracture occur at a stress level of 325 MPa (47,125 psi) when the maximum internal crack length is 1.0 mm (0.04 in.)? Why or why not?

Solution

We are asked to determine if an aircraft component will fracture for a given fracture toughness $\left(35 \text{ MPa}\sqrt{\text{m}}\right)$, stress level (325 MPa), and maximum internal crack length (1.0 mm), given that fracture occurs for the same component using the same alloy for another stress level and internal crack length. It first becomes necessary to solve for the parameter Y, using Equation 8.5, for the conditions under which fracture occurred (i.e., $\sigma = 250$ MPa and $2a = 2.0$ mm). Therefore,

$$Y = \frac{K_{Ic}}{\sigma\sqrt{\pi a}} = \frac{35 \text{ MPa}\sqrt{\text{m}}}{(250 \text{ MPa})\sqrt{(\pi)\left(\frac{2 \times 10^{-3} \text{ m}}{2}\right)}} = 2.50$$

Now we will solve for the product $Y\sigma\sqrt{\pi a}$ for the other set of conditions, so as to ascertain whether or not this value is greater than the K_{Ic} for the alloy. Thus,

$$Y\sigma\sqrt{\pi a} = (2.50)(325 \text{ MPa})\sqrt{(\pi)\left(\frac{1 \times 10^{-3} \text{ m}}{2}\right)}$$

$$= 32.2 \text{ MPa}\sqrt{\text{m}} \qquad (29.5 \text{ ksi}\sqrt{\text{in.}})$$

Therefore, fracture will not occur since this value $\left(32.3 \text{ MPa}\sqrt{\text{m}}\right)$ is less than the K_{Ic} of the material, $35 \text{ MPa}\sqrt{\text{m}}$.

8.7 Suppose that a wing component on an aircraft is fabricated from an aluminum alloy that has a plane strain fracture toughness of $40\ \text{MPa}\sqrt{\text{m}}$ ($36.4\ \text{ksi}\sqrt{\text{in.}}$). It has been determined that fracture results at a stress of 365 MPa (53,000 psi) when the maximum internal crack length is 2.5 mm (0.10 in.). For this same component and alloy, compute the stress level at which fracture will occur for a critical internal crack length of 4.0 mm (0.16 in.).

Solution

This problem asks us to determine the stress level at which an a wing component on an aircraft will fracture for a given fracture toughness $\left(40\ \text{MPa}\sqrt{\text{m}}\right)$ and maximum internal crack length (4.0 mm), given that fracture occurs for the same component using the same alloy at one stress level (365 MPa) and another internal crack length (2.5 mm). It first becomes necessary to solve for the parameter Y for the conditions under which fracture occurred using Equation 8.5. Therefore,

$$Y = \frac{K_{Ic}}{\sigma\sqrt{\pi a}} = \frac{40\ \text{MPa}\sqrt{\text{m}}}{(365\ \text{MPa})\sqrt{(\pi)\left(\dfrac{2.5 \times 10^{-3}\ \text{m}}{2}\right)}} = 1.75$$

Now we will solve for σ_c using Equation 8.6 as

$$\sigma_c = \frac{K_{Ic}}{Y\sqrt{\pi a}} = \frac{40\ \text{MPa}\sqrt{\text{m}}}{(1.75)\sqrt{(\pi)\left(\dfrac{4 \times 10^{-3}\ \text{m}}{2}\right)}} = 288\ \text{MPa}\quad(41{,}500\ \text{psi})$$

8.8 A large plate is fabricated from a steel alloy that has a plane strain fracture toughness of $55\ \text{MPa}\sqrt{\text{m}}$ ($50\ \text{ksi}\sqrt{\text{in.}}$). If, during service use, the plate is exposed to a tensile stress of 200 MPa (29,000 psi), determine the minimum length of a surface crack that will lead to fracture. Assume a value of 1.0 for Y.

Solution

For this problem, we are given values of K_{Ic} $\left(55\ \text{MPa}\sqrt{\text{m}}\right)$, σ (200 MPa), and Y (1.0) for a large plate and are asked to determine the minimum length of a surface crack that will lead to fracture. All we need do is to solve for a_c using Equation 8.7; therefore

$$a_c = \frac{1}{\pi}\left(\frac{K_{Ic}}{Y\sigma}\right)^2 = \frac{1}{\pi}\left[\frac{55\ \text{MPa}\sqrt{\text{m}}}{(1.0)(200\ \text{MPa})}\right]^2 = 0.024\ \text{m} = 24\ \text{mm}\quad (0.95\ \text{in.})$$

8.9 Calculate the maximum internal crack length allowable for a 7075-T651 aluminum alloy (Table 8.1) component that is loaded to a stress one half of its yield strength. Assume that the value of Y is 1.35.

Solution

This problem asks us to calculate the maximum internal crack length allowable for the 7075-T651 aluminum alloy in Table 8.1 given that it is loaded to a stress level equal to one-half of its yield strength. For this alloy, $K_{Ic} = 24\ \text{MPa}\sqrt{\text{m}}\ \left(22\ \text{ksi}\sqrt{\text{in.}}\right)$; also, $\sigma = \sigma_y/2$ = (495 MPa)/2 = 248 MPa (36,000 psi). Now solving for $2a_c$ using Equation 8.7 yields

$$2a_c = \frac{2}{\pi}\left(\frac{K_{Ic}}{Y\sigma}\right)^2 = \frac{2}{\pi}\left[\frac{24\ \text{MPa}\sqrt{\text{m}}}{(1.35)(248\ \text{MPa})}\right]^2 = 0.0033\ \text{m} = 3.3\ \text{mm}\quad(0.13\ \text{in.})$$

8.10 A structural component in the form of a wide plate is to be fabricated from a steel alloy that has a plane strain fracture toughness of $77.0\ \text{MPa}\sqrt{\text{m}}$ ($70.1\ \text{ksi}\sqrt{\text{in.}}$) and a yield strength of 1400 MPa (205,000 psi). The flaw size resolution limit of the flaw detection apparatus is 4.0 mm (0.16 in.). If the design stress is one half of the yield strength and the value of Y is 1.0, determine whether or not a critical flaw for this plate is subject to detection.

Solution

This problem asks that we determine whether or not a critical flaw in a wide plate is subject to detection given the limit of the flaw detection apparatus (4.0 mm), the value of K_{Ic} $\left(77\ \text{MPa}\sqrt{\text{m}}\right)$, the design stress ($\sigma_y/2$ in which σ_y = 1400 MPa), and Y = 1.0. We first need to compute the value of a_c using Equation 8.7; thus

$$a_c = \frac{1}{\pi}\left(\frac{K_{Ic}}{Y\sigma}\right)^2 = \frac{1}{\pi}\left[\frac{77\ \text{MPa}\sqrt{\text{m}}}{(1.0)\left(\dfrac{1400\ \text{MPa}}{2}\right)}\right]^2 = 0.0039\ \text{m} = 3.9\ \text{mm}\quad (0.15\ \text{in.})$$

Therefore, the critical flaw is not subject to detection since this value of a_c (3.9 mm) is less than the 4.0 mm resolution limit.

8.11 After consultation of other references, write a brief report on one or two nondestructive test techniques that are used to detect and measure internal and/or surface flaws in metal alloys.

The student should do this problem on his/her own.

Impact Fracture Testing

8.12 Following is tabulated data that were gathered from a series of Charpy impact tests on a ductile cast iron.

Temperature (°C)	Impact Energy (J)
–25	124
–50	123
–75	115
–85	100
–100	73
–110	52
–125	26
–150	9
–175	6

(a) Plot the data as impact energy versus temperature.

(b) Determine a ductile-to-brittle transition temperature as that temperature corresponding to the average of the maximum and minimum impact energies.

(c) Determine a ductile-to-brittle transition temperature as that temperature at which the impact energy is 80 J.

Solution

(a) The plot of impact energy versus temperature is shown below.

(b) The average of the maximum and minimum impact energies from the data is

$$\text{Average} = \frac{124\ \text{J} \qquad 6\ \text{J}}{2} = 65\ \text{J}$$

As indicated on the plot by the one set of dashed lines, the ductile-to-brittle transition temperature according to this criterion is about −105°C.

(c) Also, as noted on the plot by the other set of dashed lines, the ductile-to-brittle transition temperature for an impact energy of 80 J is about −95°C.

8.13 Following is tabulated data that were gathered from a series of Charpy impact tests on a tempered 4140 steel alloy.

Temperature (°C)	Impact Energy (J)
100	89.3
75	88.6
50	87.6
25	85.4
0	82.9
–25	78.9
–50	73.1
–65	66.0
–75	59.3
–85	47.9
–100	34.3
–125	29.3
–150	27.1
–175	25.0

(a) Plot the data as impact energy versus temperature.

(b) Determine a ductile-to-brittle transition temperature as that temperature corresponding to the average of the maximum and minimum impact energies.

(c) Determine a ductile-to-brittle transition temperature as that temperature at which the impact energy is 70 J.

Solution

The plot of impact energy versus temperature is shown below.

(b) The average of the maximum and minimum impact energies from the data is

$$\text{Average} = \frac{89.3\ \text{J} + 25\ \text{J}}{2} = 57.2\ \text{J}$$

As indicated on the plot by the one set of dashed lines, the ductile-to-brittle transition temperature according to this criterion is about −75°C.

(c) Also, as noted on the plot by the other set of dashed lines, the ductile-to-brittle transition temperature for an impact energy of 70 J is about −55°C.

Cyclic Stresses (Fatigue)

The S-N Curve

8.14 A fatigue test was conducted in which the mean stress was 50 MPa (7250 psi) and the stress amplitude was 225 MPa (32,625 psi).

(a) Compute the maximum and minimum stress levels.

(b) Compute the stress ratio.

(c) Compute the magnitude of the stress range.

<u>Solution</u>

(a) Given the values of σ_m (50 MPa) and σ_a (225 MPa) we are asked to compute σ_{max} and σ_{min}. From Equation 8.14

$$\sigma_m = \frac{\sigma_{max} \quad \sigma_{min}}{2} = 50 \text{ MPa}$$

Or,

$$\sigma_{max} + \sigma_{min} = 100 \text{ MPa}$$

Furthermore, utilization of Equation 8.16 yields

$$\sigma_a = \frac{\sigma_{max} \quad \sigma_{min}}{2} = 225 \text{ MPa}$$

Or,

$$\sigma_{max} - \sigma_{min} = 450 \text{ MPa}$$

Simultaneously solving these two expressions leads to

$$\sigma_{max} = 275 \text{ MPa} \ \ (40{,}000 \text{ psi})$$
$$\sigma_{min} = \ \ 175 \text{ MPa} \ \ (\ 25{,}500 \text{ psi})$$

(b) Using Equation 8.17 the stress ratio R is determined as follows:

$$R = \frac{\sigma_{min}}{\sigma_{max}} = \frac{175 \text{ MPa}}{275 \text{ MPa}} = \quad 0.64$$

(c) The magnitude of the stress range V_r is determined using Equation 8.15 as

$$V_r = V_{max} \quad V_{min} = 275 \text{ MPa} \quad (\ 175 \text{ MPa}) = 450 \text{ MPa} \ (65{,}500 \text{ psi})$$

8.15 A cylindrical 1045 steel bar (Figure 8.34) is subjected to repeated compression-tension stress cycling along its axis. If the load amplitude is 22,000 N (4950 lb_f), compute the minimum allowable bar diameter to ensure that fatigue failure will not occur. Assume a factor of safety of 2.0.

Solution

From Figure 8.34, the fatigue limit stress amplitude for this alloy is 310 MPa (45,000 psi). Stress is defined in Equation 6.1 as $\sigma = \dfrac{F}{A_0}$. For a cylindrical bar

$$A_0 = \pi\left(\frac{d_0}{2}\right)^2$$

Substitution for A_0 into the Equation 6.1 leads to

$$\sigma = \frac{F}{A_0} = \frac{F}{\pi\left(\dfrac{d_0}{2}\right)^2} = \frac{4F}{\pi d_0^2}$$

We now solve for d_0, taking stress as the fatigue limit divided by the factor of safety. Thus

$$d_0 = \sqrt{\frac{4F}{\pi\left(\dfrac{\sigma}{N}\right)}}$$

$$= \sqrt{\frac{(4)(22{,}000\ \text{N})}{(\pi)\left(\dfrac{310 \times 10^6\ \text{N/m}^2}{2}\right)}} = 13.4 \times 10^{-3}\ \text{m} = 13.4\ \text{mm}\ (0.53\ \text{in.})$$

8.16 An 8.0 mm (0.31 in.) diameter cylindrical rod fabricated from a red brass alloy (Figure 8.34) is subjected to reversed tension-compression load cycling along its axis. If the maximum tensile and compressive loads are +7500 N (1700 $\mathrm{lb_f}$) and −7500 N (−1700 $\mathrm{lb_f}$), respectively, determine its fatigue life. Assume that the stress plotted in Figure 8.34 is stress amplitude.

Solution

We are asked to determine the fatigue life for a cylindrical red brass rod given its diameter (8.0 mm) and the maximum tensile and compressive loads (+7500 N and −7500 N, respectively). The first thing that is necessary is to calculate values of σ_{max} and σ_{min} using Equation 6.1. Thus

$$\sigma_{max} = \frac{F_{max}}{A_0} = \frac{F_{max}}{\pi\left(\frac{d_0}{2}\right)^2}$$

$$= \frac{7500\ \mathrm{N}}{(\pi)\left(\frac{8.0 \times 10^{-3}\ \mathrm{m}}{2}\right)^2} = 150 \times 10^6\ \mathrm{N/m^2} = 150\ \mathrm{MPa}\ \ (22{,}500\ \mathrm{psi})$$

$$\sigma_{min} = \frac{F_{min}}{\pi\left(\frac{d_0}{2}\right)^2}$$

$$= \frac{-7500\ \mathrm{N}}{(\pi)\left(\frac{8.0 \times 10^{-3}\ \mathrm{m}}{2}\right)^2} = -150 \times 10^6\ \mathrm{N/m^2} = -150\ \mathrm{MPa}\ \ (-22{,}500\ \mathrm{psi})$$

Now it becomes necessary to compute the stress amplitude using Equation 8.16 as

$$\sigma_a = \frac{\sigma_{max} - \sigma_{min}}{2} = \frac{150\ \mathrm{MPa} - (-150\ \mathrm{MPa})}{2} = 150\ \mathrm{MPa}\ \ (22{,}500\ \mathrm{psi})$$

From Figure 8.34, for the red brass, the number of cycles to failure at this stress amplitude is about 1×10^5 cycles.

8.17 A 12.5 mm (0.50 in.) diameter cylindrical rod fabricated from a 2014-T6 alloy (Figure 8.34) is subjected to a repeated tension-compression load cycling along its axis. Compute the maximum and minimum loads that will be applied to yield a fatigue life of 1.0×10^7 cycles. Assume that the stress plotted on the vertical axis is stress amplitude, and data were taken for a mean stress of 50 MPa (7250 psi).

Solution

This problem asks that we compute the maximum and minimum loads to which a 12.5 mm (0.50 in.) diameter 2014-T6 aluminum alloy specimen may be subjected in order to yield a fatigue life of 1.0×10^7 cycles; Figure 8.34 is to be used assuming that data were taken for a mean stress of 50 MPa (7250 psi). Upon consultation of Figure 8.34, a fatigue life of 1.0×10^7 cycles corresponds to a stress amplitude of 160 MPa (23,200 psi). Or, from Equation 8.16

$$\sigma_{max} - \sigma_{min} = 2\sigma_a = (2)(160 \text{ MPa}) = 320 \text{ MPa} \ \ (46{,}400 \text{ psi})$$

Since $\sigma_m = 50$ MPa, then from Equation 8.14

$$\sigma_{max} + \sigma_{min} = 2\sigma_m = (2)(50 \text{ MPa}) = 100 \text{ MPa} \ \ (14{,}500 \text{ psi})$$

Simultaneous solution of these two expressions for σ_{max} and σ_{min} yields

$$\sigma_{max} = +210 \text{ MPa} \ \ (+30{,}400 \text{ psi})$$
$$\sigma_{min} = -110 \text{ MPa} \ \ (-16{,}000 \text{ psi})$$

Now, inasmuch as $\sigma = \dfrac{F}{A_0}$ (Equation 6.1), and $A_0 = \pi\left(\dfrac{d_0}{2}\right)^2$ then

$$F_{max} = \frac{\sigma_{max}\pi d_0^2}{4} = \frac{(210 \times 10^6 \text{ N/m}^2)(\pi)(12.5 \times 10^{-3} \text{ m})^2}{4} = 25{,}800 \text{ N} \quad (6000 \text{ lb}_f)$$

$$F_{min} = \frac{\sigma_{min}\pi d_0^2}{4} = \frac{(-110 \times 10^6 \text{ N/m}^2)(\pi)(12.5 \times 10^{-3} \text{ m})^2}{4} = -13{,}500 \text{ N} \quad (-3140 \text{ lb}_f)$$

8.18 The fatigue data for a brass alloy are given as follows:

Stress Amplitude (MPa)	Cycles to Failure
310	2×10^5
223	1×10^6
191	3×10^6
168	1×10^7
153	3×10^7
143	1×10^8
134	3×10^8
127	1×10^9

(a) Make an S–N plot (stress amplitude versus logarithm cycles to failure) using these data.

(b) Determine the fatigue strength at 5×10^5 cycles.

(c) Determine the fatigue life for 200 MPa.

Solution

(a) The fatigue data for this alloy are plotted below.

(b) As indicated by the "A" set of dashed lines on the plot, the fatigue strength at 5×10^5 cycles [log (5×10^5) = 5.7] is about 250 MPa.

(c) As noted by the “B” set of dashed lines, the fatigue life for 200 MPa is about 2 10^6 cycles (i.e., the log of the lifetime is about 6.3).

8.19 Suppose that the fatigue data for the brass alloy in Problem 8.18 were taken from torsional tests, and that a shaft of this alloy is to be used for a coupling that is attached to an electric motor operating at 1500 rpm. Give the maximum torsional stress amplitude possible for each of the following lifetimes of the coupling: (a) 1 year, (b) 1 month, (c) 1 day, and (d) 2 hours.

Solution

For each lifetime, first compute the number of cycles, and then read the corresponding fatigue strength from the above plot.

(a) Fatigue lifetime = (1 yr)(365 days/yr)(24 h/day)(60 min/h)(1500 cycles/min) = 7.9×10^8 cycles. The stress amplitude corresponding to this lifetime is about 130 MPa.

(b) Fatigue lifetime = (30 days)(24 h/day)(60 min/h)(1500 cycles/min) = 6.5×10^7 cycles. The stress amplitude corresponding to this lifetime is about 145 MPa.

(c) Fatigue lifetime = (24 h)(60 min/h)(1500 cycles/min) = 2.2×10^6 cycles. The stress amplitude corresponding to this lifetime is about 195 MPa.

(d) Fatigue lifetime = (2 h)(60 min/h)(1500 cycles/min) = 1.8×10^5 cycles. The stress amplitude corresponding to this lifetime is about 315 MPa.

8.20 The fatigue data for a ductile cast iron are given as follows:

Stress Amplitude [MPa (ksi)]	Cycles to Failure
248 (36.0)	1×10^5
236 (34.2)	3×10^5
224 (32.5)	1×10^6
213 (30.9)	3×10^6
201 (29.1)	1×10^7
193 (28.0)	3×10^7
193 (28.0)	1×10^8
193 (28.0)	3×10^8

(a) Make an S–N plot (stress amplitude versus logarithm cycles to failure) using these data.

(b) What is the fatigue limit for this alloy?

(c) Determine fatigue lifetimes at stress amplitudes of 230 MPa (33,500 psi) and 175 MPa (25,000 psi).

(d) Estimate fatigue strengths at 2×10^5 and 6×10^6 cycles.

Solution

(a) The fatigue data for this alloy are plotted below.

(b) The fatigue limit is the stress level at which the curve becomes horizontal, which is 193 MPa (28,000 psi).

(c) As noted by the “A” set of dashed lines, the fatigue lifetime at a stress amplitude of 230 MPa is about 5 u10^5 cycles (log N = 5.7). From the plot, the fatigue lifetime at a stress amplitude of 230 MPa (33,500 psi) is about 50,000 cycles (log N = 4.7). At 175 MPa (25,000 psi) the fatigue lifetime is essentially an infinite number of cycles since this stress amplitude is below the fatigue limit.

(d) As noted by the “B” set of dashed lines, the fatigue strength at 2 u 10^5 cycles (log N = 5.3) is about 240 MPa (35,000 psi); and according to the “C” set of dashed lines, the fatigue strength at 6 u 10^6 cycles (log N = 6.78) is about 205 MPa (30,000 psi).

8.21 Suppose that the fatigue data for the cast iron in Problem 8.20 were taken for rotating-bending tests, and that a rod of this alloy is to be used for an automobile axle that rotates at an average rotational velocity of 750 revolutions per minute. Give maximum lifetimes of continuous driving that are allowable for the following stress levels: (a) 250 MPa (36,250 psi), (b) 215 MPa (31,000 psi), (c) 200 MPa (29,000 psi), and (d) 150 MPa (21,750 psi).

Solution

For each stress level, first read the corresponding lifetime from the above plot, then convert it into the number of cycles.

(a) For a stress level of 250 MPa (36,250 psi), the fatigue lifetime is approximately 90,000 cycles. This translates into (9×10^4 cycles)(1 min/750 cycles) = 120 min.

(b) For a stress level of 215 MPa (31,000 psi), the fatigue lifetime is approximately 2×10^6 cycles. This translates into (2×10^6 cycles)(1 min/750 cycles) = 2670 min = 44.4 h.

(c) For a stress level of 200 MPa (29,000 psi), the fatigue lifetime is approximately 1×10^7 cycles. This translates into (1×10^7 cycles)(1 min/750 cycles) = 1.33×10^4 min = 222 h.

(d) For a stress level of 150 MPa (21,750 psi), the fatigue lifetime is essentially infinite since we are below the fatigue limit [193 MPa (28,000 psi)].

8.22 Three identical fatigue specimens (denoted A, B, and C) are fabricated from a nonferrous alloy. Each is subjected to one of the maximum-minimum stress cycles listed below; the frequency is the same for all three tests.

Specimen	σ_{max} (MPa)	σ_{min} (MPa)
A	+450	–350
B	+400	–300
C	+340	–340

(a) Rank the fatigue lifetimes of these three specimens from the longest to the shortest.

(b) Now justify this ranking using a schematic S–N plot.

Solution

In order to solve this problem, it is necessary to compute both the mean stress and stress amplitude for each specimen. Since from Equation 8.14, mean stresses are the specimens are determined as follows:

$$\sigma_m = \frac{\sigma_{max} + \sigma_{min}}{2}$$

$$\sigma_m(A) = \frac{450\ \text{MPa} + (-350\ \text{MPa})}{2} = 50\ \text{MPa}$$

$$\sigma_m(B) = \frac{400\ \text{MPa} + (-300\ \text{MPa})}{2} = 50\ \text{MPa}$$

$$\sigma_m(C) = \frac{340\ \text{MPa} + (-340\ \text{MPa})}{2} = 0\ \text{MPa}$$

Furthermore, using Equation 8.16, stress amplitudes are computed as

$$\sigma_a = \frac{\sigma_{max} - \sigma_{min}}{2}$$

$$\sigma_a(A) = \frac{450\ \text{MPa} - (-350\ \text{MPa})}{2} = 400\ \text{MPa}$$

$$\sigma_a(B) = \frac{400\ \text{MPa} - (-300\ \text{MPa})}{2} = 350\ \text{MPa}$$

$$\sigma_a(C) = \frac{340\ \text{MPa} - (-340\ \text{MPa})}{2} = 340\ \text{MPa}$$

On the basis of these results, the fatigue lifetime for specimen C will be greater than specimen B, which in turn will be greater than specimen A. This conclusion is based upon the following S-N plot on which curves are plotted for two σ_m values.

8.23 Cite five factors that may lead to scatter in fatigue life data.

Solution

Five factors that lead to scatter in fatigue life data are (1) specimen fabrication and surface preparation, (2) metallurgical variables, (3) specimen alignment in the test apparatus, (4) variation in mean stress, and (5) variation in test cycle frequency.

Crack Initiation and Propagation

Factors That Affect Fatigue Life

8.24 Briefly explain the difference between fatigue striations and beachmarks both in terms of (a) size and (b) origin.

Solution

(a) With regard to size, beachmarks are normally of macroscopic dimensions and may be observed with the naked eye; fatigue striations are of microscopic size and it is necessary to observe them using electron microscopy.

(b) With regard to origin, beachmarks result from interruptions in the stress cycles; each fatigue striation is corresponds to the advance of a fatigue crack during a single load cycle.

8.25 List four measures that may be taken to increase the resistance to fatigue of a metal alloy.

Solution

Four measures that may be taken to increase the fatigue resistance of a metal alloy are:

(1) Polish the surface to remove stress amplification sites.

(2) Reduce the number of internal defects (pores, etc.) by means of altering processing and fabrication techniques.

(3) Modify the design to eliminate notches and sudden contour changes.

(4) Harden the outer surface of the structure by case hardening (carburizing, nitriding) or shot peening.

Generalized Creep Behavior

8.26 Give the approximate temperature at which creep deformation becomes an important consideration for each of the following metals: nickel, copper, iron, tungsten, lead, and aluminum.

Solution

Creep becomes important at about 0.4T_m, T_m being the absolute melting temperature of the metal. (The melting temperatures in degrees Celsius are found inside the front cover of the book.)

For Ni, 0.4T_m = (0.4)(1455 + 273) = 691 K or 418°C (785°F)
For Cu, 0.4T_m = (0.4)(1085 + 273) = 543 K or 270°C (518°F)
For Fe, 0.4T_m = (0.4)(1538 + 273) = 725 K or 450°C (845°F)
For W, 0.4T_m = (0.4)(3410 + 273) = 1473 K or 1200°C (2190°F)
For Pb, 0.4T_m = (0.4)(327 + 273) = 240 K or −33°C (−27°F)
For Al, 0.4T_m = (0.4)(660 + 273) = 373 K or 100°C (212°F)

8.27 The following creep data were taken on an aluminum alloy at 400°C (750°F) and a constant stress of 25 MPa (3660 psi). Plot the data as strain versus time, then determine the steady-state or minimum creep rate. Note: The initial and instantaneous strain is not included.

Time (min)	Strain	Time (min)	Strain
0	0.000	16	0.135
2	0.025	18	0.153
4	0.043	20	0.172
6	0.065	22	0.193
8	0.078	24	0.218
10	0.092	26	0.255
12	0.109	28	0.307
14	0.120	30	0.368

Solution

These creep data are plotted below

The steady-state creep rate ($\Delta\epsilon/\Delta t$) is the slope of the linear region (i.e., the straight line that has been superimposed on the curve) as

$$\frac{\Delta\epsilon}{\Delta t} = \frac{0.230 - 0.09}{30\ \text{min} - 10\ \text{min}} = 7.0 \times 10^{-3}\ \text{min}^{-1}$$

Stress and Temperature Effects

8.28 A specimen 750 mm (30 in.) long of an S-590 alloy (Figure 8.31) is to be exposed to a tensile stress of 80 MPa (11,600 psi) at 815°C (1500°F). Determine its elongation after 5000 h. Assume that the total of both instantaneous and primary creep elongations is 1.5 mm (0.06 in.).

Solution

From the 815°C line in Figure 8.31, the steady state creep rate $\dot{\epsilon}_s$ is about 5.5×10^{-6} h^{-1} at 80 MPa. The steady state creep strain, ϵ_s, therefore, is just the product of $\dot{\epsilon}_s$ and time as

$$\epsilon_s = \dot{\epsilon}_s \times \text{(time)}$$

$$= \left(5.5 \times 10^{-6}\ \text{h}^{-1}\right)(5{,}000\ \text{h}) = 0.0275$$

Strain and elongation are related as in Equation 6.2; solving for the steady state elongation, Δl_s, leads to

$$\Delta l_s = l_0 \epsilon_s = (750\ \text{mm})\left(0.0275\right) = 20.6\ \text{mm}\quad (0.81\ \text{in.})$$

Finally, the total elongation is just the sum of this Δl_s and the total of both instantaneous and primary creep elongations [i.e., 1.5 mm (0.06 in.)]. Therefore, the total elongation is 20.6 mm + 1.5 mm = 22.1 mm (0.87 in.).

8.29 For a cylindrical S-590 alloy specimen (Figure 8.31) originally 10 mm (0.40 in.) in diameter and 500 mm (20 in.) long, what tensile load is necessary to produce a total elongation of 145 mm (5.7 in.) after 2,000 h at 730°C (1350°F)? Assume that the sum of instantaneous and primary creep elongations is 8.6 mm (0.34 in.).

Solution

It is first necessary to calculate the steady state creep rate so that we may utilize Figure 8.31 in order to determine the tensile stress. The steady state elongation, Δl_s, is just the difference between the total elongation and the sum of the instantaneous and primary creep elongations; that is,

$$\Delta l_s = 145 \text{ mm} - 8.6 \text{ mm} = 136.4 \text{ mm} \quad (5.36 \text{ in.})$$

Now the steady state creep rate $\dot{\varepsilon}_s$ is just

$$\dot{\varepsilon}_s = \frac{\Delta \varepsilon}{\Delta t} = \frac{\dfrac{\Delta l_s}{l_0}}{\Delta t} = \frac{\dfrac{136.4 \text{ mm}}{500 \text{ mm}}}{2{,}000 \text{ h}}$$

$$= 1.36 \times 10^{-4} \text{ h}^{-1}$$

Employing the 730°C line in Figure 8.31, a steady state creep rate of 1.36×10^{-4} h^{-1} corresponds to a stress σ of about 200 MPa (or 29,000 psi) [since log $(1.36 \times 10^{-4}) = -3.866$]. From this we may compute the tensile load using Equation 6.1 as

$$F = \sigma A_0 = \sigma \pi \left(\frac{d_0}{2}\right)^2$$

$$= \left(200 \times 10^6 \text{ N/m}^2\right)(\pi)\left(\frac{10.0 \times 10^{-3} \text{ m}}{2}\right)^2 = 15{,}700 \text{ N} \quad (3645 \text{ lb}_f)$$

8.30 If a component fabricated from an S-590 alloy (Figure 8.30) is to be exposed to a tensile stress of 300 MPa (43,500 psi) at 650°C (1200°F), estimate its rupture lifetime.

Solution

This problem asks us to calculate the rupture lifetime of a component fabricated from an S-590 alloy exposed to a tensile stress of 300 MPa at 650°C. All that we need do is read from the 650°C line in Figure 8.30 the rupture lifetime at 300 MPa; this value is about 600 h.

8.31 A cylindrical component constructed from an S-590 alloy (Figure 8.30) has a diameter of 12 mm (0.50 in.). Determine the maximum load that may be applied for it to survive 500 h at 925°C (°F).

Solution

We are asked in this problem to determine the maximum load that may be applied to a cylindrical S-590 alloy component that must survive 500 h at 925°C. From Figure 8.30, the stress corresponding to 500 h is about 50 MPa (7,250 psi). Since stress is defined in Equation 6.1 as $\sigma = F/A_0$, and for a cylindrical specimen, $A_0 = \pi\left(\frac{d_0}{2}\right)^2$, then

$$F = \sigma A_0 = \sigma\pi\left(\frac{d_0}{2}\right)^2$$

$$= \left(50 \times 10^6 \text{ N/m}^2\right)(\pi)\left(\frac{12 \times 10^{-3}\text{ m}}{2}\right)^2 = 5655 \text{ N} \quad (1424 \text{ lb}_f)$$

8.32 From Equation 8.19, if the logarithm of $\dot{\varepsilon}_s$ LV SORWWHG YHUVXV WKH ORJDULWKP

should result, the slope of which is the stress exponent n. Using Figure 8.31, determine the value of n for the S-590 alloy at 925°C, and for the initial (i.e., lower-temperature) straight line segments at each of 650°C, 730°C, and 815°C.

Solution

The slope of the line from a log $\dot{\varepsilon}_s$ versus log σ plot yields the value of n in Equation 8.19; that is

$$n = \frac{\Delta \log \dot{\varepsilon}_s}{\Delta \log \sigma}$$

We are asked to determine the values of n for the creep data at the four temperatures in Figure 8.31 [i.e., at 925°C, and for the initial (i.e., lower-temperature) straight line segments at each of 650°C, 730°C, and 815°C]. This is accomplished by taking ratios of the differences between two log $\dot{\varepsilon}_s$ and log σ values. (Note: Figure 8.31 plots log σ versus log $\dot{\varepsilon}_s$; therefore, values of n are equal to the reciprocals of the slopes of the straight-line segments.)

Thus for 650°C

$$n = \frac{\Delta \log \dot{\varepsilon}_s}{\Delta \log \sigma} = \frac{\log\left(10^{-1}\right) - \log\left(10^{-5}\right)}{\log (545\ \text{MPa}) - \log (240\ \text{MPa})} = 11.2$$

While for 730°C

$$n = \frac{\Delta \log \dot{\varepsilon}_s}{\Delta \log \sigma} = \frac{\log 1 - \log\left(10^{-6}\right)}{\log (430\ \text{MPa}) - \log (125\ \text{MPa})} = 11.2$$

And at 815°C

$$n = \frac{\Delta \log \dot{\varepsilon}_s}{\Delta \log \sigma} = \frac{\log 1 - \log\left(10^{-6}\right)}{\log (320\ \text{MPa}) - \log (65\ \text{MPa})} = 8.7$$

And, finally at 925°C

$$n = \frac{\Delta \log \dot{\varepsilon}_s}{\Delta \log \sigma} = \frac{\log 10^{2} - \log\left(10^{-5}\right)}{\log (350\ \text{MPa}) - \log (44\ \text{MPa})} = 7.8$$

8.33 (a) Estimate the activation energy for creep (i.e., Q_c in Equation 8.20) for the S-590 alloy having the steady-state creep behavior shown in Figure 8.31. Use data taken at a stress level of 300 MPa (43,500 psi) and temperatures of 650°C and 730°C. Assume that the stress exponent n is independent of temperature. (b) Estimate $\dot{\varepsilon}_s$ at 600°C (873 K) and 300 MPa.

Solution

(a) We are asked to estimate the activation energy for creep for the S-590 alloy having the steady-state creep behavior shown in Figure 8.31, using data taken at σ = 300 MPa and temperatures of 650°C and 730°C. Since σ is a constant, Equation 8.20 takes the form

$$\dot{\varepsilon}_s = K_2 \sigma^n \exp\left(-\frac{Q_c}{RT}\right) = K_2' \exp\left(-\frac{Q_c}{RT}\right)$$

where K_2' is now a constant. (Note: the exponent n has about the same value at these two temperatures per Problem 8.32.) Taking natural logarithms of the above expression

$$\ln \dot{\varepsilon}_s = \ln K_2' - \frac{Q_c}{RT}$$

For the case in which we have creep data at two temperatures (denoted as T_1 and T_2) and their corresponding steady-state creep rates ($\dot{\varepsilon}_{s_1}$ and $\dot{\varepsilon}_{s_2}$), it is possible to set up two simultaneous equations of the form as above, with two unknowns, namely K_2' and Q_c. Solving for Q_c yields

$$Q_c = -\frac{R\left(\ln \dot{\varepsilon}_{s_1} - \ln \dot{\varepsilon}_{s_2}\right)}{\left[\dfrac{1}{T_1} - \dfrac{1}{T_2}\right]}$$

Let us choose T_1 as 650°C (923 K) and T_2 as 730°C (1003 K); then from Figure 8.31, at σ = 300 MPa, $\dot{\varepsilon}_{s_1} = 8.9 \times 10^{-5}\ \text{h}^{-1}$ and $\dot{\varepsilon}_{s_2} = 1.3 \times 10^{-2}\ \text{h}^{-1}$. Substitution of these values into the above equation leads to

$$Q_c = -\frac{(8.31\ \text{J/mol-K})\left[\ln\left(8.9 \times 10^{-5}\right) - \ln\left(1.3 \times 10^{-2}\right)\right]}{\left[\dfrac{1}{923\ \text{K}} - \dfrac{1}{1003\ \text{K}}\right]}$$

$$= 480{,}000\ \text{J/mol}$$

(b) We are now asked to estimate $\dot{\varepsilon}_s$ at 600°C (873 K) and 300 MPa. It is first necessary to determine the value of K_2', which is accomplished using the first expression above, the value of Q_c, and one value each of $\dot{\varepsilon}_s$ and T (say $\dot{\varepsilon}_{s_1}$ and T_1). Thus,

$$K_2' = \dot{\varepsilon}_{s_1} \exp\left(\frac{Q_c}{RT_1}\right)$$

$$= (8.9 \times 10^{-5}\ \text{h}^{-1}) \exp\left[\frac{480{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(923\ \text{K})}\right] = 1.34 \times 10^{23}\ \text{h}^{-1}$$

Now it is possible to calculate $\dot{\varepsilon}_s$ at 600°C (873 K) and 300 MPa as follows:

$$\dot{\varepsilon}_s = K_2' \exp\left(-\frac{Q_c}{RT}\right)$$

$$= (1.34 \times 10^{23}\ \text{h}^{-1}) \exp\left[-\frac{480{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(873\ \text{K})}\right]$$

$$= 2.47 \times 10^{-6}\ \text{h}^{-1}$$

8.34 Steady-state creep rate data are given below for nickel at 1000°C (1273 K):

$\dot{\epsilon}_s$ (s^{-1})	σ [MPa (psi)]
10^{-4}	15 (2175)
10^{-6}	4.5 (650)

If it is known that the activation energy for creep is 272,000 J/mol, compute the steady-state creep rate at a temperature of 850°C (1123 K) and a stress level of 25 MPa (3625 psi).

Solution

Taking natural logarithms of both sides of Equation 8.20 yields

$$\ln \dot{\epsilon}_s = \ln K_2 + n \ln \sigma - \frac{Q_c}{RT}$$

With the given data there are two unknowns in this equation--namely K_2 and n. Using the data provided in the problem statement we can set up two independent equations as follows:

$$\ln\left(1 \times 10^{-4}\ s^{-1}\right) = \ln K_2 + n \ln(15\ \text{MPa}) - \frac{272{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(1273\ \text{K})}$$

$$\ln\left(1 \times 10^{-6}\ s^{-1}\right) = \ln K_2 + n \ln(4.5\ \text{MPa}) - \frac{272{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(1273\ \text{K})}$$

Now, solving simultaneously for n and K_2 leads to $n = 3.825$ and $K_2 = 466\ s^{-1}$. Thus it is now possible to solve for $\dot{\epsilon}_s$ at 25 MPa and 1123 K using Equation 8.20 as

$$\dot{\epsilon}_s = K_2 \sigma^n \exp\left(-\frac{Q_c}{RT}\right)$$

$$= \left(466\ s^{-1}\right)(25\ \text{MPa})^{3.825} \exp\left[-\frac{272{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(1123\ \text{K})}\right]$$

$$= 2.28 \times 10^{-5}\ s^{-1}$$

8.35 Steady-state creep data taken for a stainless steel at a stress level of 70 MPa (10,000 psi) are given as follows:

$\dot{\varepsilon}_s$ (s^{-1})	T (K)
1.0×10^{-5}	977
2.5×10^{-3}	1089

If it is known that the value of the stress exponent n for this alloy is 7.0, compute the steady-state creep rate at 1250 K and a stress level of 50 MPa (7250 psi).

Solution

Taking natural logarithms of both sides of Equation 8.20 yields

$$\ln \dot{\varepsilon}_s = \ln K_2 + n \ln \sigma - \frac{Q_c}{RT}$$

With the given data there are two unknowns in this equation--namely K_2 and Q_c. Using the data provided in the problem statement we can set up two independent equations as follows:

$$\ln\left(1.0 \times 10^{-5}\ s^{-1}\right) = \ln K_2 + (7.0)\ln(70\ \text{MPa}) - \frac{Q_c}{(8.31\ \text{J/mol-K})(977\ \text{K})}$$

$$\ln\left(2.5 \times 10^{-3}\ s^{-1}\right) = \ln K_2 + (7.0)\ln(70\ \text{MPa}) - \frac{Q_c}{(8.31\ \text{J/mol-K})(1089\ \text{K})}$$

Now, solving simultaneously for K_2 and Q_c leads to $K_2 = 2.55 \times 10^{5}\ s^{-1}$ and Q_c = 436,000 J/mol. Thus, it is now possible to solve for $\dot{\varepsilon}_s$ at 50 MPa and 1250 K using Equation 8.20 as

$$\dot{\varepsilon}_s = K_2 \sigma^n \exp\left(-\frac{Q_c}{RT}\right)$$

$$= \left(2.55 \times 10^{5}\ s^{-1}\right)(50\ \text{MPa})^{7.0} \exp\left[-\frac{436{,}000\ \text{J/mol}}{(8.31\ \text{J/mol-K})(1250\ \text{K})}\right]$$

$$= 0.118\ s^{-1}$$

Alloys for High-Temperature Use

8.36 Cite three metallurgical/processing techniques that are employed to enhance the creep resistance of metal alloys.

Solution

Three metallurgical/processing techniques that are employed to enhance the creep resistance of metal alloys are (1) solid solution alloying, (2) dispersion strengthening by using an insoluble second phase, and (3) increasing the grain size or producing a grain structure with a preferred orientation.

DESIGN PROBLEMS

8.D1 Each student (or group of students) is to obtain an object/structure/component that has failed. It may come from your home, an automobile repair shop, a machine shop, etc. Conduct an investigation to determine the cause and type of failure (i.e., simple fracture, fatigue, creep). In addition, propose measures that can be taken to prevent future incidents of this type of failure. Finally, submit a report that addresses the above issues.

Each student or group of students is to submit their own report on a failure analysis investigation that was conducted.

8.D2 (a) For the thin-walled spherical tank discussed in Design Example 8.1, on the basis of critical crack size criterion [as addressed in part (a)], rank the following polymers from longest to shortest critical crack length: nylon 6,6 (50% relative humidity), polycarbonate, poly(ethylene terephthalate), and poly(methyl methacrylate). Comment on the magnitude range of the computed values used in the ranking relative to those tabulated for metal alloys as provided in Table 8.3. For these computations, use data contained in Tables B.4 and B.5 in Appendix B.

(b) Now rank these same four polymers relative to maximum allowable pressure according to the leak-before-break criterion, as described in the (b) portion of Design Example 8.1. As above, comment on these values in relation to those for the metal alloys that are tabulated in Table 8.4.

Solution

(a) This portion of the problem calls for us to rank four polymers relative to critical crack length in the wall of a spherical pressure vessel. In the development of Design Example 8.1, it was noted that critical crack length is proportional to the square of the K_{Ic}–σ_y ratio. Values of K_{Ic} and σ_y as taken from Tables B.4 and B.5 are tabulated below. (Note: when a range of σ_y or K_{Ic} values is given, the average value is used.)

Material	$K_{Ic}\ (\mathrm{MPa}\sqrt{\mathrm{m}})$	σ_y (MPa)
Nylon 6,6	2.75	51.7
Polycarbonate	2.2	62.1
Poly(ethylene terephthlate)	5.0	59.3
Poly(methyl methacrylate)	1.2	63.5

On the basis of these values, the four polymers are ranked per the squares of the K_{Ic}–σ_y ratios as follows:

Material	$\left(\frac{K_{Ic}}{\sigma_y}\right)^2$ (mm)
PET	7.11
Nylon 6,6	2.83
PC	1.26
PMMA	0.36

These values are smaller than those for the metal alloys given in Table 8.3, which range from 0.93 to 43.1 mm.

(b) Relative to the leak-before-break criterion, the K_{Ic}^2 - V_y ratio is used. The four polymers are ranked according to values of this ratio as follows:

Material	$\frac{K_{Ic}^2}{V_y}$ (MPa- m)
PET	0.422
Nylon 6,6	0.146
PC	0.078
PMMA	0.023

These values are all smaller than those for the metal alloys given in Table 8.4, which values range from 1.2 to 11.2 MPa-m.

Data Extrapolation Methods

8.D3 An S-590 alloy component (Figure 8.32) must have a creep rupture lifetime of at least 100 days at 500°C (773 K). Compute the maximum allowable stress level.

Solution

This problem asks that we compute the maximum allowable stress level to give a rupture lifetime of 100 days for an S-590 iron component at 773 K. It is first necessary to compute the value of the Larson-Miller parameter as follows:

$$T(20 + \log t_r) = (773\ \text{K})\left\{20 + \log\left[(100\ \text{days})(24\ \text{h/day})\right]\right\}$$

$$= 18.1 \times 10^3$$

From the curve in Figure 8.32, this value of the Larson-Miller parameter corresponds to a stress level of about 530 MPa (77,000 psi).

8.D4 Consider an S-590 alloy component (Figure 8.32) that is subjected to a stress of 200 MPa (29,000 psi). At what temperature will the rupture lifetime be 500 h?

Solution

We are asked in this problem to calculate the temperature at which the rupture lifetime is 500 h when an S-590 iron component is subjected to a stress of 200 MPa (29,000 psi). From the curve shown in Figure 8.32, at 200 MPa, the value of the Larson-Miller parameter is 22.5×10^3 (K-h). Thus,

$$22.5 \times 10^3 \text{ (K - h)} = T\left(20 + \log t_r\right)$$

$$= T\left[20 + \log(500 \text{ h})\right]$$

Or, solving for T yields T = 991 K (718°C).

8.D5 For an 18-8 Mo stainless steel (Figure 8.35), predict the time to rupture for a component that is subjected to a stress of 80 MPa (11,600 psi) at 700°C (973 K).

Solution

This problem asks that we determine, for an 18-8 Mo stainless steel, the time to rupture for a component that is subjected to a stress of 80 MPa (11,600 psi) at 700°C (973 K). From Figure 8.35, the value of the Larson-Miller parameter at 80 MPa is about 23.5×10^3, for T in K and t_r in h. Therefore,

$$23.5 \times 10^3 = T\left(20 + \log t_r\right)$$

$$= 973\left(20 + \log t_r\right)$$

And, solving for t_r

$$24.15 = 20 + \log t_r$$

which leads to $t_r = 1.42 \times 10^4$ h = 1.6 yr.

8.D6 Consider an 18-8 Mo stainless steel component (Figure 8.35) that is exposed to a temperature of 500°C (773 K). What is the maximum allowable stress level for a rupture lifetime of 5 years? 20 years?

Solution

We are asked in this problem to calculate the stress levels at which the rupture lifetime will be 5 years and 20 years when an 18-8 Mo stainless steel component is subjected to a temperature of 500°C (773 K). It first becomes necessary to calculate the value of the Larson-Miller parameter for each time. The values of t_r corresponding to 5 and 20 years are 4.38×10^4 h and 1.75×10^5 h, respectively. Hence, for a lifetime of 5 years

$$T(20 + \log t_r) = 773\left[20 + \log(4.38 \times 10^4)\right] \cong 19.05 \times 10^3$$

And for t_r = 20 years

$$T(20 + \log t_r) = 773\left[20 + \log(1.75 \times 10^5)\right] \cong 19.51 \times 10^3$$

Using the curve shown in Figure 8.35, the stress values corresponding to the five- and twenty-year lifetimes are approximately 260 MPa (37,500 psi) and 225 MPa (32,600 psi), respectively.

which yields a value for m'_{sugar} of 2667 g. Subtracting the latter from the former of these sugar concentrations yields the amount of sugar that precipitated out of the solution upon cooling, m''_{sugar}; that is

$$m''_{sugar} = m_{sugar} - m'_{sugar} = 5022\text{ g} - 2667\text{ g} = 2355\text{ g}$$

9.2 At 500°C (930°F), what is the maximum solubility (a) of Cu in Ag? (b) Of Ag in Cu?

Solution

(a) From Figure 9.7, the maximum solubility of Cu in Ag at 500°C corresponds to the position of the β–(α + β) phase boundary at this temperature, or to about 2 wt% Cu.

(b) From this same figure, the maximum solubility of Ag in Cu corresponds to the position of the α–(α + β) phase boundary at this temperature, or about 1.5 wt% Ag.

Microstructure

9.3 Cite three variables that determine the microstructure of an alloy.

Solution

Three variables that determine the microstructure of an alloy are (1) the alloying elements present, (2) the concentrations of these alloying elements, and (3) the heat treatment of the alloy.

Phase Equilibria

9.4 What thermodynamic condition must be met for a state of equilibrium to exist?

Solution

In order for a system to exist in a state of equilibrium the free energy must be a minimum for some specified combination of temperature, pressure, and composition.

One-Component (or Unary) Phase Diagrams

9.5 Consider a specimen of ice that is at –10°C and 1 atm pressure. Using Figure 9.2, the pressure–temperature phase diagram for H_2O, determine the pressure to which the specimen must be raised or lowered to cause it (a) to melt, and (b) to sublime.

Solution

The figure below shows the pressure–temperature phase diagram for H_2O, Figure 10.2; a vertical line has been constructed at -10°C, and the location on this line at 1 atm pressure (point B) is also noted.

(a) Melting occurs, (by changing pressure) as, moving vertically (upward) at this temperature, we cross the Ice–Liquid phase boundary. This occurs at approximately 570 atm; thus, the pressure of the specimen must be raised from 1 to 570 atm.

(b) In order to determine the pressure at which sublimation occurs at this temperature, we move vertically downward from 1 atm until we cross the Ice–Vapor phase boundary. This intersection occurs at approximately 0.0023 atm.

9.6 At a pressure of 0.01 atm, determine (a) the melting temperature for ice, and (b) the boiling temperature for water.

Solution

The melting temperature for ice and the boiling temperature for water at a pressure of 0.01 atm may be determined from the pressure-temperature diagram for this system, Figure 10.2, which is shown below; a horizontal line has been constructed across this diagram at a pressure of 0.01 atm.

The melting and boiling temperatures for ice at a pressure of 0.01 atm may be determined by moving horizontally across the pressure-temperature diagram at this pressure. The temperature corresponding to the intersection of the Ice-Liquid phase boundary is the melting temperature, which is approximately 1°C. On the other hand, the boiling temperature is at the intersection of the horizontal line with the Liquid-Vapor phase boundary—approximately 16°C.

Binary Isomorphous Systems

9.7 Given here are the solidus and liquidus temperatures for the germanium-silicon system. Construct the phase diagram for this system and label each region.

Composition (wt% Si)	Solidus Temperature (°C)	Liquidus Temperature (°C)
0	938	938
10	1005	1147
20	1065	1226
30	1123	1278
40	1178	1315
50	1232	1346
60	1282	1367
70	1326	1385
80	1359	1397
90	1390	1408
100	1414	1414

Solution

The germanium-silicon phase diagram is constructed below.

Interpretation of Phase Diagrams

9.8 Cite the phases that are present and the phase compositions for the following alloys:

(a) 90 wt% Zn-10 wt% Cu at 400°C (750°F)

(b) 75 wt% Sn-25 wt% Pb at 175°C (345°F)

(c) 55 wt% Ag-45 wt% Cu at 900°C (1650°F)

(d) 30 wt% Pb-70 wt% Mg at 425°C (795°F)

(e) 2.12 kg Zn and 1.88 kg Cu at 500°C (930°F)

(f) 37 lb_m Pb and 6.5 lb_m Mg at 400°C (750°F)

(g) 8.2 mol Ni and 4.3 mol Cu at 1250°C (2280°F)

(h) 4.5 mol Sn and 0.45 mol Pb at 200°C (390°F)

Solution

This problem asks that we cite the phase or phases present for several alloys at specified temperatures.

(a) That portion of the Cu-Zn phase diagram (Figure 9.19) that pertains to this problem is shown below; the point labeled “A” represents the 90 wt% Zn-10 wt% Cu composition at 400°C.

As may be noted, point A lies within the ε and η phase field. A tie line has been constructed at 400°C; its intersection with the ε – ε + η phase boundary is at 87 wt% Zn, which corresponds to the composition of the ε phase. Similarly, the tie-line intersection with the ε + η – η phase boundary occurs at 97 wt% Zn, which is the composition of the η phase. Thus, the phase compositions are as follows:

$$C_H = 87 \text{ wt\% Zn-13 wt\% Cu}$$
$$C_K = 97 \text{ wt\% Zn-3 wt\% Cu}$$

(b) That portion of the Pb-Sn phase diagram (Figure 9.8) that pertains to this problem is shown below; the point labeled "B" represents the 75 wt% Sn-25 wt% Pb composition at 175°C.

As may be noted, point B lies within the α + β phase field. A tie line has been constructed at 175°C; its intersection with the α–(α + β) phase boundary is at 16 wt% Sn, which corresponds to the composition of the α phase. Similarly, the tie-line intersection with the (α + β)–β phase boundary occurs at 97 wt% Sn, which is the composition of the β phase. Thus, the phase compositions are as follows:

$$C_\alpha = 16 \text{ wt\% Sn-84 wt\% Pb}$$
$$C_\beta = 97 \text{ wt\% Sn-3 wt\% Pb}$$

(c) The Ag-Cu phase diagram (Figure 9.7) is shown below; the point labeled "C" represents the 55 wt% Ag-45 wt% Cu composition at 900°C.

As may be noted, point C lies within the Liquid phase field. Therefore, only the liquid phase is present; its composition is 55 wt% Ag-45 wt% Cu.

(d) The Mg-Pb phase diagram (Figure 9.20) is shown below; the point labeled "D" represents the 30 wt% Pb-70 wt% Mg composition at 425°C.

As may be noted, point D lies within the D phase field. Therefore, only the D phase is present; its composition is 30 wt% Pb-70 wt% Mg.

(e) For an alloy composed of 2.12 kg Zn and 1.88 kg Cu and at 500qC, we must first determine the Zn and Cu concentrations, as

$$C_{Zn} \quad \frac{2.12\,\text{kg}}{2.12\,\text{kg} \quad 1.88\,\text{kg}} \; u\,100 \quad 53\,\text{wt\%}$$

$$C_{Cu} \quad \frac{1.88\,\text{kg}}{2.12\,\text{kg} \quad 1.88\,\text{kg}} \; u\,100 \quad 47\,\text{wt\%}$$

That portion of the Cu-Zn phase diagram (Figure 9.19) that pertains to this problem is shown below; the point labeled “E” represents the 53 wt% Zn-47 wt% Cu composition at 500qC.

As may be noted, point E lies within the E + J phase field. A tie line has been constructed at 500qC; its intersection with the E – E + J phase boundary is at 49 wt% Zn, which corresponds to the composition of the E phase. Similarly, the tie-line intersection with the E + J – J phase boundary occurs at 58 wt% Zn, which is the composition of the J phase. Thus, the phase compositions are as follows:

$$C_E = 49\text{ wt\% Zn-51 wt\% Cu}$$

$$C_J = 58\text{ wt\% Zn-42 wt\% Cu}$$

(f) For an alloy composed of 37 lb_m Pb and 6.5 lb_m Mg and at 400qC, we must first determine the Pb and Mg concentrations, as

$$C_{Pb} \quad \frac{37\ lb_m}{37\ lb_m \quad 6.5\ lb_m} \ u\ 100 \quad 85\text{ wt\%}$$

$$C_{Mg} \quad \frac{6.5\ lb_m}{37\ lb_m \quad 6.5\ lb_m} \ u\ 100 \quad 15\text{ wt\%}$$

That portion of the Mg-Pb phase diagram (Figure 9.20) that pertains to this problem is shown below; the point labeled "F" represents the 85 wt% Pb-15 wt% Mg composition at 400qC.

As may be noted, point F lies within the L + Mg_2Pb phase field. A tie line has been constructed at 400°C; it intersects the vertical line at 81 wt% Pb, which corresponds to the composition of Mg_2Pb. Furthermore, the tie line intersection with the L + Mg_2Pb-L phase boundary is at 93 wt% Pb, which is the composition of the liquid phase. Thus, the phase compositions are as follows:

$$C_{Mg_2Pb} = 81 \text{ wt\% Pb-19 wt\% Mg}$$

$$C_L = 93 \text{ wt\% Pb-7 wt\% Mg}$$

(g) For an alloy composed of 8.2 mol Ni and 4.3 mol Cu and at 1250°C, it is first necessary to determine the Ni and Cu concentrations, which we will do in wt% as follows:

$$n'_{Ni} = n_{m_{Ni}} A_{Ni} = (8.2 \text{ mol})(58.69 \text{ g/mol}) = 481.3 \text{ g}$$

$$n'_{Cu} = n_{m_{Cu}} A_{Cu} = (4.3 \text{ mol})(63.55 \text{ g/mol}) = 273.3 \text{ g}$$

$$C_{Ni} = \frac{481.3 \text{ g}}{481.3 \text{ g} + 273.3 \text{ g}} \times 100 = 63.8 \text{ wt\%}$$

$$C_{Cu} = \frac{273.3 \text{ g}}{481.3 \text{ g} + 273.3 \text{ g}} \times 100 = 36.2 \text{ wt\%}$$

The Cu-Ni phase diagram (Figure 9.3a) is shown below; the point labeled "G" represents the 63.8 wt% Ni-36.2 wt% Cu composition at 1250°C.

As may be noted, point G lies within the α phase field. Therefore, only the α phase is present; its composition is 63.8 wt% Ni–36.2 wt% Cu.

(h) For an alloy composed of 4.5 mol Sn and 0.45 mol Pb and at 200°C, it is first necessary to determine the Sn and Pb concentrations, which we will do in weight percent as follows:

$$n'_{Sn} = n_{m_{Sn}} A_{Sn} = (4.5 \text{ mol})(118.71 \text{ g/mol}) = 534.2 \text{ g}$$

$$n'_{Pb} = n_{m_{Pb}} A_{Pb} = (0.45 \text{ mol})(207.2 \text{ g/mol}) = 93.2 \text{ g}$$

$$C_{Sn} = \frac{534.2 \text{ g}}{534.2 \text{ g} + 93.2 \text{ g}} \times 100 = 85.1 \text{ wt\%}$$

$$C_{Pb} = \frac{93.2 \text{ g}}{534.2 \text{ g} + 93.2 \text{ g}} \times 100 = 14.9 \text{ wt\%}$$

That portion of the Pb–Sn phase diagram (Figure 9.8) that pertains to this problem is shown below; the point labeled "H" represents the 85.1 wt% Sn–14.9 wt% Pb composition at 200°C.

As may be noted, point H lies within the E + L phase field. A tie line has been constructed at 200 C; its intersection with the L – (E + L) phase boundary is at 74 wt% Sn, which corresponds to the composition of the L phase. Similarly, the tie-line intersection with the (E + L) – E phase boundary occurs at 97.5 wt% Sn, which is the composition of the E phase. Thus, the phase compositions are as follows:

$$C_E = 97.5 \text{ wt\% Sn-}2.5 \text{ wt\% Pb}$$

$$C_L = 74 \text{ wt\% Sn-}26 \text{ wt\% Pb}$$

9.9 Is it possible to have a copper–nickel alloy that, at equilibrium, consists of a liquid phase of composition 20 wt% Ni–80 wt% Cu and also an *α* phase of composition 37 wt% Ni–63 wt% Cu? If so, what will be the approximate temperature of the alloy? If this is not possible, explain why.

Solution

It is not possible to have a Cu-Ni alloy, which at equilibrium, consists of a liquid phase of composition 20 wt% Ni-80 wt% Cu and an α phase of composition 37 wt% Ni-63 wt% Cu. From Figure 9.3**a**, a single tie line does not exist within the α + L region that intersects the phase boundaries at the given compositions. At 20 wt% Ni, the L-(α + L) phase boundary is at about 1200°C, whereas at 37 wt% Ni the (L + α)-α phase boundary is at about 1230°C.

9.10 Is it possible to have a copper-zinc alloy that, at equilibrium, consists of an ε phase of composition 80 wt% Zn-20 wt% Cu, and also a liquid phase of composition 95 wt% Zn-5 wt% Cu? If so, what will be the approximate temperature of the alloy? If this is not possible, explain why.

Solution

It is not possible to have a Cu-Zn alloy, which at equilibrium consists of an ε phase of composition 80 wt% Zn-20 wt% Cu and also a liquid phase of composition 95 wt% Zn-5 wt% Cu. From Figure 9.19 a single tie line does not exist within the ε + L region which intersects the phase boundaries at the given compositions. At 80 wt% Zn, the ε-(ε + L) phase boundary is at about 575°C, whereas at 95 wt% Zn the (ε + L)-L phase boundary is at about 490°C.

9.11 A copper-nickel alloy of composition 70 wt% Ni-30 wt% Cu is slowly heated from a temperature of 1300°C (2370°F).

(a) At what temperature does the first liquid phase form?

(b) What is the composition of this liquid phase?

(c) At what temperature does complete melting of the alloy occur?

(d) What is the composition of the last solid remaining prior to complete melting?

Solution

Shown below is the Cu-Ni phase diagram (Figure 9.3a) and a vertical line constructed at a composition of 70 wt% Ni-30 wt% Cu.

(a) Upon heating from 1300°C, the first liquid phase forms at the temperature at which this vertical line intersects the α-(α + L) phase boundary--i.e., about 1345°C.

(b) The composition of this liquid phase corresponds to the intersection with the (α + L)-L phase boundary, of a tie line constructed across the α + L phase region at 1345°C--i.e., 59 wt% Ni;

(c) Complete melting of the alloy occurs at the intersection of this same vertical line at 70 wt% Ni with the (α + L)-L phase boundary--i.e., about 1380°C;

(d) The composition of the last solid remaining prior to complete melting corresponds to the intersection with D-(D + L) phase boundary, of the tie line constructed across the D + L phase region at 1380qC—i.e., about 79 wt% Ni.

9.12 A 50 wt% Pb-50 wt% Mg alloy is slowly cooled from 700°C (1290°F) to 400°C (750°F).

(a) At what temperature does the first solid phase form?

(b) What is the composition of this solid phase?

(c) At what temperature does the liquid solidify?

(d) What is the composition of this last remaining liquid phase?

Solution

Shown below is the Mg-Pb phase diagram (Figure 9.20) and a vertical line constructed at a composition of 50 wt% Pb-50 wt% Mg.

(a) Upon cooling from 700°C, the first solid phase forms at the temperature at which a vertical line at this composition intersects the L-(α + L) phase boundary—i.e., about 560°C;

(b) The composition of this solid phase corresponds to the intersection with the α-(α + L) phase boundary, of a tie line constructed across the α + L phase region at 560°C—i.e., 21 wt% Pb-79 wt% Mg;

(c) Complete solidification of the alloy occurs at the intersection of this same vertical line at 50 wt% Pb with the eutectic isotherm—i.e., about 465°C;

(d) The composition of the last liquid phase remaining prior to complete solidification corresponds to the eutectic composition—i.e., about 67 wt% Pb-33 wt% Mg.

9.13 For an alloy of composition 74 wt% Zn-26 wt% Cu, cite the phases present and their compositions at the following temperatures: 850°C, 750°C, 680°C, 600°C, and 500°C.

Solution

This problem asks us to determine the phases present and their concentrations at several temperatures, for an alloy of composition 74 wt% Zn-26 wt% Cu. From Figure 9.19 (the Cu-Zn phase diagram), which is shown below with a vertical line constructed at the specified composition:

At 850°C, a liquid phase is present; C_L = 74 wt% Zn-26 wt% Cu

At 750°C, J and liquid phases are present; C_J = 67 wt% Zn-33 wt% Cu; C_L = 77 wt% Zn-23 wt% Cu

At 680°C, G and liquid phases are present; C_G = 73 wt% Zn-27 wt% Cu; C_L = 82 wt% Zn-18 wt% Cu

At 600°C, the G phase is present; C_G = 74 wt% Zn-26 wt% Cu

At 500°C, J and H phases are present; C_J = 69 wt% Zn-31 wt% Cu; C_H = 78 wt% Zn-22 wt% Cu

9.14 Determine the relative amounts (in terms of mass fractions) of the phases for the alloys and temperatures given in Problem 9.8.

Solution

This problem asks that we determine the phase mass fractions for the alloys and temperatures in Problem 9.8.

(a) From Problem 9.8a, H and K phases are present for a 90 wt% Zn-10 wt% Cu alloy at 400qC, as represented in the portion of the Cu-Zn phase diagram shown below (at point A).

Furthermore, the compositions of the phases, as determined from the tie line are

C_H = 87 wt% Zn-13 wt% Cu

C_K = 97 wt% Zn-3 wt% Cu

Inasmuch as the composition of the alloy C_0 = 90 wt% Zn, application of the appropriate lever rule expressions (for compositions in weight percent zinc) leads to

$$W_H = \frac{C_K \quad C_0}{C_K \quad C_H} = \frac{97 \quad 90}{97 \quad 87} = 0.70$$

$$W_K = \frac{C_0 \quad C_H}{C_K \quad C_H} = \frac{90 \quad 87}{97 \quad 87} = 0.30$$

(b) From Problem 9.8b, D and E phases are present for a 75 wt% Sn-25 wt% Pb alloy at 175qC, as represented in the portion of the Pb-Sn phase diagram shown below (at point B).

Furthermore, the compositions of the phases, as determined from the tie line are

C_D = 16 wt% Sn-84 wt% Pb

C_E = 97 wt% Sn-3 wt% Pb

Inasmuch as the composition of the alloy C_0 = 75 wt% Sn, application of the appropriate lever rule expressions (for compositions in weight percent tin) leads to

$$W_D = \frac{C_E \quad C_0}{C_E \quad C_D} = \frac{97 \quad 75}{97 \quad 16} = 0.27$$

$$W_E = \frac{C_0 \quad C_D}{C_E \quad C_D} = \frac{75 \quad 16}{97 \quad 16} = 0.73$$

(c) From Problem 9.8c, just the liquid phase is present for a 55 wt% Ag-45 wt% Cu alloy at 900qC, as may be noted in the Ag-Cu phase diagram shown below (at point C)—i.e., W_L = 1.0

(d) From Problem 9.8d, just the D phase is present for a 30 wt% Pb-70 wt% Mg alloy at 425°C, as may be noted in the Mg-Pb phase diagram shown below (at point D)—i.e., $W_D = 1.0$

(e) From Problem 9.8e, E and J phases are present for an alloy composed of 2.12 kg Zn and 1.88 kg Cu (i.e., of composition 53 wt% Zn-47 wt% Cu) at 500°C. This is represented in the portion of the Cu-Zn phase diagram shown below (at point E).

Furthermore, the compositions of the phases, as determined from the tie line are

C_E = 49 wt% Zn-51 wt% Cu

C_J = 58 wt% Zn-42 wt% Cu

Inasmuch as the composition of the alloy C_0 = 53 wt% Zn and application of the appropriate lever rule expressions (for compositions in weight percent zinc) leads to

$$W_E = \frac{C_J - C_0}{C_J - C_E} = \frac{58 - 53}{58 - 49} = 0.56$$

$$W_J = \frac{C_0 - C_E}{C_J - C_E} = \frac{53 - 49}{58 - 49} = 0.44$$

(f) From Problem 9.8f, L and Mg_2Pb phases are present for an alloy composed of 37 lb_m Pb and 6.5 lb_m Mg (85 wt% Pb-15 wt% Mg) at 400°C. This is represented in the portion of the Pb-Mg phase diagram shown below (at point F).

Furthermore, the compositions of the phases, as determined from the tie line are

C_{Mg_2Pb} = 81 wt% Pb-19 wt% Mg

C_L = 93 wt% Pb-7 wt% Mg

Inasmuch as the composition of the alloy C_0 = 85 wt% Pb and application of the appropriate lever rule expressions (for compositions in weight percent lead) leads to

$$W_{Mg_2Pb} = \frac{C_L - C_0}{C_L - C_{Mg_2Pb}} = \frac{93 - 85}{93 - 81} = 0.67$$

$$W_L = \frac{C_0 - C_{Mg_2Pb}}{C_L - C_{Mg_2Pb}} = \frac{85 - 81}{93 - 81} = 0.33$$

(g) From Problem 9.8g, just the α phase is present (i.e., W_α = 1.0) for an alloy composed of 8.2 mol Ni and 4.3 mol Cu (i.e., 63.8 wt% Ni-36.2 wt% Cu) at 1250°C; such may be noted (as point G) in the Cu-Ni phase diagram shown below.

(h) From Problem 9.8h, β and L phases are present for an alloy composed of 4.5 mol Sn and 0.45 mol Pb (85.1 wt% Sn-14.9 wt% Pb) and at 200°C. This is represented in the portion of the Pb-Sn phase diagram shown below (at point H).

Furthermore, the compositions of the phases, as determined from the tie line are

C_E = 97.5 wt% Sn-2.5 wt% Pb

C_L = 74 wt% Sn-26 wt% Pb

Inasmuch as the composition of the alloy C_0 = 85.1 wt% Sn, application of the appropriate lever rule expressions (for compositions in weight percent lead) leads to

$$W_E = \frac{C_0 - C_L}{C_E - C_L} = \frac{85.1 - 74}{97.5 - 74} = 0.47$$

$$W_L = \frac{C_E - C_0}{C_E - C_L} = \frac{97.5 - 85.1}{97.5 - 74} = 0.53$$

9.15 A 1.5-kg specimen of a 90 wt% Pb–10 wt% Sn alloy is heated to 250°C (480°F); at this temperature it is entirely an α-phase solid solution (Figure 9.8). The alloy is to be melted to the extent that 50% of the specimen is liquid, the remainder being the α phase. This may be accomplished either by heating the alloy or changing its composition while holding the temperature constant.

(a) To what temperature must the specimen be heated?

(b) How much tin must be added to the 1.5-kg specimen at 250°C to achieve this state?

Solution

(a) Probably the easiest way to solve this part of the problem is by trial and error—that is, on the Pb–Sn phase diagram (Figure 9.8), moving vertically at the given composition, through the α + L region until the tie-line lengths on both sides of the given composition are the same. This occurs at approximately 295°C (560°F).

(b) We can also produce a 50% liquid solution at 250°C, by adding Sn to the alloy. At 250°C and within the α + L phase region

$$C_\alpha = 14 \text{ wt\% Sn-86 wt\% Pb}$$
$$C_L = 34 \text{ wt\% Sn-66 wt\% Pb}$$

Let C_0 be the new alloy composition to give $W_\alpha = W_L = 0.5$. Then,

$$W_\alpha = 0.5 = \frac{C_L - C_0}{C_L - C_\alpha} = \frac{34 - C_0}{34 - 14}$$

And solving for C_0 gives 24 wt% Sn. Now, let m_{Sn} be the mass of Sn added to the alloy to achieve this new composition. The amount of Sn in the original alloy is

$$(0.10)(1.5 \text{ kg}) = 0.15 \text{ kg}$$

Then, using a modified form of Equation 4.3

$$\left[\frac{0.15 \text{ kg} + m_{Sn}}{1.5 \text{ kg} + m_{Sn}}\right] \times 100 = 24$$

And, solving for m_{Sn} (the mass of tin to be added), yields $m_{Sn} = 0.276$ kg.

9.16 A magnesium-lead alloy of mass 5.5 kg consists of a solid α phase that has a composition that is just slightly below the solubility limit at 200°C (390°F).

(a) What mass of lead is in the alloy?

(b) If the alloy is heated to 350°C (660°F), how much more lead may be dissolved in the α phase without exceeding the solubility limit of this phase?

Solution

(a) This portion of the problem asks that we calculate, for a Pb-Mg alloy, the mass of lead in 5.5 kg of the solid α phase at 200°C just below the solubility limit. From Figure 9.20, the solubility limit for the α phase at 200°C corresponds to the position (composition) of the α-α + Mg_2Pb phase boundary at this temperature, which is about 5 wt% Pb. Therefore, the mass of Pb in the alloy is just (0.05)(5.5 kg) = 0.28 kg.

(b) At 350°C, the solubility limit of the α phase increases to approximately 25 wt% Pb. In order to determine the additional amount of Pb that may be added (m_{Pb}), we utilize a modified form of Equation 4.3 as

$$C_{Pb} = 25\,\text{wt\%} = \frac{0.28\,\text{kg} + m_{Pb}}{5.5\,\text{kg} + m_{Pb}} \times 100$$

Solving for m_{Pb} yields m_{Pb} = 1.46 kg.

9.17 A 90 wt% Ag-10 wt% Cu alloy is heated to a temperature within the E + liquid phase region. If the composition of the liquid phase is 85 wt% Ag, determine:

(a) The temperature of the alloy

(b) The composition of the E phase

(c) The mass fractions of both phases

Solution

(a) In order to determine the temperature of a 90 wt% Ag-10 wt% Cu alloy for which E and liquid phases are present with the liquid phase of composition 85 wt% Ag, we need to construct a tie line across the E + L phase region of Figure 9.7 that intersects the liquidus line at 85 wt% Ag; this is possible at about 850 qC.

(b) The composition of the E phase at this temperature is determined from the intersection of this same tie line with solidus line, which corresponds to about 95 wt% Ag.

(c) The mass fractions of the two phases are determined using the lever rule, Equations 9.1 and 9.2 with C_0 = 90 wt% Ag, C_L = 85 wt% Ag, and C_E = 95 wt% Ag, as

$$W_E = \frac{C_0 \quad C_L}{C_E \quad C_L} = \frac{90 \quad 85}{95 \quad 85} = 0.50$$

$$W_L = \frac{C_E \quad C_0}{C_E \quad C_L} = \frac{95 \quad 90}{95 \quad 85} = 0.50$$

9.18 A 30 wt% Sn-70 wt% Pb alloy is heated to a temperature within the α + liquid phase region. If the mass fraction of each phase is 0.5, estimate:

(a) The temperature of the alloy

(b) The compositions of the two phases

Solution

(a) We are given that the mass fractions of α and liquid phases are both 0.5 for a 30 wt% Sn-70 wt% Pb alloy and asked to estimate the temperature of the alloy. Using the appropriate phase diagram, Figure 9.8, by trial and error with a ruler, a tie line within the α + L phase region that is divided in half for an alloy of this composition exists at about 230°C.

(b) We are now asked to determine the compositions of the two phases. This is accomplished by noting the intersections of this tie line with both the solidus and liquidus lines. From these intersections, C_α = 15 wt% Sn, and C_L = 43 wt% Sn.

9.19 For alloys of two hypothetical metals A and B, there exist DQ .U$FK SKDVH-rich phase DQG D %. From the mass fractions of both phases for two different alloys provided in the table below, (which are at the same WHPSHUDWXUH GHWHUPLQH WKH FRPSRVLWLRQ RI WKH SKDVH ERXQGDU temperature.

Alloy Composition	)UDFWLI Phase	)UDFWI Phase
60 wt% A–40 wt% B	0.57	0.43
30 wt% A–70 wt% B	0.14	0.86

Solution

The problem is to solve for compositions at the phase boundaries for both D and E phases (i.e., C_D and C_E). We may set up two independent lever rule expressions, one for each composition, in terms of C_D and C_E as follows:

$$W_{D1} = 0.57 = \frac{C_E \quad C_{01}}{C_E \quad C_D} = \frac{C_E \quad 60}{C_E \quad C_D}$$

$$W_{D2} = 0.14 = \frac{C_E \quad C_{02}}{C_E \quad C_D} = \frac{C_E \quad 30}{C_E \quad C_D}$$

In these expressions, compositions are given in wt% of A. Solving for C_D and C_E from these equations, yield

C_D = 90 (or 90 wt% A–10 wt% B)

C_E = 20.2 (or 20.2 wt% A–79.8 wt% B)

9.20 A hypothetical A-B alloy of composition 55 wt% B-45 wt% A at some temperature is found to consist RI PDVV IUDFWLRQV RI IRU ERWK DQG SKDVHV ,I WKH FRPSRVLWLRQ RI WKH SKDVH LV 90 wt% B-10 wt% A, what is Z WKH FRPSRVLWLRQ RI WKH . SKDVH"

Solution

For this problem, we are asked to determine the composition of the E phase given that

$$C_0 = 55 \text{ (or 55 wt\% B-45 wt\% A)}$$

$$C_E = 90 \text{ (or 90 wt\% B-10 wt\% A)}$$

$$W_D = W_E = 0.5$$

If we set up the lever rule for W_D

$$W_D = 0.5 = \frac{C_E \quad C_0}{C_E \quad C_D} = \frac{90 \quad 55}{90 \quad C_D}$$

And solving for C_D

$$C_D = 20 \text{ (or 20 wt\% B-80 wt\% A)}$$

9.21 Is it possible to have a copper-silver alloy of composition 50 wt% Ag-50 wt% Cu, which, at equilibrium, consists of D Q GS K D V H V having mass fractions W_D = 0.60 and W_E = 0.40? If so, what will be the approximate temperature of the alloy? If such an alloy is not possible, explain why.

Solution

It is not possible to have a Cu-Ag alloy of composition 50 wt% Ag-50 wt% Cu which consists of mass fractions W_D = 0.60 and W_E = 0.40. Using the appropriate phase diagram, Figure 9.7, and, using Equations 9.1 and 9.2 let us determine W_D and W_E at just below the eutectic temperature and also at room temperature. At just below the eutectic, C_D = 8.0 wt% Ag and C_E = 91.2 wt% Ag; thus,

$$W_D = \frac{C_E \quad C_0}{C_E \quad C_D} \quad \frac{91.2 \quad 50}{91.2 \quad 8} \quad 0.50$$

$$W_E = 1.00 \quad W_D = 1.00 \quad 0.50 = 0.50$$

Furthermore, at room temperature, C_D = 0 wt% Ag and C_E = 100 wt% Ag; employment of Equations 9.1 and 9.2 yields

$$W_D \quad \frac{C_E \quad C_0}{C_E \quad C_D} \quad \frac{100 \quad 50}{100 \quad 0} \quad 0.50$$

And, W_E = 0.50. Thus, the mass fractions of the D and E phases, upon cooling through the D + E phase region will remain approximately constant at about 0.5, and will never have values of W_D = 0.60 and W_E = 0.40 as called for in the problem.

9.22 For 11.20 kg of a magnesium-lead alloy of composition 30 wt% Pb-70 wt% Mg, is it possible, at equilibrium, to have and Mg_2Pb phases having respective masses of 7.39 kg and 3.81 kg? If so, what will be the approximate temperature of the alloy? If such an alloy is not possible, explain why.

Solution

Yes, it is possible to have a 30 wt% Pb-70 wt% Mg alloy which has masses of 7.39 kg and 3.81 kg for the D and Mg_2Pb phases, respectively. In order to demonstrate this, it is first necessary to determine the mass fraction of each phase as follows:

$$W_D = \frac{m_D}{m_D \quad m_{Mg_2Pb}} = \frac{7.39 \text{ kg}}{7.39 \text{ kg} \quad 3.81 \text{ kg}} = 0.66$$

$$W_{Mg_2Pb} = 1.00 \quad 0.66 = 0.34$$

Now, if we apply the lever rule expression for W_D

$$W_D = \frac{C_{Mg_2Pb} \quad C_0}{C_{Mg_2Pb} \quad C_D}$$

Since the Mg_2Pb phase exists only at 81 wt% Pb, and C_0 = 30 wt% Pb

$$W_D = 0.66 = \frac{81 \quad 30}{81 \quad C_D}$$

Solving for C_D from this expression yields C_D = 3.7 wt% Pb. The position along the D + Mg_2Pb) phase boundary of Figure 9.20 corresponding to this composition is approximately 190 qC.

9.23 Derive Equations 9.6a and 9.7a, which may be used to convert mass fraction to volume fraction, and vice versa.

Solution

This portion of the problem asks that we derive Equation 9.6a, which is used to convert from phase weight fraction to phase volume fraction. Volume fraction of phase D, V_D, is defined by Equation 9.5 as

$$V_D = \frac{v_D}{v_D \quad v_E} \qquad (9.S1)$$

where v_D and v_E are the volumes of the respective phases in the alloy. Furthermore, the density of each phase is equal to the ratio of its mass and volume, or upon rearrangement

$$v_D = \frac{m_D}{U_D} \qquad (9.S2a)$$

$$v_E = \frac{m_E}{U_E} \qquad (9.S2b)$$

Substitution of these expressions into Equation 9.S1 leads to

$$V_D = \frac{\dfrac{m_D}{U_D}}{\dfrac{m_D}{U_D} \quad \dfrac{m_E}{U_E}} \qquad (9.S3)$$

in which m's and U's denote masses and densities, respectively. Now, the mass fractions of the D and E phases (i.e., W_D and W_E) are defined in terms of the phase masses as

$$W_D = \frac{m_D}{m_D \quad m_E} \qquad (9.S4a)$$

$$W_E = \frac{m_E}{m_D \quad m_E} \qquad (9.S4b)$$

Which, upon rearrangement yield

$$m_D = W_D\left(m_D + m_E\right) \tag{9.S5a}$$

$$m_E = W_E\left(m_D + m_E\right) \tag{9.S5b}$$

Incorporation of these relationships into Equation 9.S3 leads to

$$V_D \quad \frac{\frac{W_D\left(m_D + m_E\right)}{\rho_D}}{\frac{W_D\left(m_D + m_E\right)}{\rho_D} \quad \frac{W_E\left(m_D + m_E\right)}{\rho_E}}$$

$$V_D = \frac{\frac{W_D}{\rho_D}}{\frac{W_D}{\rho_D} \quad \frac{W_E}{\rho_E}} \tag{9.S6}$$

which is the desired equation.

For this portion of the problem we are asked to derive Equation 9.7a, which is used to convert from phase volume fraction to mass fraction. Mass fraction of the D phase is defined as

$$W_D = \frac{m_D}{m_D \quad m_E} \tag{9.S7}$$

From Equations 9.S2a and 9.S2b

$$m_D = v_D \rho_D \tag{9.S8a}$$

$$m_E = v_E \rho_E \tag{9.S8b}$$

Substitution of these expressions into Equation 9.S7 yields

$$W_D = \frac{v_D \rho_D}{v_D \rho_D \quad v_E \rho_E} \tag{9.S9}$$

From Equation 9.5 and its equivalent for v_E the following may be written:

$$v_D = V_D(v_D + v_E) \tag{9.S10a}$$

$$v_E = V_E(v_D + v_E) \tag{9.S10b}$$

Substitution of Equations 9.S10a and 9.S10b into Equation 9.S9 yields

$$W_D = \frac{V_D(v_D + v_E)\,U_D}{V_D(v_D + v_E)\,U_D \quad V_E(v_D + v_E)\,U_E}$$

$$W_D = \frac{V_D U_D}{V_D U_D \quad V_E U_E} \tag{9.S11}$$

which is the desired expression.

9.24 Determine the relative amounts (in terms of volume fractions) of the phases for the alloys and temperatures given in Problem 9.8a, b, and c. Below are given the approximate densities of the various metals at the alloy temperatures:

Metal	Temperature (°C)	Density (g/cm^3)
Ag	900	9.97
Cu	400	8.77
Cu	900	8.56
Pb	175	11.20
Sn	175	7.22
Zn	400	6.83

Solution

This problem asks that we determine the phase volume fractions for the alloys and temperatures in Problems 9.8a, b, and c. This is accomplished by using the technique illustrated in Example Problem 9.3, and also the results of Problems 9.8 and 9.14.

(a) This is a Cu-Zn alloy at 400°C, wherein

C_H = 87 wt% Zn-13 wt% Cu
C_K = 97 wt% Zn-3 wt% Cu
W_H = 0.70
W_K = 0.30
U_{Cu} = 8.77 g/cm^3
U_{Zn} = 6.83 g/cm^3

Using these data it is first necessary to compute the densities of the H and K phases using Equation 4.10a. Thus

$$U_H = \frac{100}{\dfrac{C_{Zn(H)}}{U_{Zn}} \quad \dfrac{C_{Cu(H)}}{U_{Cu}}}$$

$$= \frac{100}{\dfrac{87}{6.83\ \text{g/cm}^3} \quad \dfrac{13}{8.77\ \text{g/cm}^3}} = 7.03\ \text{g/cm}^3$$

$$\rho_K = \frac{100}{\dfrac{C_{Zn(K)}}{\rho_{Zn}} \quad \dfrac{C_{Cu(K)}}{\rho_{Cu}}}$$

$$= \frac{100}{\dfrac{97}{6.83\ \text{g/cm}^3} \quad \dfrac{3}{8.77\ \text{g/cm}^3}} = 6.88\ \text{g/cm}^3$$

Now we may determine the V_H and V_K values using Equation 9.6. Thus,

$$V_H = \frac{\dfrac{W_H}{\rho_H}}{\dfrac{W_H}{\rho_H} \quad \dfrac{W_K}{\rho_K}}$$

$$= \frac{\dfrac{0.70}{7.03\ \text{g/cm}^3}}{\dfrac{0.70}{7.03\ \text{g/cm}^3} \quad \dfrac{0.30}{6.88\ \text{g/cm}^3}} = 0.70$$

$$V_K = \frac{\dfrac{W_K}{\rho_K}}{\dfrac{W_H}{\rho_H} \quad \dfrac{W_K}{\rho_K}}$$

$$= \frac{\dfrac{0.30}{6.88\ \text{g/cm}^3}}{\dfrac{0.70}{7.03\ \text{g/cm}^3} \quad \dfrac{0.30}{6.88\ \text{g/cm}^3}} = 0.30$$

(b) This is a Pb-Sn alloy at 175°C, wherein

C_D = 16 wt% Sn-84 wt% Pb

C_E = 97 wt% Sn-3 wt% Pb

$W_D = 0.27$

$W_E = 0.73$

$U_{Sn} = 7.22\ \text{g/cm}^3$

$U_{Pb} = 11.20\ \text{g/cm}^3$

Using this data it is first necessary to compute the densities of the D and E phases. Thus

$$U_D = \frac{100}{\dfrac{C_{Sn(D)}}{U_{Sn}} \quad \dfrac{C_{Pb(D)}}{U_{Pb}}}$$

$$= \frac{100}{\dfrac{16}{7.22\ \text{g/cm}^3} \quad \dfrac{84}{11.20\ \text{g/cm}^3}} = 10.29\ \text{g/cm}^3$$

$$U_E = \frac{100}{\dfrac{C_{Sn(E)}}{U_{Sn}} \quad \dfrac{C_{Pb(E)}}{U_{Pb}}}$$

$$= \frac{100}{\dfrac{97}{7.22\ \text{g/cm}^3} \quad \dfrac{3}{11.20\ \text{g/cm}^3}} = 7.30\ \text{g/cm}^3$$

Now we may determine the V_D and V_E values using Equation 9.6. Thus,

$$V_D = \frac{\dfrac{W_D}{U_D}}{\dfrac{W_D}{U_D} \quad \dfrac{W_E}{U_E}}$$

$$= \frac{\dfrac{0.27}{10.29\ \text{g/cm}^3}}{\dfrac{0.27}{10.29\ \text{g/cm}^3} \quad \dfrac{0.73}{7.30\ \text{g/cm}^3}} = 0.21$$

$$V_E = \frac{\dfrac{W_E}{U_E}}{\dfrac{W_D}{U_D} \quad \dfrac{W_E}{U_E}}$$

$$= \frac{\dfrac{0.73}{7.30\,\text{g/cm}^3}}{\dfrac{0.27}{10.29\,\text{g/cm}^3} \quad \dfrac{0.73}{7.30\,\text{g/cm}^3}} = 0.79$$

(c) This is a Ag-Cu alloy at 900 C, wherein only the liquid phase is present. Therefore, $V_L = 1.0$.

Development of Microstructure in Isomorphous Alloys

9.25 (a) Briefly describe the phenomenon of coring and why it occurs.

(b) Cite one undesirable consequence of coring.

Solution

(a) Coring is the phenomenon whereby concentration gradients exist across grains in polycrystalline alloys, with higher concentrations of the component having the lower melting temperature at the grain boundaries. It occurs, during solidification, as a consequence of cooling rates that are too rapid to allow for the maintenance of the equilibrium composition of the solid phase.

(b) One undesirable consequence of a cored structure is that, upon heating, the grain boundary regions will melt first and at a temperature below the equilibrium phase boundary from the phase diagram; this melting results in a loss in mechanical integrity of the alloy.

Mechanical Properties of Isomorphous Alloys

9.26 It is desirable to produce a copper-nickel alloy that has a minimum noncold-worked tensile strength of 350 MPa (50,750 psi) and a ductility of at least 48%EL. Is such an alloy possible? If so, what must be its composition? If this is not possible, then explain why.

<u>Solution</u>

From Figure 9.6a, a tensile strength greater than 350 MPa (50,750 psi) is possible for compositions between about 22.5 and 98 wt% Ni. On the other hand, according to Figure 9.6b, ductilities greater than 48%EL exist for compositions less than about 8 wt% and greater than about 98 wt% Ni. Therefore, the stipulated criteria are met only at a composition of 98 wt% Ni.

Binary Eutectic Systems

9.27 A 45 wt% Pb-55 wt% Mg alloy is rapidly quenched to room temperature from an elevated temperature in such a way that the high-temperature microstructure is preserved. This microstructure is found to F R Q V L V W R I W K H $_2$Pb, S K D V H D Q G 0 J having respective mass fractions of 0.65 and 0.35. Determine the approximate temperature from which the alloy was quenched.

Solution

We are asked to determine the approximate temperature from which a 45 wt% Pb-55 wt% Mg alloy was quenched, given the mass fractions D and Mg$_2$Pb phases. We can write a lever-rule expression for the mass fraction of the D phase as

$$W_D = 0.65 = \frac{C_{Mg_2Pb} \quad C_0}{C_{Mg_2Pb} \quad C_D}$$

The value of C_0 is stated as 45 wt% Pb-55 wt% Mg, and C_{Mg_2Pb} is 81 wt% Pb-19 wt% Mg, which is independent of temperature (Figure 9.20); thus,

$$0.65 = \frac{81 \quad 45}{81 \quad C_D}$$

which yields

$$C_D = 25.6 \text{ wt\% Pb}$$

The temperature at which the –(D + Mg$_2$Pb) phase boundary (Figure 9.20) has a value of 25.6 wt% Pb is about 360 C (680 F).

Development of Microstructure in Eutectic Alloys

9.28 Briefly explain why, upon solidification, an alloy of eutectic composition forms a microstructure consisting of alternating layers of the two solid phases.

Solution

Upon solidification, an alloy of eutectic composition forms a microstructure consisting of alternating layers of the two solid phases because during the solidification atomic diffusion must occur, and with this layered configuration the diffusion path length for the atoms is a minimum.

9.29 What is the difference between a phase and a microconstituent?

Solution

A “phase” is a homogeneous portion of the system having uniform physical and chemical characteristics, whereas a “microconstituent” is an identifiable element of the microstructure (that may consist of more than one phase).

9.30 Is it possible to have a copper-silver alloy in which the mass fractions of primary and total are 0.68 and 0.925, respectively, at 775°C (1425°F)? Why or why not?

Solution

This problem asks if it is possible to have a Cu-Ag alloy for which the mass fractions of primary E and total E are 0.68 and 0.925, respectively at 775°C. In order to make this determination we need to set up the appropriate lever rule expression for each of these quantities. From Figure 9.7 and at 775°C, C_D = 8.0 wt% Ag, C_E = 91.2 wt% Ag, and $C_{eutectic}$ = 71.9 wt% Ag.

For primary E

$$W_E = \frac{C_0 \quad C_{eutectic}}{C_E \quad C_{eutectic}} = \frac{C_0 \quad 71.9}{91.2 \quad 71.9} = 0.68$$

Solving for C_0 gives C_0 = 85 wt% Ag.

Now the analogous expression for total E

$$W_E = \frac{C_0 \quad C_D}{C_E \quad C_D} = \frac{C_0 \quad 8.0}{91.2 \quad 8.0} = 0.925$$

And this value of C_0 is 85 wt% Ag. Therefore, since these two C_0 values are the same (85 wt% Ag), this alloy is possible

9.31 For 6.70 kg of a magnesium-lead alloy, is it possible to have the masses of primary . and total . of 4.23 kg and 6.00 kg, respectively, at 460qC (860qF)? Why or why not?

Solution

This problem asks if it is possible to have a Mg-Pb alloy for which the masses of primary D and total D are 4.23 kg and 6.00 kg, respectively in 6.70 kg total of the alloy at 460qC. In order to make this determination we first need to convert these masses to mass fractions. Thus,

$$W_D = \frac{4.23\,\text{kg}}{6.70\,\text{kg}} = 0.631$$

$$W_D = \frac{6.00\,\text{kg}}{6.70\,\text{kg}} = 0.896$$

Next it is necessary to set up the appropriate lever rule expression for each of these quantities. From Figure 9.20 and at 460qC, C_D = 41 wt% Pb, C_{Mg_2Pb} = 81 wt% Pb, and $C_{eutectic}$ = 66 wt% Pb

For primary D

$$W_D = \frac{C_{eutectic} \quad C_0}{C_{eutectic} \quad C_D} = \frac{66 \quad C_0}{66 \quad 41} = 0.631$$

And solving for C_0 gives C_0 = 50.2 wt% Pb.

Now the analogous expression for total D

$$W_D = \frac{C_{Mg_2Pb} \quad C_0}{C_{Mg_2Pb} \quad C_D} = \frac{81 \quad C_0}{81 \quad 41} = 0.896$$

And this value of C_0 is 45.2 wt% Pb. Therefore, since these two C_0 values are different, this alloy is not possible

9.32 For a copper-silver alloy of composition 25 wt% Ag-75 wt% Cu and at 775qC (1425qF) do the following:

(a) Determine the mass fractions of D Q G S K D V H V

(b) Determine the mass fractions of primary and eutectic microconstituents.

(c) Determine the mass fraction of eutectic.

Solution

(a) This portion of the problem asks that we determine the mass fractions of D and E phases for an 25 wt% Ag-75 wt% Cu alloy (at 775qC). In order to do this it is necessary to employ the lever rule using a tie line that extends entirely across the D + E phase field. From Figure 9.7 and at 775qC, C_D = 8.0 wt% Ag, C_E = 91.2 wt% Ag, and $C_{eutectic}$ = 71.9 wt% Sn. Therefore, the two lever-rule expressions are as follows:

$$W_D = \frac{C_E \quad C_0}{C_E \quad C_D} = \frac{91.2 \quad 25}{91.2 \quad 8.0} = 0.796$$

$$W_E = \frac{C_0 \quad C_D}{C_E \quad C_D} = \frac{25 \quad 8.0}{91.2 \quad 8.0} = 0.204$$

(b) Now it is necessary to determine the mass fractions of primary D and eutectic microconstituents for this same alloy. This requires us to utilize the lever rule and a tie line that extends from the maximum solubility of Ag in the D phase at 775qC (i.e., 8.0 wt% Ag) to the eutectic composition (71.9 wt% Ag). Thus

$$W_{D'} = \frac{C_{eutectic} Ê C_0}{C_{eutectic} Ê C_D} = \frac{71.9 \quad 25}{71.9 \quad 8.0} = 0.734$$

$$W_e = \frac{C_0 \quad C_D}{C_{eutectic} \quad C_D} = \frac{25 \quad 8.0}{71.9 \quad 8.0} = 0.266$$

(c) And, finally, we are asked to compute the mass fraction of eutectic D, W_{eD}. This quantity is simply the difference between the mass fractions of total D and primary D as

$$W_{eD} = W_D – W_{D'} = 0.796 – 0.734 = 0.062$$

9.33 The microstructure of a lead-tin alloy at 180°C (355°F) consists of primary and eutectic structures. If the mass fractions of these two microconstituents are 0.57 and 0.43, respectively, determine the composition of the alloy.

Solution

Since there is a primary E microconstituent present, then we know that the alloy composition, C_0 is between 61.9 and 97.8 wt% Sn (Figure 9.8). Furthermore, this figure also indicates that C_E = 97.8 wt% Sn and $C_{eutectic}$ = 61.9 wt% Sn. Applying the appropriate lever rule expression for W_E

$$W_E = \frac{C_0 - C_{eutectic}}{C_E - C_{eutectic}} = \frac{C_0 - 61.9}{97.8 - 61.9} = 0.57$$

and solving for C_0 yields C_0 = 82.4 wt% Sn.

9.34 Consider the hypothetical eutectic phase diagram for metals A and B, which is similar to that for the lead-tin system, Figure 9.8. Assume that (1) D Q G phases exist at the A and B extremities of the phase diagram, respectively; (2) the eutectic composition is 47 wt% B-53 wt% A; and (3) the composition of the phase at the eutectic temperature is 92.6 wt% B-7.4 wt% A. Determine the composition of an alloy that will yield primary . and total . mass fractions of 0.356 and 0.693, respectively.

Solution

We are given a hypothetical eutectic phase diagram for which $C_{eutectic}$ = 47 wt% B, C_E = 92.6 wt% B at the eutectic temperature, and also that W_D = 0.356 and W_D = 0.693; from this we are asked to determine the composition of the alloy. Let us write lever rule expressions for W_D and W_D

$$W_D = \frac{C_E - C_0}{C_E - C_D} = \frac{92.6 - C_0}{92.6 - C_D} = 0.693$$

$$W_D = \frac{C_{eutectic} - C_0}{C_{eutectic} - C_D} = \frac{47 - C_0}{47 - C_D} = 0.356$$

Thus, we have two simultaneous equations with C_0 and C_D as unknowns. Solving them for C_0 gives C_0 = 32.6 wt% B.

9.35 For an 85 wt% Pb-15 wt% Mg alloy, make schematic sketches of the microstructure that would be observed for conditions of very slow cooling at the following temperatures: 600°C (1110°F), 500°C (930°F), 270°C (520°F), and 200°C (390°F). Label all phases and indicate their approximate compositions.

Solution

The illustration below is the Mg-Pb phase diagram (Figure 9.20). A vertical line at a composition of 85 wt% Pb-15 wt% Mg has been drawn, and, in addition, horizontal arrows at the four temperatures called for in the problem statement (i.e., 600°C, 500°C, 270°C, and 200°C).

On the basis of the locations of the four temperature-composition points, schematic sketches of the four respective microstructures along with phase compositions are represented as follows:

9.36 For a 68 wt% Zn-32 wt% Cu alloy, make schematic sketches of the microstructure that would be observed for conditions of very slow cooling at the following temperatures: 1000°C (1830°F), 760°C (1400°F), 600°C (1110°F), and 400°C (750°F). Label all phases and indicate their approximate compositions.

Solution

The illustration below is the Cu-Zn phase diagram (Figure 9.19). A vertical line at a composition of 68 wt% Zn-32 wt% Cu has been drawn, and, in addition, horizontal arrows at the four temperatures called for in the problem statement (i.e., 1000°C, 760°C, 600°C, and 400°C).

On the basis of the locations of the four temperature-composition points, schematic sketches of the four respective microstructures along with phase compositions are represented as follows:

CHAPTER 2

ATOMIC STRUCTURE AND INTERATOMIC BONDING

PROBLEM SOLUTIONS

Fundamental Concepts

Electrons in Atoms

2.1 *Cite the difference between atomic mass and atomic weight.*

Solution

Atomic mass is the mass of an individual atom, whereas atomic weight is the average (weighted) of the atomic masses of an atom's naturally occurring isotopes.