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.

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.

<table>
<thead>
<tr>
<th>Line Number</th>
<th>No. Grains Intersected</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>11</td>
</tr>
<tr>
<td>2</td>
<td>10</td>
</tr>
<tr>
<td>3</td>
<td>9</td>
</tr>
<tr>
<td>4</td>
<td>8.5</td>
</tr>
<tr>
<td>5</td>
<td>7</td>
</tr>
<tr>
<td>6</td>
<td>10</td>
</tr>
<tr>
<td>7</td>
<td>8</td>
</tr>
</tbody>
</table>

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\( \times \) according to Equation 4.16. Inasmuch as the magnification is 100\( \times \), 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.

![Micrograph](image)

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

\[
n = \frac{\log N}{\log 2} + 1
\]

\[
= \frac{\log 10}{\log 2} + 1 = 4.3
\]

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

\[
n = \frac{\log N_{M} + 2 \log \left( \frac{M}{100} \right)}{\log 2} + 1
\]

\[
= \frac{\log 8 + 2 \log \left( \frac{600}{100} \right)}{\log 2} + 1 = 9.2
\]

CHAPTER 5

5.1 Briefly explain the difference between self-diffusion and interdiffusion.

Solution

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.

5.4 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.

5.6 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 m² at 500 °C. Assume a diffusion coefficient of \( 1.0 \times 10^{-8} \) m²/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

\[ M = JAt = -DA \frac{\Delta C}{\Delta x} \]

\[ = -(1.0 \times 10^{-8} \text{ m}^2/\text{s})(0.20 \text{ m}^2)(3600 \text{ s/h}) \left( \frac{0.6 - 2.4 \text{ kg/m}^3}{5 \times 10^{-3} \text{ m}} \right) \]

\[ = 2.6 \times 10^{-3} \text{ kg/h} \]

5.17 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

\[ D = (2.4 \times 10^{-5} \text{ m}^2/\text{s}) \exp\left[ -\frac{189,000 \text{ J/mol}}{(8.31 \text{ J/mol-K})(650 + 273 \text{ K})} \right] \]

\[ = 4.8 \times 10^{-16} \text{ m}^2/\text{s} \]

Note: this problem may also be solved using the “Diffusion” module in the VMSE software. Open the “Diffusion” module, click on the “D 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 $4.7 \times 10^{-16} \text{ m}^2/\text{s}$. 
5.21 The diffusion coefficients for iron in nickel are given at two temperatures:

<table>
<thead>
<tr>
<th>T (K)</th>
<th>D (m²/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1273</td>
<td>9.4 × 10⁻¹⁶</td>
</tr>
<tr>
<td>1473</td>
<td>2.4 × 10⁻¹⁴</td>
</tr>
</tbody>
</table>

(a) Determine the values of $D_0$ and the activation energy $Q_d$.

(b) What is the magnitude of $D$ at 1100°C (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 m²/s), we get

\[
Q_d = -R \left[ \ln \left( \frac{D_1}{D_2} \right) \frac{1}{T_1 - T_2} \right]
\]

\[
= - (8.31 \text{ J/mol - K}) \frac{\ln (9.4 \times 10^{-16}) - \ln (2.4 \times 10^{-14})}{1273 \text{ K} - 1473 \text{ K}}
\]

\[
= 252,400 \text{ J/mol}
\]

Now, solving for $D_0$ from Equation 5.8 (and using the 1273 K value of $D$)

\[
D_0 = D_1 \exp \left( \frac{Q_d}{RT_1} \right)
\]

\[
= (9.4 \times 10^{-16} \text{ m}^2/\text{s}) \exp \left[ \frac{252,400 \text{ J/mol}}{(8.31 \text{ J/mol - K})(1273 \text{ K})} \right]
\]
(b) Using these values of \( D_0 \) and \( Q_d \), \( D \) at 1373 K is just

\[
D = (2.2 \times 10^{-5} \text{ m}^2/\text{s}) \exp\left(\frac{-252,400 \text{ J/mol}}{(8.31 \text{ J/mol} \cdot \text{K})(1373 \text{ K})}\right)
\]

\[
= 5.4 \times 10^{-15} \text{ m}^2/\text{s}
\]

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 \( 2.17 \times 10^{-5} \text{ m}^2/\text{s} \) 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 \( 5.4 \times 10^{-15} \text{ m}^2/\text{s} \).