

Question 1

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/cm³ and 55.85 g/mol, respectively.

Solution:

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

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

$$\begin{aligned} N_v &= \frac{(6.022 \times 10^{23} \text{ atoms/mol})(7.65 \text{ g/cm}^3)}{55.85 \text{ g/mol}} \exp\left[-\frac{1.08 \text{ eV/atom}}{(8.62 \times 10^{-5} \text{ eV/atom-K})(850^\circ\text{C} + 273 \text{ K})}\right] \\ &= 1.18 \times 10^{18} \text{ cm}^{-3} = 1.18 \times 10^{24} \text{ m}^{-3} \end{aligned}$$

Question 2:

- Describe the substitutional and interstitial diffusion mechanisms in solid metals
- Cite two reasons why interstitial diffusion is normally more rapid than vacancy diffusion
- Describe the factors that affect diffusion and discuss their effects

Solution:

- During the substitutional diffusion of atoms in a solid alloy crystal lattice, solute atoms move into positions of solvent atoms in the matrix through a vacancy mechanism. In interstitial diffusion, small solute atoms move between the interstices of the solvent lattice.
- 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.
- The diffusion coefficient, D , is a function of temperature, concentration and crystal structure. Also, in addition to the lattice diffusion which has been mainly considered, significant amount of diffusion may take place by other methods like along the grain boundaries, surfaces, or dislocations. Moreover the diffusion may take place not only by concentration gradient, but also by local state of stress, electric, or magnetic field, or temperature gradient. The effect of concentration on diffusion coefficient in dilute solutions, or over a small range

of concentration is not much. The crystal structure also effects the diffusion coefficient. BCC crystal structure has atomic packing factor of 0.68 with a void fraction of 0.32, whereas FCC has a void fraction of 0.26. At a given temperature, diffusion and self-diffusion occurs about one hundred times more rapidly in ferrite (BCC) than in austenite (FCC). The rate of diffusion is faster in a distorted crystal structure due to elastic strains, or extensive cold working. As grain boundary diffusion is faster than that within the grains, thus diffusion is faster in fine grained materials, particularly when the grain sizes are in the ultra-fine grain range.

Question 3

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 below.

<i>Diffusing Species</i>	<i>Host Metal</i>	$D_0(m^2/s)$	<i>Activation Energy Q_d</i>		<i>Calculated Values</i>	
			<i>kJ/mol</i>	<i>eV/atom</i>	<i>T(°C)</i>	<i>D(m²/s)</i>
Fe	α -Fe (BCC)	2.8×10^{-4}	251	2.60	500	3.0×10^{-21}
					900	1.8×10^{-15}
Fe	γ -Fe (FCC)	5.0×10^{-5}	284	2.94	900	1.1×10^{-17}
					1100	7.8×10^{-16}
C	α -Fe	6.2×10^{-7}	80	0.83	500	2.4×10^{-12}
					900	1.7×10^{-10}
C	γ -Fe	2.3×10^{-5}	148	1.53	900	5.9×10^{-12}
					1100	5.3×10^{-11}
Cu	Cu	7.8×10^{-5}	211	2.19	500	4.2×10^{-19}
Zn	Cu	2.4×10^{-5}	189	1.96	500	4.0×10^{-18}
Al	Al	2.3×10^{-4}	144	1.49	500	4.2×10^{-14}
Cu	Al	6.5×10^{-5}	136	1.41	500	4.1×10^{-14}
Mg	Al	1.2×10^{-4}	131	1.35	500	1.9×10^{-13}
Cu	Ni	2.7×10^{-5}	256	2.65	500	1.3×10^{-22}

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 $x = 2 \text{ mm} = 2 \times 10^{-3} \text{ m}$. 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	$\operatorname{erf}(z)$
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)

$$D = (2.3 \times 10^{-5} \text{ m}^2/\text{s}) \exp\left[-\frac{148,000 \text{ J/mol}}{(8.31 \text{ J/mol}\cdot\text{K})(1273 \text{ K})}\right]$$

$$= 1.93 \times 10^{-11} \text{ m}^2/\text{s}$$

Thus,

$$0.854 = \frac{2 \times 10^{-3} \text{ m}}{(2)\sqrt{(1.93 \times 10^{-11} \text{ m}^2/\text{s})(t)}}$$

$$\text{Solving for } t \text{ yields } t = 7.1 \times 10^4 \text{ s} = 19.7 \text{ h}$$

Question 4

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 1100°C (1373 K)?

Solution:

$$\ln D_1 = \ln D_0 - \frac{Q_d}{R} \left(\frac{1}{T_1} \right)$$

$$\ln D_2 = \ln D_0 - \frac{Q_d}{R} \left(\frac{1}{T_2} \right)$$

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

$$\begin{aligned} Q_d &= -R \frac{\ln D_1 - \ln D_2}{\frac{1}{T_1} - \frac{1}{T_2}} \\ &= -(8.31 \text{ J/mol-K}) \frac{[\ln(9.4 \times 10^{-16}) - \ln(2.4 \times 10^{-14})]}{\frac{1}{1273 \text{ K}} - \frac{1}{1473 \text{ K}}} \\ &= 252,400 \text{ J/mol} \end{aligned}$$

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

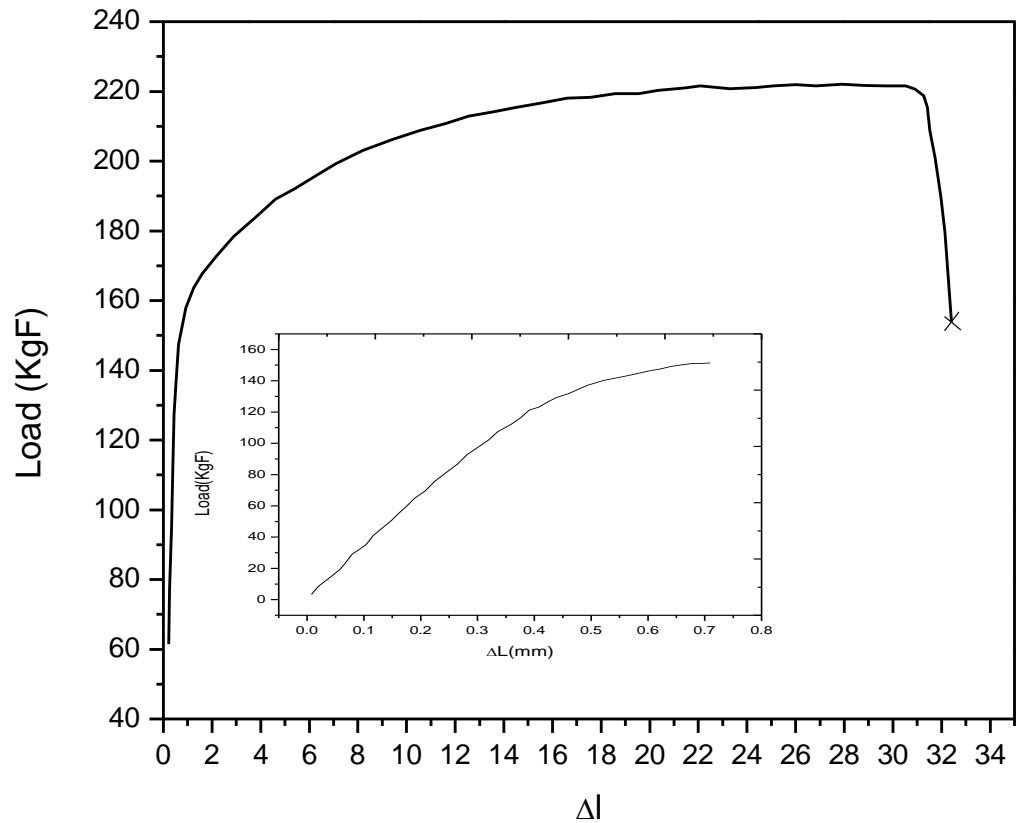
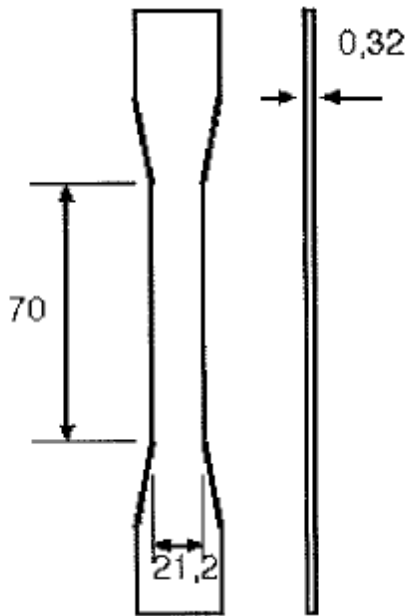
$$\begin{aligned} D_0 &= D_1 \exp\left(\frac{Q_d}{RT_1}\right) \\ &= (9.4 \times 10^{-16} \text{ m}^2/\text{s}) \exp\left[\frac{252,400 \text{ J/mol}}{(8.31 \text{ J/mol-K})(1273 \text{ K})}\right] \\ &= 2.2 \times 10^{-5} \text{ m}^2/\text{s} \end{aligned}$$

- (b) Using these values of D_0 and Q_d , D at 1373 K is just

$$D = (2.2 \times 10^{-5} \text{ m}^2/\text{s}) \exp\left[-\frac{252,400 \text{ J/mol}}{(8.31 \text{ J/mol-K})(1373 \text{ K})}\right] = 5.4 \times 10^{-15} \text{ m}^2/\text{s}$$

Question 5

Determine the 0.2% offset Yield Strength, the Percent Elongation and the Tensile Strength for the specimen with the dimensions given below in mm.

**Solution:**

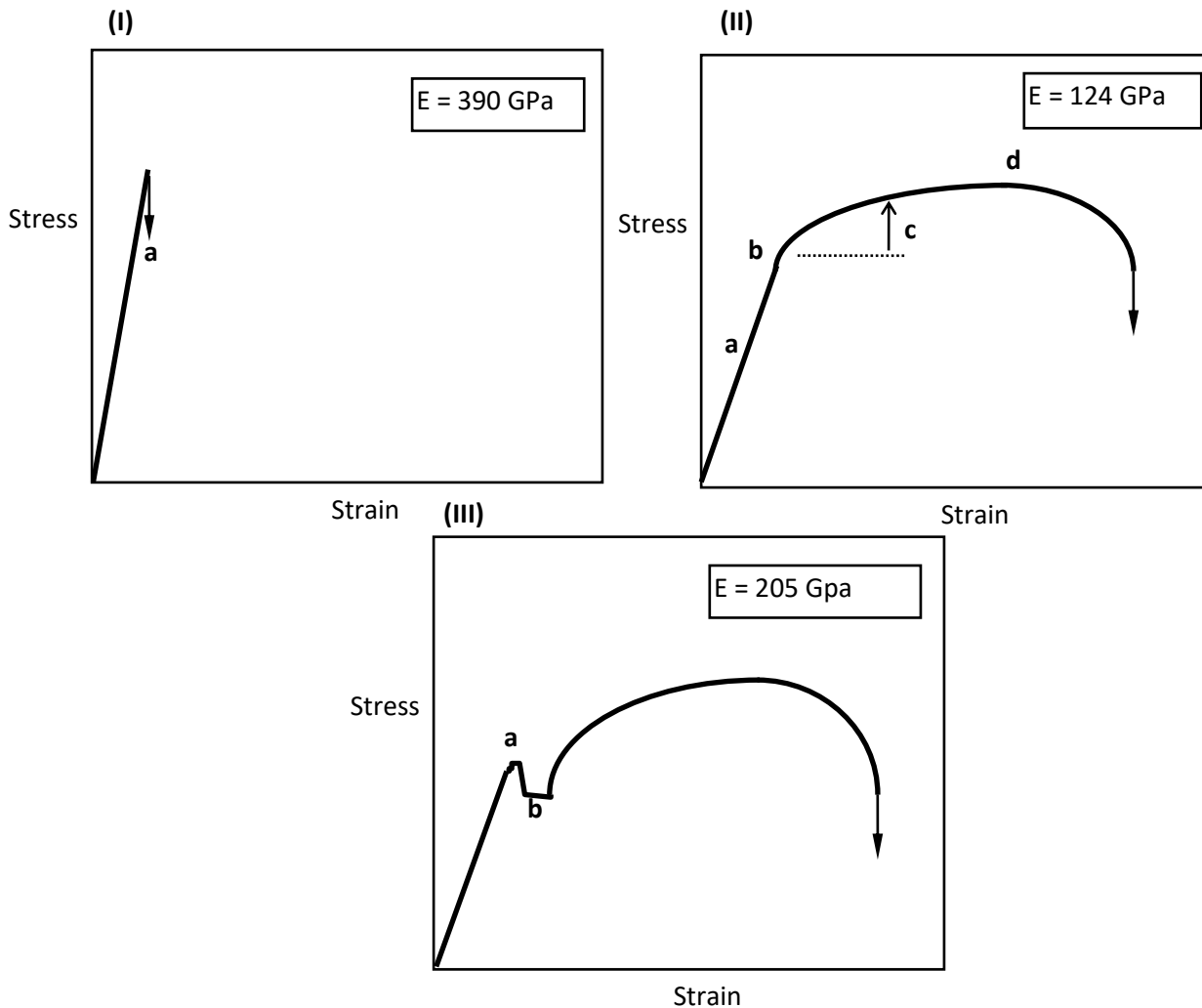
The elongation can be calculated from the Load x Displacement curve. If we consider $l_f=33\text{mm}$ then

$$\%EL = \frac{l_f - l_0}{l_0} \times 100 = \frac{(70 + 33) - 70}{70} \times 100 = 47.1\%$$

Question 6

Describe in detail the main features of the stress-strain curves shown in the following figures at the key points labelled a,b,c etc.

Using the information given suggest the material that each curve might belong to?

**Solution:**

I) This stress-strain curve represents a linear elastic material (i.e. no plastic deformation). (a) point represents fracture. This is a typical mechanical behavior of a brittle material such as a ceramic

II) Ductile metal. a: elastic deformation; b: yielding; c: plastic deformation; d: tensile strength and the onset of necking – a ductile material such as copper

III) Ductile metal with a clear yield. a: upper yield point; b: lower yield point - steel