

Tabulation of Error Function Values

$z$	$\text{erf}(z)$	$z$	$\text{erf}(z)$	$z$	$\text{erf}(z)$
0	0	0.55	0.5633	1.3	0.9340
0.025	0.0282	0.60	0.6039	1.4	0.9523
0.05	0.0564	0.65	0.6420	1.5	0.9661
0.10	0.1125	0.70	0.6778	1.6	0.9763
0.15	0.1680	0.75	0.7112	1.7	0.9838
0.20	0.2227	0.80	0.7421	1.8	0.9891
0.25	0.2763	0.85	0.7707	1.9	0.9928
0.30	0.3286	0.90	0.7970	2.0	0.9953
0.35	0.3794	0.95	0.8209	2.2	0.9981
0.40	0.4284	1.0	0.8427	2.4	0.9993
0.45	0.4755	1.1	0.8802	2.6	0.9998
0.50	0.5205	1.2	0.9103	2.8	0.9999

**Problem 1**

Nitrogen from a gaseous phase is to be diffused into pure iron. If the surface concentration is maintained at 0.2 wt. % N, what will be the concentration at 0.3 mm from the surface after 5 hours? The diffusion coefficient for N in Fe is  $2.5 \times 10^{-11} \text{ m}^2/\text{sec}$ .

$C_s = 0.2 \text{ wt.\% N}$      $C_0 = 0$      $x = 0.3 \text{ mm}$      $t = 5 \text{ hrs}$

$$\frac{C_x - C_0}{C_s - C_0} = 1 - \text{erf} \left( \frac{x}{2\sqrt{Dt}} \right)$$

$$\frac{C_x}{0.2} = 1 - \text{erf} \left[ \frac{0.3 \times 10^{-3} \text{ m}}{2\sqrt{2.5 \times 10^{-11} \text{ m}^2/\text{sec} \cdot 5 \text{ hrs} \cdot 3600 \text{ sec/hr}}} \right]$$

$\frac{C_x}{0.2} = 1 - \text{erf}(0.22)$

From table	$z$	$\text{erf}(z)$
	0.20	0.2227
	0.22	x
	0.25	0.2763

$$\frac{C_x}{0.2} = 1 - 0.244$$

$\Rightarrow \boxed{C_x = 0.15 \text{ wt.\% N}}$     Linear interpolation

$$\frac{x - 0.2227}{0.22 - 0.20} = \frac{0.2763 - 0.2227}{0.25 - 0.20}$$

**Problem 2**

The fraction of vacancies in a metal at  $800^{\circ}\text{C}$  is  $2.86 \times 10^{-4}$ . What is the fraction of vacancies at  $1100^{\circ}\text{C}$ ?

$$n_v = 2.86 \times 10^{-4} \text{ at } 800^{\circ}\text{C} = 1073\text{K}$$

$$n_v = \exp\left(\frac{-Q}{RT}\right) = 2.86 \times 10^{-4} = \exp\left(\frac{-Q}{8.62 \times 10^{-5} \frac{\text{eV}}{\text{atomK}} \cdot 1073\text{K}}\right)$$

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

$$\text{At } 1100^{\circ}\text{C} = 1373\text{K}$$

$$n_v = \exp\left[\frac{-0.75}{8.62 \times 10^{-5} \cdot 1373}\right] \Rightarrow \boxed{n_v = 1.7 \times 10^{-3}}$$

**Problem 3**

An alloy contains 30 wt.% zinc and 70 wt.% copper. What is the concentration of Zn (in atoms of Zn/m<sup>3</sup>) in the alloy?

DATA:  $A_{Cu} = 63.55 \text{ gm/mole}$ ,  $A_{Zn} = 65.41 \text{ gm/mole}$ ,  $\rho_{Cu} = 8.94 \text{ gm/cm}^3$ ,  $\rho_{Zn} = 7.13 \text{ gm/cm}^3$

30 wt% Zn      70 wt% Cu

$$N_{Zn} = \frac{N_A C_{Zn}}{\frac{C_{Zn} A_{Zn}}{\rho_{Zn}} + \frac{A_{Zn}}{\rho_{Cu}} (100 - C_{Zn})}$$

$$N_{Zn} = \frac{6.02 \times 10^{23} \frac{\text{atoms}}{\text{mole}} \cdot 30 \text{ wt}\%}{\frac{(30 \text{ wt}\%) (65.41 \frac{\text{gm}}{\text{mole}})}{7.13 \frac{\text{gm}}{\text{cm}^3}} + \frac{(65.41 \frac{\text{gm}}{\text{mole}}) (70 \text{ wt}\%)}{8.94 \frac{\text{gm}}{\text{cm}^3}}} = \boxed{2.29 \times 10^{22} \frac{\text{atoms}}{\text{cm}^3}} \\ = 2.29 \times 10^{28} \frac{\text{atoms}}{\text{m}^3}$$

**Problem 4**

Lithium has an atomic radius of 0.152 nm, a density of 0.534 gm/cm<sup>3</sup> and atomic weight,  $A_{Li} = 6.94$  gm/mole. Determine if the structure is BCC or FCC.

$$r = 0.152 \text{ nm} \quad \rho = 0.534 \text{ gm/cm}^3 \quad A_{Li} = 6.94 \text{ gm/mole}$$

$$\rho = \frac{n A_{Li}}{V_c N_A} \quad V_{c_{FCC}} = a_{FCC}^3 = (2r\sqrt{2})^3 \quad n=4$$
$$V_{c_{BCC}} = a_{BCC}^3 = \left(\frac{4r}{\sqrt{3}}\right)^3 \quad n=2$$

For FCC

$$\rho = \frac{4 (6.94 \text{ gm/mole})}{(2 \times 0.152 \times 10^{-7} \text{ cm} \sqrt{2})^3 \cdot 6.02 \times 10^{23} \frac{\text{atoms}}{\text{mole}}} = 0.58 \frac{\text{gm}}{\text{cm}^3}$$

For BCC

$$\rho = \frac{2 \text{ atoms} (6.94 \text{ gm/mole})}{\left(\frac{4 \times 0.152 \times 10^{-7} \text{ cm}}{\sqrt{3}}\right)^3 \cdot 6.02 \times 10^{23} \frac{\text{atoms}}{\text{mole}}} = 0.533 \frac{\text{gm}}{\text{mole}}$$

$\Rightarrow$  BCC

**Problem 5**

Put your answer in the boxes to the right.

(answer)

<p>An x-ray diffraction pattern from a FCC crystal has a peak at <math>2\theta = 45^\circ</math> that is indexed to the (111) plane. What is the lattice parameter? The x-ray wavelength = 0.154 nm.</p> <p>(a) 0.201 nm (b) 0.348 nm (c) 0.189 nm (d) none of the above</p>	b
<p>The grain size of a material can be determined by:</p> <p>(a) optical microscopy (b) x-ray diffraction (c) the density (d) all of the above</p>	a
<p>A metallic bond forms by the:</p> <p>(a) formation of an electron cloud surrounding the atoms (b) sharing of electrons between the atoms (c) transfer of an electron from one atom to the other (d) none of the above</p>	a
<p>A close packed plane in the BCC structure is the:</p> <p>(a) <math>(\bar{1}01)</math> (b) (001) (c) <math>(\bar{1}11)</math> (d) none of the above</p>	a
<p>T/F Steady state diffusion occurs when the concentration gradient changes with the diffusion time.</p>	F

$$2d_{hkl} \sin \theta_{hkl} = n\lambda \quad n = 1$$

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

$$\frac{2a}{\sqrt{1^2 + 1^2 + 1^2}} \sin(22.5^\circ) = 0.154 \text{ nm}$$

$$a = 0.348 \text{ nm}$$