HW 1	**Inorganic Materials Chemistry**	**Name:**	
Points:	**C7780**	**Date:**	
Max. 100 points	**Fall 2017**	**A**	

1. (35 pts) Application of Fick's Second Law of Diffusion (Non-Steady-State Diffusion) to diffusion of carbon into iron:

$$\frac{d\,C_x}{d\,t} = \frac{d}{d\,x}\left(D\frac{d\,C_x}{d\,x}\right)$$

The rate of change of composition at position x with time, t, is equal to the rate of change of the product of the diffusivity, D, times the rate of change of the concentration gradient, dC_x/dx, with respect to distance, x.
Consider diffusion from a surface where the concentration of diffusing species is always constant into a material volume. This solution applies to gas diffusion into a solid as in carburization of steels or doping of semiconductors.

Boundary Conditions
For $t = 0$, $C = C_o$ at $0 < x$
For $t > 0$ $C = C_s$ at $x = 0$ and $C = C_o$ at $x = \infty$

Solution:

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

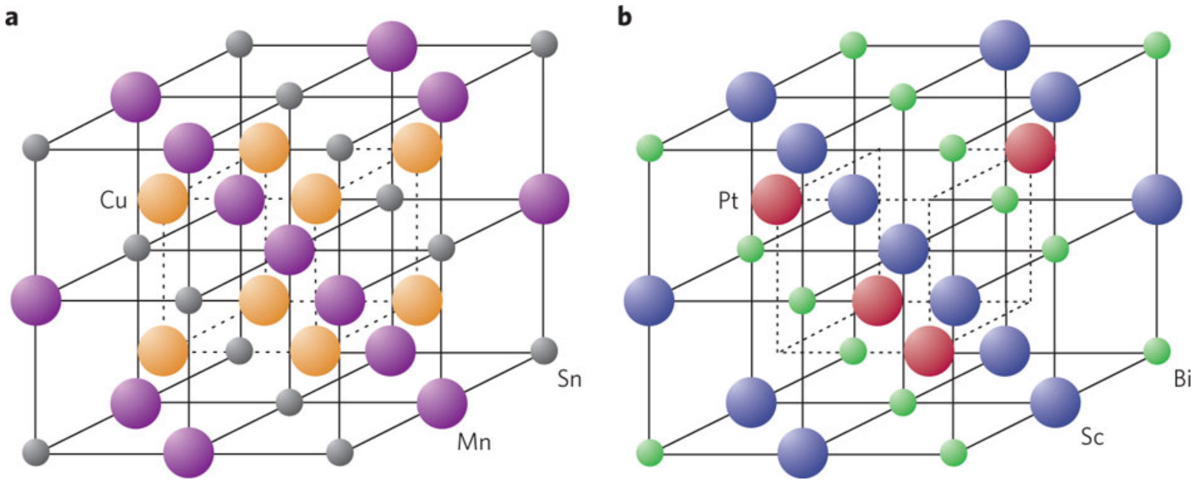
where C_s = surface concentration
C_o = initial uniform bulk concentration
C_x = concentration of element at distance x from surface at time t
x = distance from surface
D = diffusivity of diffusing species in host lattice
t = time
erf = error function

TABLE 5.1 Tabulation of Error Function Values

z	*erf*(*z*)	*z*	*erf*(*z*)	*z*	*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

To harden the surface of steel above that of its interior may be accomplished by increasing the surface concentration of carbon in a process termed carburizing; the steel piece is exposed, at an elevated temperature, to an atmosphere rich in a hydrocarbon gas, such as methane (CH_4). Consider one such alloy that initially has a uniform carbon concentration of 0.25 wt% and is to be treated at 950 °C. If the concentration of carbon at the surface is suddenly brought to and maintained at 1.20 wt%, how long will it take to achieve a carbon content of 0.80 wt% at a position 0.5 mm below the surface? The diffusion coefficient for carbon in iron at this temperature is $1.6\ 10^{-11}\ m^2/s$; assume that the steel piece is semi-infinite.

2. (10 pts) Give stoichiometric formulas for the cubic structures in the picture below. **a** = Heusler compound, **b** = Half-Heusler compound.



3. (20 pts) $CaWO_4$ has the scheelite structure where the W^{6+} ions are tetrahedrally coordinated. Use the bond valence rules (Second Pauling's Rule) to decide if the WO_4 tetrahedra share corners, i.e. oxygens are bridging, or the WO_4 tetrahedra are isolated, i.e. oxygens are terminal. Show your bond strength calculation.

4. (35 pts) $FeTiO_3$ (mineral Ilmenite) possesses the **corundum** structure – an hcp array of oxides with cations filling 2/3 of octahedral holes. Use the bond valence rules (Second Pauling's Rule) to decide which oxidation states are present: Fe(II) Ti(IV) or Fe(III) Ti(III).

Bond Distances (d_{exp}, Å)	Tabulated reference values	Constants
Fe–O = 3×2.07 and 3×2.20	R_0(Fe–O) = 1.795 Å	b = 0.30
Ti–O = 3×1.88 and 3×2.09	R_0(Ti–O) = 1.815 Å	b = 0.37

Check for oxygen valence (what is the coordination number of O?): each oxygen is bound to Fe and Ti with both bond distances.