Exercise for the Lecture on Materials Science

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Exercise Sheet 2

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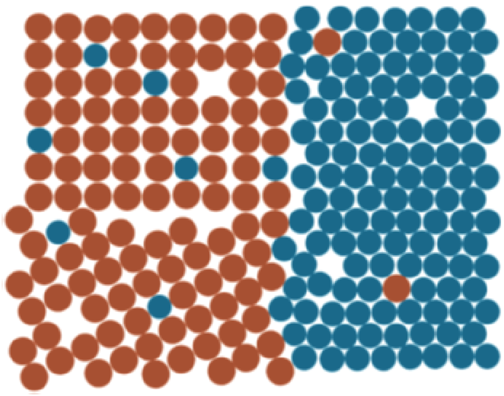
Problem 1: Defects

1. Calculate the fraction of vacancies in lead (Pb) at its melting temperature of 327 °C (600 K). Use a vacancy formation energy of $Q_v = 0.55\,\mathrm{eV}$.

2. Calculate the vacancy formation energy Q_v in aluminum, assuming that the number of vacancies N_V at 500 °C (773 K) is $7.57 \times 10^{23}\,\mathrm{m}^{-3}$.
   The molar mass and density (at 500 °C) for aluminum are $26.98\,\mathrm{g/mol}$ and $2.62\,\mathrm{g/cm}^3$.

3. Consider the schematic structure shown below. Are the following statements true or false? Justify your answers!



   (a) Two phases are visible, each consisting of two components.
   (b) The red phase has a higher vacancy concentration than the blue phase.
   (c) The red structure contains seven interstitial atoms.
   (d) Only one phase boundary is shown.
   (e) Three grain boundaries are shown.

Problem 2: Solid Solutions

Using the following table name the elements you would expect to form

1. a substitutional solid solution, and
2. an interstitial solid solution

with copper (Cu). Justify your answer!

Element	Atomic Radius (nm)	Crystal Structure	Electronegativity	Valency
Cu	0.1278	fcc	1.9	+2
C	0.071		2.55	+4
H	0.046		2.2	+1
O	0.060		3.44	-2
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

Problem 3: Steady-State Diffusion: Fick's First Law

The principles of diffusion form the basis for thermochemical processes such as nitriding, in which nitrogen is introduced into the edge zone of iron-based materials. Nitriding and nitrocarburising (with the addition of C) are used for the targeted improvement of wear resistance, hardness, mechanical strength and corrosion resistance.

A 1.5 mm thick steel sheet is exposed to a nitrogen atmosphere at 1200 °C. At this temperature, the diffusion coefficient for nitrogen in steel is $6.0 \times 10^{-11}\,\mathrm{m^2/s}$, and the diffusion flux density is $1.2 \times 10^{-7}\,\mathrm{kg/(m^2 \cdot s)}$.

Additionally, the nitrogen concentration at the surface of the steel sheet is $4\,\mathrm{kg/m^3}$. Determine the depth at which the nitrogen concentration in the steel sheet falls to $2.0\,\mathrm{kg/m^3}$, assuming a linear concentration profile.

Problem 4: Non-Steady-State Diffusion: Fick's Second Law

1. Determine the carburizing time required to achieve a carbon concentration of 0.45 % at a position of 2 mm in an iron-carbon alloy that initially contains 0.20 % C. The surface concentration is to be maintained at 1.30 % C, and the treatment is carried out at 1000 °C. The activation energy for diffusion is $Q_D = 148\,\mathrm{kJ\,mol^{-1}}$, and the temperature-independent pre-exponential factor is $D_0 = 2.3 \times 10^{-5}\,\mathrm{m^2\,s^{-1}}$. Use the error function data provided below (erf).

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

2. For a steel alloy, a 10-hour carburizing treatment increases the carbon concentration at a distance of 2.5 mm to 0.45 wt%. Estimate the time required to reach the same concentration at a depth of 5 mm under identical conditions.

Problem 5: Activation Energy

The measured self-diffusion coefficients for an aluminum sample are listed below. Plot the data appropriately to determine the activation energy.

T (°C)	50	100	150	200	250	300	350	400
D ($\mathrm{nm^2/s}$)	4×10^{-7}	2×10^{-4}	5×10^{-3}	5×10^{-2}	1.1	19	210	1620