Project No.1

Modelling of Diffusion and the Kirkendall effect!

Ref.

Phase Transformations in Metals and Alloy, Porter & Easterling Ch.2

Stability of microstructure in metallic systems, Martin, Doherty and Cantor, pp. 28-40

Theoretical basis:

Fick's 2. Law of diffusion

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial c}{\partial x} \right)$$

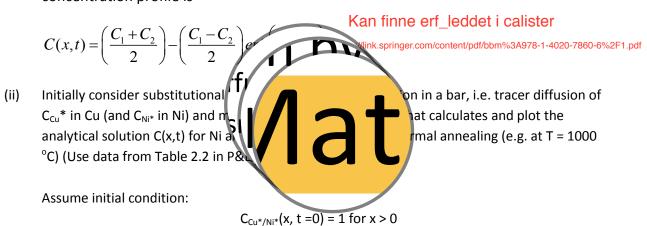
If D independent of concentration(/position)

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

Part I: Substitutional-self diffusion ("tracer diffusion")

(i) Consider two "semi-infinite" bars of different initial composition C_1 and C_2 , which are joined at x = 0, and annealed after welding:

Assume 1-D diffusion (diffusion only along bar(s)). Derive from Fick's 2 law and by using the relevant boundary conditions that the relevant solution for the concentration profile is



 $C_{Cu^*/Ni^*}(x, t = 0) = 0 \text{ for } x < 0$

Calculate and plot the concentration gradient for the range [-1:+1] mm after 30 hrs.

(i) Implement a numerical solution using <u>finite</u> differences and compare with the analytical solution!

Mind the choice of time step and spatial discretization to avoid numerical instabilities!

Basis for calculations: Length of bar (diffusion couple); I = 2 mm.

What are the appropriate boundary conditions at the ends of the bar?

(ii) Extend the numerical solution to account for non-isothermal annealing. Assume a linear temperature profile between T = $700\,^{\circ}$ C and T = $1000\,^{\circ}$ C (e.g. heating $10\,^{\circ}$ K/hr) and redo the calculations for Cu. What changes has to be made to your code?

Compare with the results above.

"Initial Home work":

(i) Derive from Fick's 2 law and by using the relevant boundary conditions that the relevant solution for the concentration profile is (or alt. just confirm by substitution in Fick's 2 law that the relevant solution is

$$C(x,t) = \left(\frac{C_1 + C_2}{2}\right) - \left(\frac{C_1 - C_2}{2}\right) erf\left(\frac{x}{2\sqrt{Dt}}\right)$$

- (ii) Find from literature appropriate values for D_0 and Q to calculate the diffusion coefficient as a function of T (D(T)
- (iii) Identify (from literature/internet) an appropriate (explicit) "Finite Difference scheme" to use for the calculations!
- (iv) Identify (if appropriate) the relevant stability requirement (i.e. conditions for choice of Δt and Δx (spatial resolution)?
- (v) What are appropriate boundary conditions at the end of the bar?

Part II: Substitutional diffusin in Cu/Ni diffusion couple (Kirkendall-effect):

Darkens equations:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left(\tilde{D} \frac{\partial C}{\partial x} \right)$$

$$\tilde{D} = X_B D_A + X_A D_B$$

$$v = (D_A - D_B) \frac{\partial X_A}{\partial x}$$

Generalized diffusion equation:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left(\tilde{D} \frac{\partial C}{\partial x} \right)$$

Interdiffusion coefficient

$$\tilde{D} = X_B D_A + X_A D_B$$

Assume in this case a diffusion couple with initial condition:

$$C_{Cu}(x, t = 0) = 1 (C_{Ni}(x, t = 0) = 0 \text{ for } x > 0$$

$$C_{Cu}(x, t = 0) = 0 (C_{Ni}(x, t = 0) = 1 \text{ for } x < 0$$

Tasks:

- (i) Use data from Fig. 2.21 in Porter&Easterling and calculate and plot \tilde{D} , D_A , D_B as a function of alloy composition (X_A)! Assume a log-linear dependency on concentration.
- (ii) Consider the necessary changes that has to be made to the finite difference scheme used above (search the internet and/or other literature)!
- (iii) Calculate the diffusion profile (afo postion and time) across the Cu-Ni diffusion couple (cf. Fig. 2.3 in Martin, Doherty & Cantor)!
- (iv) Calculate the flux of Cu and Ni atoms, respectively across the diffusion couple (i.e. $J_{Cu}(x)$ and $J_{Ni}(x)$; cf. Eqs. 2.39, 2.40 Porter&Easterling)
 - Calculate the velocity with which the lattice plane(s) migrate, v_{KS-plane}(x) (Eq. 2.47).
 - Estimate /calculate the total amount of Cu (or Ni) that has diffused across the (initial) midplane of the diffusion couple after ~300 hrs!

The graphs in part (iii) should preferably be displayed for different times between start and stop ($\sim 300 \text{ hrs}$)!