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

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

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https://link.springer.com/content/pdf/bbm%3A978-1-4020-7860-6%2F1.pdf

(ii) Initially consider substitutional self-diffusion by tracer diffusion in a bar, i.e. tracer diffusion of C_{Cu}* in Cu (and C_{Ni*} in Ni) and make a small Matlab-program that calculates and plot the analytical solution C(x,t) for Ni and Cu, respectively, for isothermal annealing (e.g. at T = 1000 ^{o}C) (Use data from Table 2.2 in P&E!).

Assume initial condition:

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

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

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

while loop

(i) Implement a numerical solution using finite 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); l = 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 ^{o}C and T = 1000 ^{o}C (e.g. heating 10 ^{o}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:

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

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

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

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:

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

$C_{Cu}(x, t=0) = 0$ ($C_{Ni}(x, t=0) = 1$ 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, $v_{KS\text{-}plane}(x)$ (Eq. 2.47).
- Estimate /calculate the total amount of Cu (or Ni) that has diffused across the (initial) mid-plane of the diffusion couple after ~300 hrs!

The graphs in part (iii) should preferably be displayed for different times between start and stop (~ 300 hrs)!