

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

$$C(x,t) = \left( \frac{C_1 + C_2}{2} \right) - \left( \frac{C_1 - C_2}{2} \right) e^{-\frac{x^2}{4Dt}}$$

Kan finne erf\_leddet i calister

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

- (ii) Initially consider substitutional diffusion of Cu in a bar, i.e. tracer diffusion of  $C_{Cu}^*$  in Cu (and  $C_{Ni}^*$  in Ni) and numerically calculate and plot the analytical solution  $C(x,t)$  for Ni and Cu after thermal annealing (e.g. at  $T = 1000^\circ\text{C}$ ) (Use data from Table 2.2 in P&E).

Assume initial condition:

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

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

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

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);  $l = 2 \text{ mm}$ .

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  $T = 700 \text{ }^\circ\text{C}$  and  $T = 1000 \text{ }^\circ\text{C}$  (e.g. heating  $10 \text{ }^\circ\text{K/hr}$ ) 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

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

- (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  $\Delta t$  and  $\Delta x$  (spatial resolution)?
- (v) What are appropriate boundary conditions at the end of the bar?

## Part II: Substitutional diffusion 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:

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

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

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 position 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.  $J_{\text{Cu}}(x)$  and  $J_{\text{Ni}}(x)$ ; cf. Eqs. 2.39, 2.40 Porter&Easterling)  
- **Calculate the velocity with which the lattice plane(s) migrate,  $v_{\text{KS-plane}}(x)$  (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)!**