MM3110 : Computational Materials Engineering Lab
Session dated 11-Sep-2017
Illustation of uphill diffusion

Task: Consider a 1D domain and show how uphill diffusion takes place with appropriate value of regular solution parameter.

Let us consider a very dilute solute with a concentration C_i, atom fraction x_i and a chemical potential in the solution phase μ_i. Subscripts for evolution equation are omitted for simplicity. M is the mobility of the species under consideration.

Use modified Fick's law for diffusion of solute as:

$$\vec{J} = -M\vec{\nabla}\mu$$

Fick's second law:

$$\frac{\partial C}{\partial t} = M\nabla^2\mu$$

Take the excess Gibbs energy term for solution as $\Omega x_i(1 - x_i)$.

Chemical potential of a species i in a binary alloy can then be taken as:

$$\mu_i = \mu_i^0 + \Omega\,(1 - x_i)^2 + RT\,\ln\,(x_i)$$

Plot the phase separation for the case when Ω is positive. How does the G versus x_i plot look like at different temperatures? What is the critical temperature above which the solution has miscibility gap? For a temperature below the critical temperature, we need to show that diffusion is uphill.

For the purpose of converting compositions to atom fractions, use species as Cu and Ni with atomic weights as 63.5 and 58.6, respectively.

Watch out for the Neumann's stability criterion for 1D:

$$\frac{M\Delta t}{\Delta x^2} \leq 0.5$$

Take a step profile of initial concentration and show how it evolves with time to illustrate downhill and uphill diffusion regimes. Use finite difference method with explicit time marching scheme.