Phase Separation of a Binary Alloy

Phase Separation describes the change of a binary alloy from a uniform mixed state to that of a spatially seperated two phase structure. This change takes place, when the temperature is rapidly reduced below a critical temperature.

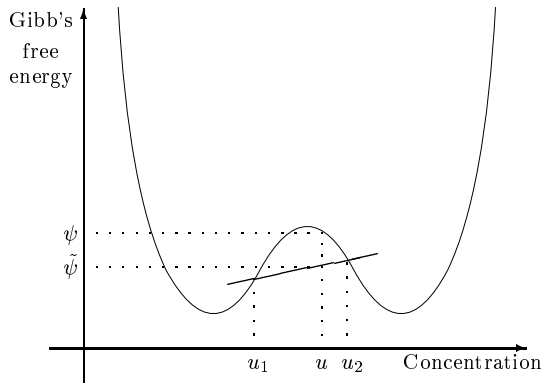

Figure 1: Gibb's free energies ψ and $\tilde{\psi}$ of a mixed state u and two phase structures u_1, u_2

Associated to this phenomenon is a Gibb's free energy ψ, which has the double well form shown in Figure 1. Comparing the Gibb's free energy of two phase structures with that of a mixed state leads to the phase diagram depicted schematically in Figure 2. The spinodal and the conodal line seperate stable, unstable and metastable concentrations.

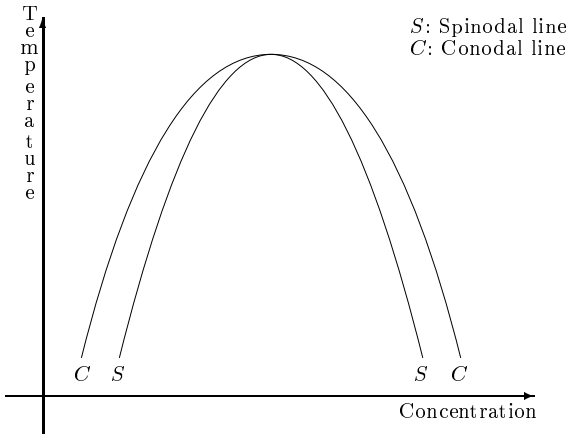

Figure 2: Phase diagram with spinodal line (S) and conodal line (C)

The mathematical model is due to Cahn and Hilliard:

$$\begin{aligned} \partial_t u &= \triangle w, \\ w &= \psi'(u) - \gamma \triangle u \end{aligned}$$

in $\Omega \subset I\!R^n$, $t > 0$, subject to the boundary conditions $\frac{\partial u}{\partial \nu} = \frac{\partial w}{\partial \nu} = 0$ on $\partial\Omega$ and initial condition $u(\cdot, 0) = 0$ in Ω, where u denotes the concentration, w the chemical potential and γ is a prescribed positive constant.

These equations can be studied numerically using a finite element method. The two and three dimensional computational studies are based on piecewise linear elements in space together with a Crank–Nicholson time discretization. This requires the solution of a nonlinear system of equations at each time step. To solve these equations a predictor–corrector method is used.