Cahn - Hilliard Equation

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1 Introduction

Aim

To derive the Cahn-Hilliard equation to model spinodal decomposition.

Strategy

- Treat Gibbs energy as a functional
- Derive the chemical potential for such a system
- Use Fick's law to understand the composition evolution

Assumptions

- The system has cubic symmetry
- The gibbs energy is a quadratic in c

Derivation

Gibbs energy formulation

The total Gibbs' energy of the system is given by,

$$F(x,y,z,c,\nabla c,\nabla^2 c) = \int f(c,\nabla c,\nabla^2 c)dV, \tag{1}$$

Expanding Gibbs' function using Taylor's approximation, we get

$$f = f(c) + \frac{\partial f}{\partial(\nabla c)_i}(\nabla c)_i + \frac{\partial f}{\partial(\nabla^2 c)_{ij}}(\nabla^2 c)_{ij} + \frac{1}{2!}\frac{\partial f}{\partial(\nabla c)_i \partial(\nabla c)_j}(\nabla c)_i(\nabla c)_j,$$

$$\alpha_i = \frac{\partial f}{\partial(\nabla c)_i},$$

$$\beta_{ij} = \frac{\partial f}{\partial(\nabla^2 c)_{ij}},$$

$$\gamma_{ij} = \frac{\partial f}{\partial(\nabla c)_i \partial(\nabla c)_j},$$

$$f = f(c) + \alpha_i(\nabla c)_i + \beta_{ij}(\nabla^2 c)_{ij} + \frac{1}{2}\gamma_{ij}(\nabla c)_i(\nabla c)_j,$$

Simplifying the third term in the above equation, we get,

$$\int \beta_{ij}(\nabla^2 c)_{ij} dV,$$

$$= \int \beta_{ij}\frac{\partial^2 c}{\partial x_i \partial x_j}dV,$$

$$= \int \beta_{ij}\frac{\partial}{\partial x_i}\Big(\frac{\partial c}{\partial x_j}\Big)dV,$$

$$= \Big[\beta_{ij}(\nabla c)_j\Big]_s - \int \frac{\partial \beta_{ij}}{\partial x_i}(\nabla c)_j dV,$$

$$= -\int \frac{\partial \beta_{ij}}{\partial c}(\nabla c)_i(\nabla c)_j dV,$$

$$f = f(c) + \alpha_i(\nabla c)_i + \left[\frac{\gamma_{ij}}{2} - \frac{\partial \beta_{ij}}{\partial c}\right](\nabla c)_i(\nabla c)_j,$$
$$f = f(c) + \alpha_i(\nabla c)_i + \kappa_{ij}(\nabla c)_i(\nabla c)_j,$$

Since, we assumed that the material has cubic symmetry, we can assume $\alpha_i = 0$ and $\kappa_{ij} = \kappa\delta_{ij}$ by invoking Neumann's principle.

Chemical Potential

$$\frac{\delta F}{\delta c} = \mu,$$
$$F = \int \Big[f(c) + \kappa(\nabla c)^2\Big] dV,$$
$$\frac{\delta F}{\delta c} = \frac{\partial f}{\partial c} - 2\kappa\nabla^2 c$$

Fick's Law

$$J = -M\nabla\mu,$$
$$\frac{\partial c}{\partial t} = -\nabla J,$$
$$\frac{\partial c}{\partial t} = M\nabla^2\mu,$$
$$\frac{\partial c}{\partial t} = M\nabla^2\Big(\frac{\partial f}{\partial c} - 2\kappa\nabla^2 c\Big),$$

Thus simplifying the above equation gives, Cahn-Hilliard Equation,

$$\frac{\partial c}{\partial t} = Mf''\nabla^2 c - 2\kappa M\nabla^4 c \tag{2}$$