

MSE-483 : Advanced Phase Transformations

Lecture 10 : Cahn-Hilliard equation

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Cahn – Hilliard equation (spinodal decomposition)

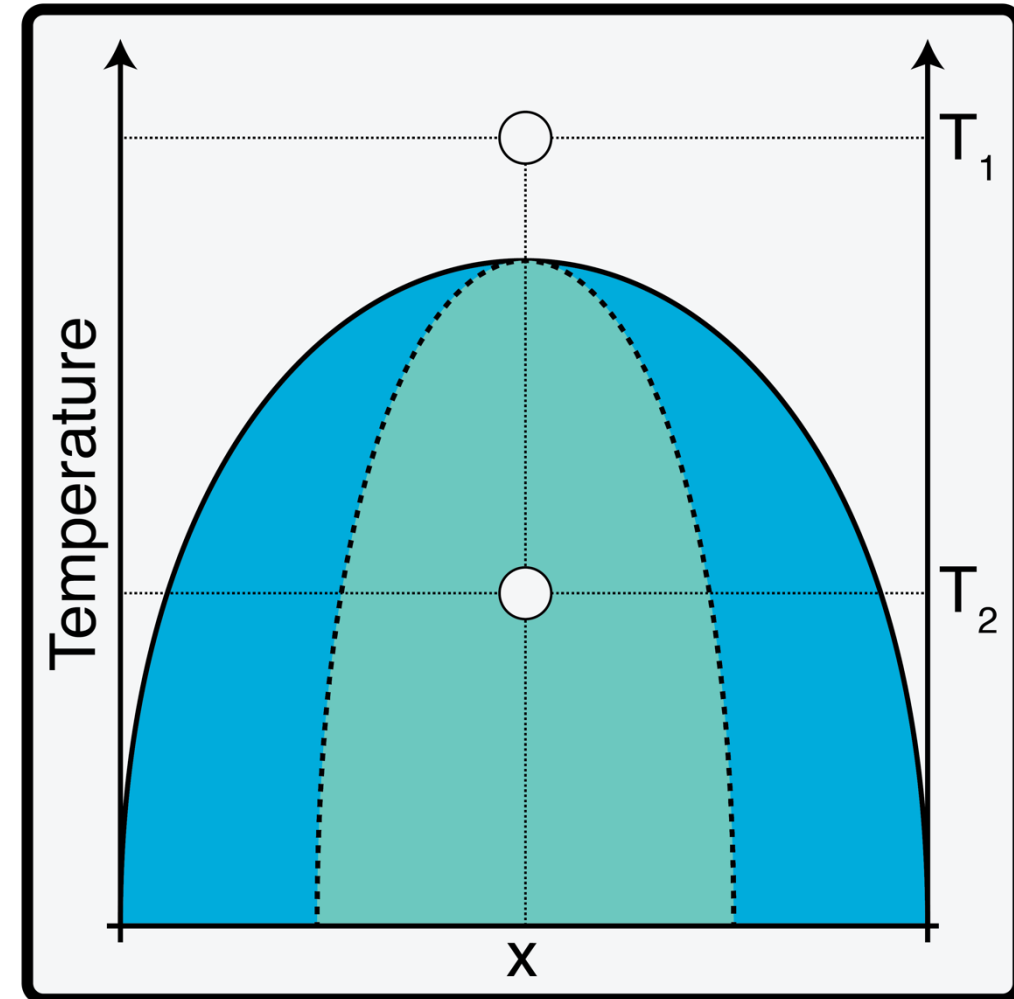
Total Free Energy :
$$G = \int \left(g(x_1, x_2, \dots, T) + \sum_{ijk} \alpha_{jk}^i \nabla_j x_i \nabla_k x_i \right) d^3 r$$

Evolution equations

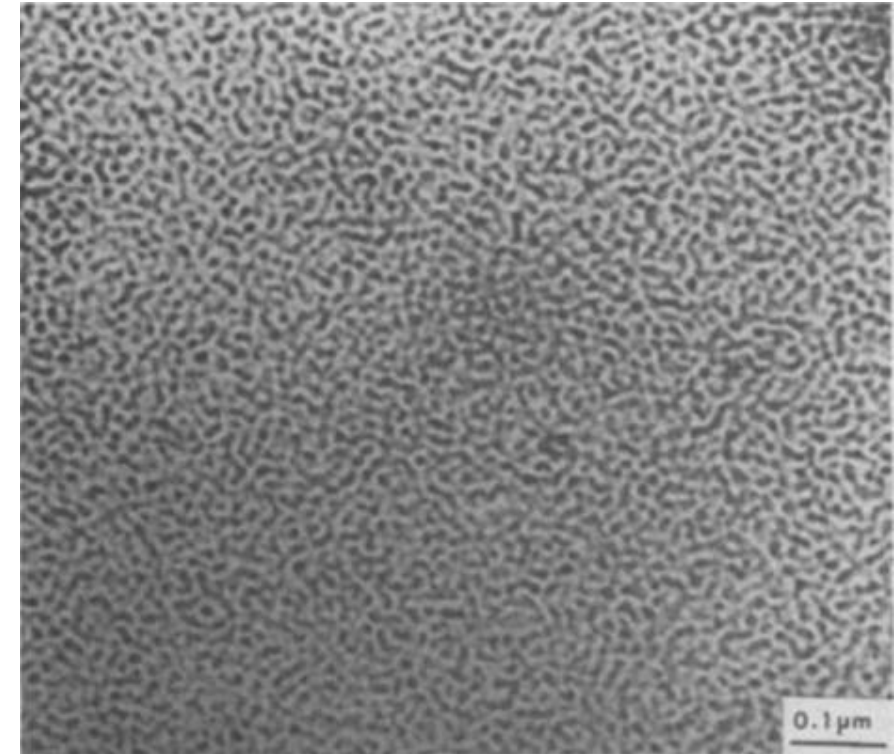
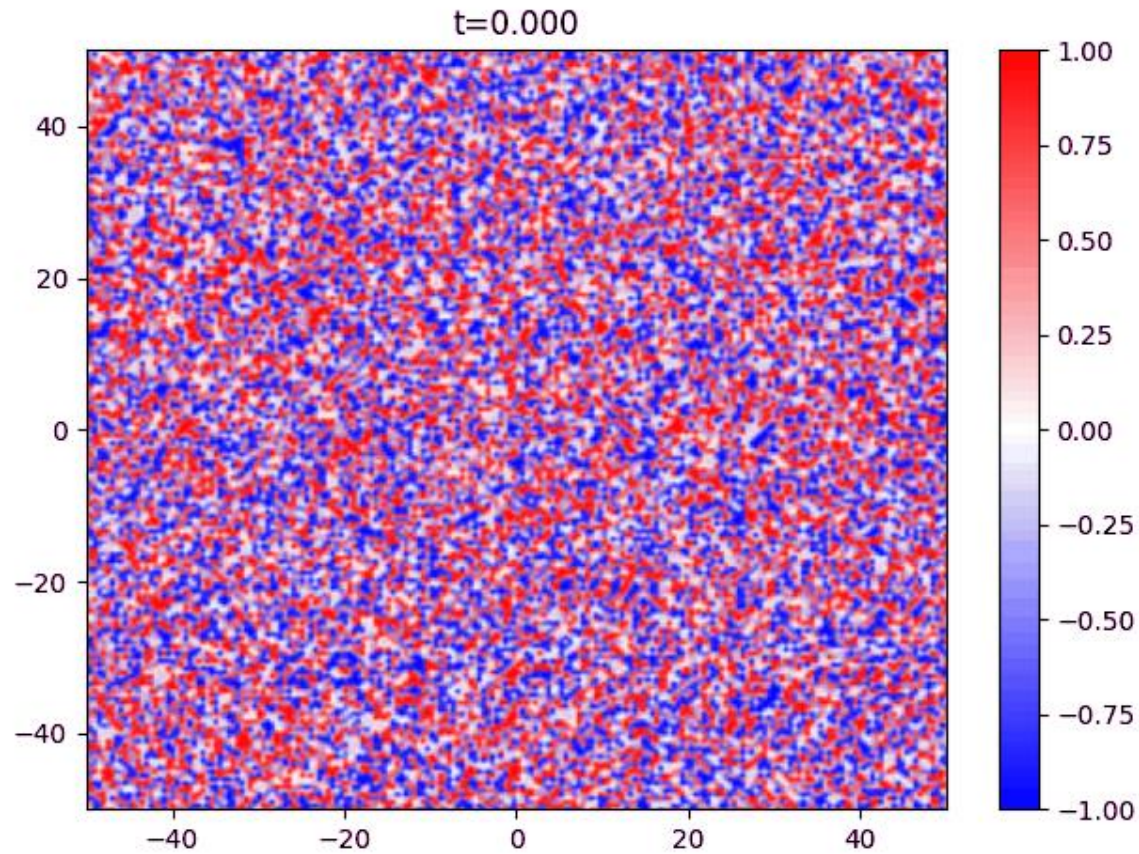
Cahn-Hilliard equation :
$$\frac{\partial c_i(\vec{r}, t)}{\partial t} = \nabla M_{ij} \nabla \frac{\delta G}{\delta c_j(\vec{r}, t)}$$

Inputs to the phenomenological models:

- Free energies
- Gradient energy coefficients
- Transport coefficients

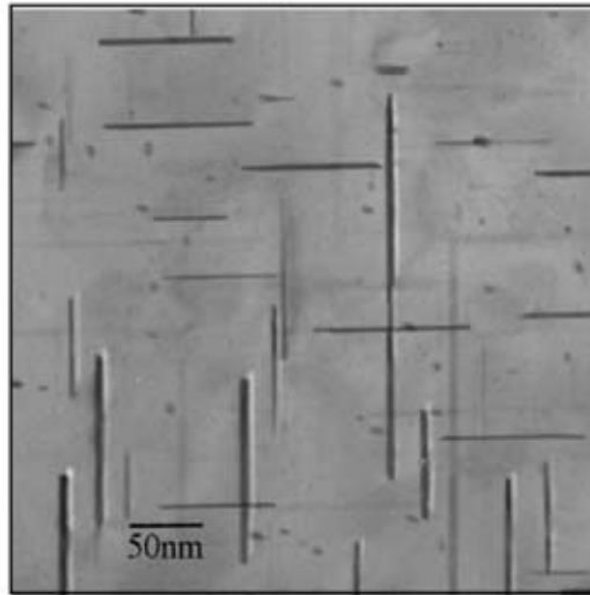
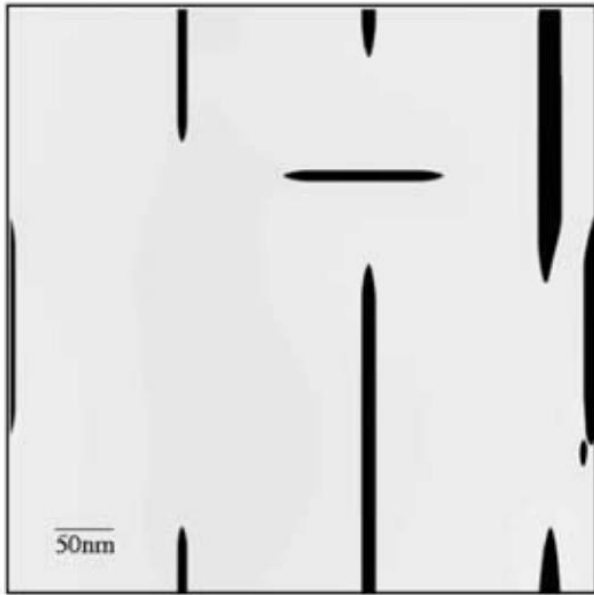


Microstructure simulation

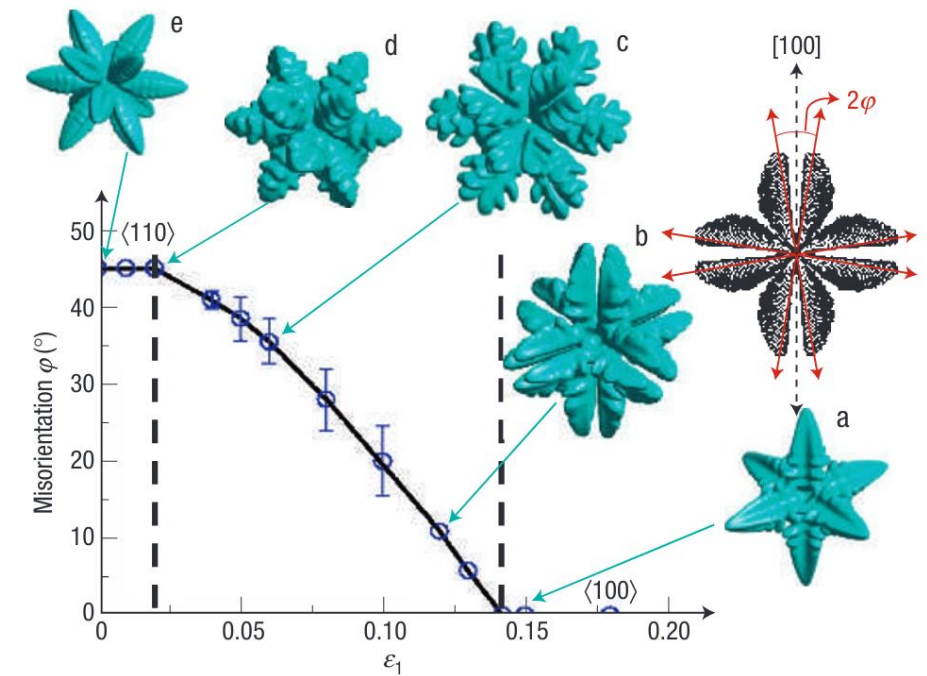


Some examples

Precipitation in an Al-Cu alloy



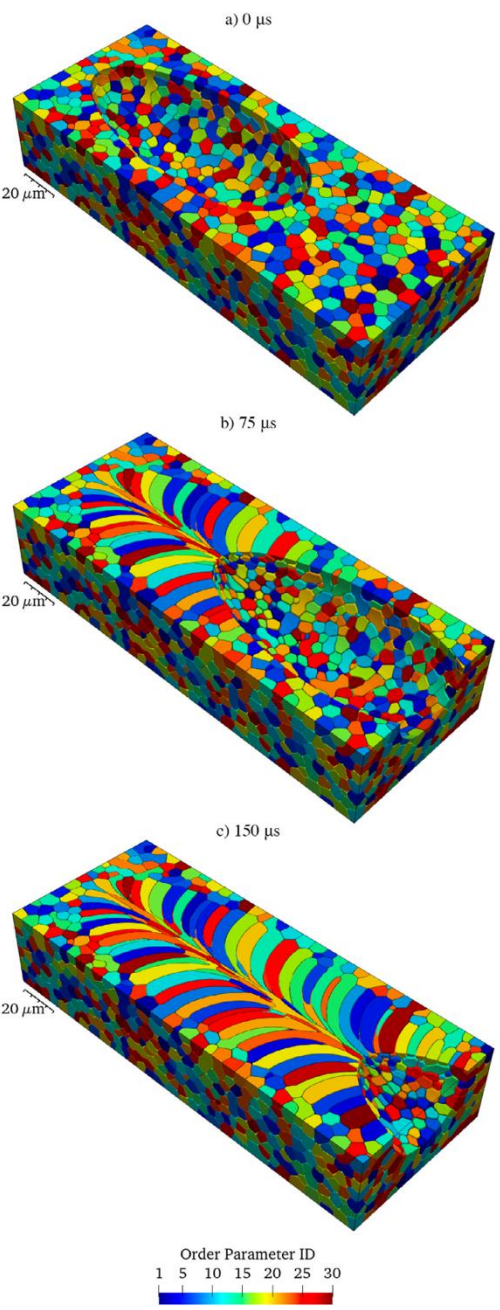
Solidification modeling



Vaithyanathan, V., Wolverton, C. & Chen, L. Q. Multiscale modeling of θ' precipitation in Al-Cu binary alloys. *Acta Materialia* 52, 2973–2987 (2004).

Haxhimali, T., Karma, A., Gonzales, F. & Rappaz, M. Orientation selection in dendritic evolution. *Nature Mater* 5, 660–664 (2006).

Some examples



Additive
manufacturing of
stainless steel

Phase field modeling of battery electrodes

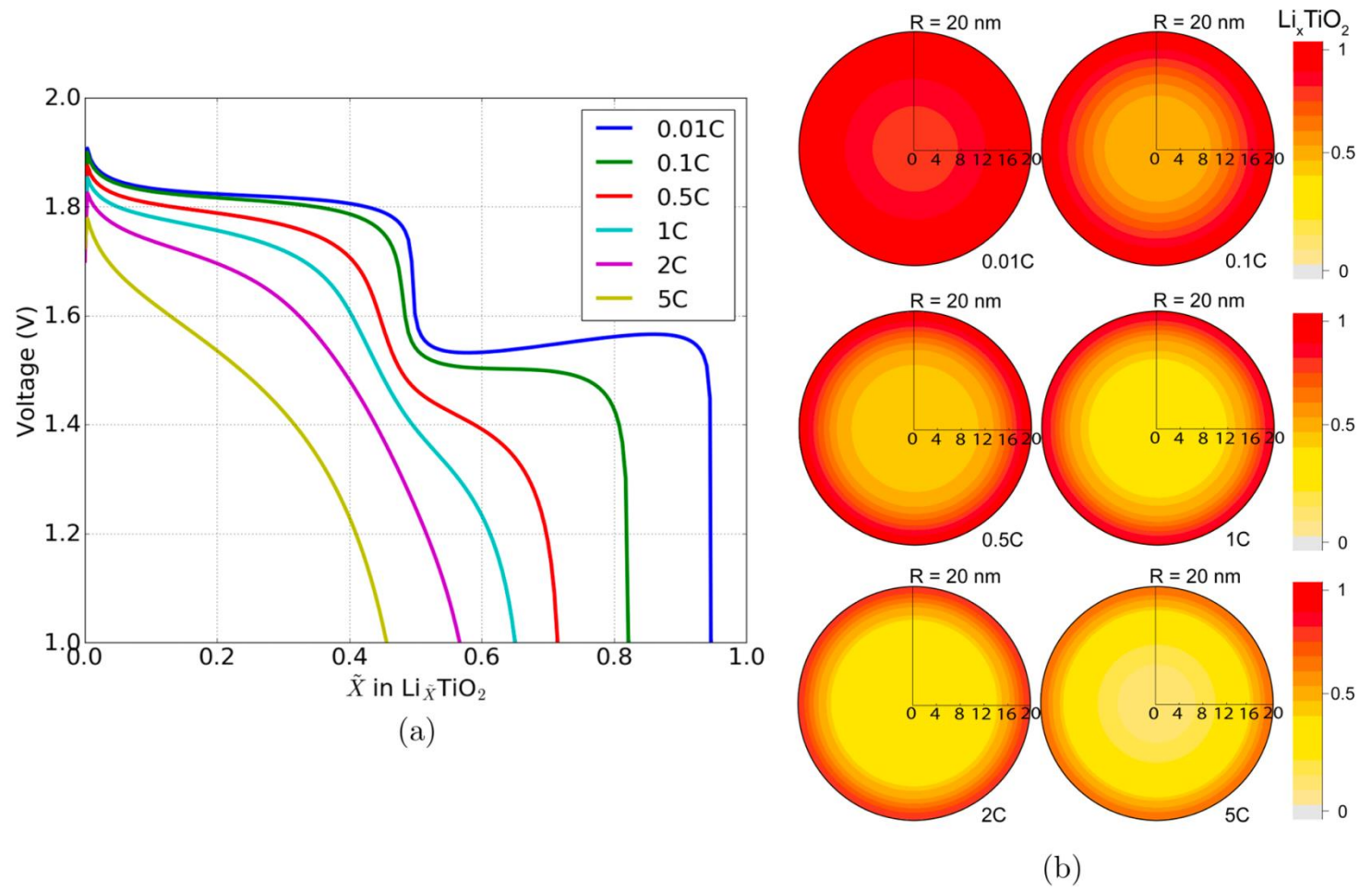


FIG. 3. (a) Voltages profiles vs average concentration ($\tilde{X}$) and (b) final concentration profiles in the particle at different C rates.

De Klerk, N. J. J., Vasileiadis, A., Smith, R. B., Bazant, M. Z. & Wagemaker, M. Explaining key properties of lithiation in TiO_2 -anatase Li-ion battery electrodes using phase-field modeling. *Phys. Rev. Materials* 1, 025404 (2017).
Chadwick, A. F. & Voorhees, P. W. The development of grain structure during additive manufacturing. *Acta Materialia* 211, 116862 (2021).