Friedrich-Alexander-Universität
Faculty of Engineering

Department Materials Science

WW8: Materials Simulation

Practical: Phase-Field Method

Basics and Application in Materials Science

Leon Pyka (22030137)

Supervision:

Contents

1 Introduction

Phase-field simulation is a versatile application in the toolbox of materials simulation. It is often used for simulations of phase transitions, dislocation evolution, fracture simulations etc. The following practicals aim is to get a practical introduction into the subject. In two separate tasks a 1D single-component solidification simulation, calculation of a bulk energy density coefficient and gradient energy density coefficient are going to be conducted.

2 Task 1: 1D Single-Component Solidification

To simulate a 1D single-component solidification we utilize the following energy density:

$$F = \int \left(f_0 \phi^2 (1-\phi)^2 + \frac{K_\phi}{2} |\nabla \phi|^2 \right) d\vec{r} \tag{1}$$

As soldification is a a non-conservative process, the kinetics are governed by the Allen-Cahn equation (for the homogeneous, isotropic case).

$$\frac{\partial \phi}{\partial t} = -L \frac{\delta F}{\delta \phi} \tag{2}$$

Here the functional derivative $\frac{\delta F}{\delta \phi}$ of an energy functional eq. 3a can be evaluated as eq. 3b.

$$F = \int f(\vec{r}, \phi, \nabla \phi) d\vec{r} \tag{3a}$$

$$\frac{\delta F}{\delta \phi} = \frac{\partial f}{\partial \phi} - \nabla \cdot \frac{\partial f}{\partial (\nabla \phi)} \tag{3b}$$

Solving the functional derivative from eq. 2 yields:

$$\frac{\delta F}{\delta \phi} = 2 f_0 \phi (1-\phi)^2 + 2 f_0 \phi^2 (\phi - 1) - K_\phi \nabla^2 \phi \Leftrightarrow \tag{4a}$$

$$\Leftrightarrow 2 f_0 (2\phi^3 - \phi^2 + \phi) - K_\phi \nabla^2 \phi \tag{4b}$$

Inserting the result into eq. 2 results in:

$$\frac{\partial \phi}{\partial t} = -L\Big[2f_0(2\phi^3 - \phi^2 + \phi) - K_\phi \nabla^2 \phi\Big] \tag{5}$$