1 Basics of the Multi-phase Field Model

In the multi-phase field model [?, ?], each microstructural constituent i, e.g. grain, is defined by a phase field variable ϕ_i. The value of the phase field variable represents the local fraction of the relevant constituent. Therefore, a constraint exists among the variables:

$$\sum \phi_i = 1 \tag{1}$$

Inside the constituent i, the value of ϕ_i is 1 while the values of other phase field variables is 0. The interface is a mixture of various constituents, within which there are at least two phase field variables whose value is between 0 and 1. Each constituent can be assigned a set of attributes, e.g. phase, crystallographic orientation and stored energy.

The phase field equations which describe the pair-wise interaction of adjacent constituents are given by:

$$\frac{\partial \phi_i}{\partial t} = \sum_{i \neq j} m_{ij} \left\{ \sigma_{ij} I_{ij} + \frac{\pi}{\eta} \sqrt{\phi_i \phi_j} \Delta G_{ij}^{driv} \right\} \tag{2}$$

with

$$I_{ij} = \left[\left(\phi_j \nabla^2 \phi_i - \phi_i \nabla^2 \phi_j \right) + \frac{\pi^2}{2\eta^2} \left(\phi_i - \phi_j \right) \right] \tag{3}$$

where I_{ij} is a generalized curvature term, m_{ij} and σ_{ij} are mobility and energy of the interface between i and j, η is the interface thickness and ΔG_{ij}^{driv} is the driving force.

The mobilities are assumed to obey an Arrhenius relationship, i.e.:

$$m_{ij} = m_{ij}^0 exp \left(\frac{Q_{ij}^m}{RT} \right) \tag{4}$$

where R is the ideal gas constant, T is the temperature, m_{ij}^0 is the pre-factor and Q_{ij}^m is the activation energy.

Solute diffusion occurs during austenite formation and the austenite-to-ferrite transformation in low-carbon steels. In the present approach, it is assumed that only the interstitial, i.e. carbon, can redistribute by long-range diffusion, which is described by:

$$\frac{dC^C}{dt} = \sum_i \left(\nabla \left(D_i^C \phi_i \nabla C_i^C \right) \right) \tag{5}$$

where D_i^C is carbon diffusivity in phase i, C_i^C is the carbon concentration in phase i and C^C is the local concentration given by:

The carbon diffusivity D_i^C obeys an Arrhenius relationship, given by:

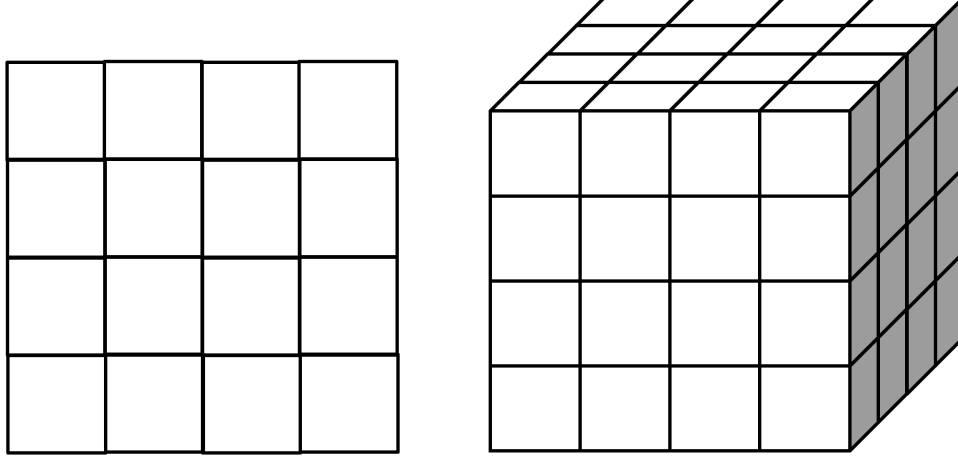$$D_i^C = D_i^{C0} exp \left(-Q_i^C / RT \right) \tag{6}$$

Figure 1: Schematic of the grid structure in the computational domain.

where D_i^{C0} is the pre-factor and Q_i^C is the activation energy.

In order to calculate the carbon concentration C_i^C and C_j^C within the interface, it is further assumed that the local redistribution between phases is described by

$$\frac{C_i^C}{C_j^C} = \frac{C_i^*}{C_j^*} \qquad (7)$$

where the paraequilibrium carbon concentration C_i^* is calculated with Thermo-Calc®.

2   Numerical Techniques

The phase field equations (Eq. 2) and diffusion equations (Eq. 5) are nonlinear partial differential equations (PDE). The finite difference method is used to solve the PDEs in a discretized computational domain. The computational domains used in this study are square in 2D and cubic in 3D. Thus the domain is simply discretized into a Cartesian grid having the same grid spacing Δx in all directions (Fig. 1). Periodic boundary conditions are assumed in the simulations using computer-constructed microstructures. Since experimental micrographs are used as the initial microstructures in the simulations of cyclic phase transformation, insulate boundary conditions are used, i.e. $\frac{\partial \phi_i}{\partial \mathbf{n}} = 0$ where $\mathbf{n}$ denotes the normal to the boundary.

A sparse data structure is used to store variables on each grid point, including the indice and values of non-zero phase field variables as well as local solute concentrations. The detailed description of the data structure can be found in [?].

Centered finite difference with the nearest neighbors (5-point stencil in 2D and 7-point stencil in 3D) is used to discretize the first and second derivatives. For example, the gradient and Laplacian of ϕ at grid point (i, j, k) in a 3D domain are given by:

$$\nabla \phi_{i,j,k} = \frac{\partial \phi_{i,j,k}}{\partial \mathbf{n}} = \left(\frac{\phi_{i+1,j,k} - \phi_{i-1,j,k}}{2\Delta x}, \frac{\phi_{i,j+1,k} - \phi_{i,j-1,k}}{2\Delta x}, \frac{\phi_{i,j,k+1} - \phi_{i,j,k-1}}{2\Delta x} \right) \tag{8}$$

and

$$\begin{aligned} \nabla^2 \phi_{i,j,k} &= \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} \\ &= \frac{\phi_{i+1,j,k} + \phi_{i-1,j,k} + \phi_{i,j+1,k} + \phi_{i,j-1,k} + \phi_{i,j,k+1} + \phi_{i,j,k-1} - 6\phi_{i,j,k}}{\Delta x^2} \end{aligned} \tag{9}$$

The Forward Euler method is used to implement the integration in the time domain for both phase field and diffusion equations, e.g.

$$\left(\frac{\partial \phi_i}{\partial t} \right)^t = \frac{\phi_i^{t+\Delta t} - \phi_i^t}{\Delta t} \tag{10}$$

where Δt is the time step, ϕ_i^t is the current value of ϕ_i, $\phi_i^{t+\Delta t}$ is the value for the next time step. The Forward Euler method is conditionally stable and requires the time step to fulfill the following constraint:

$$\Delta t < \Delta t_c = min \left(\frac{\Delta x^2}{2Dim \cdot max\left(m_{ij}\sigma_{ij} \right)}, \frac{\Delta x^2}{2Dim \cdot max\left(D_i^C \right)} \right) \tag{11}$$

where Dim is the domain dimensionality.