

# Simulation of lower bainitic transformation with the phase-field method considering carbide formation



M. Düsing, R. Mahnken\*

Chair of Engineering Mechanics, University of Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany

## ARTICLE INFO

### Article history:

Received 10 June 2015

Received in revised form 19 August 2015

Accepted 21 August 2015

### Keywords:

Phase-field

Bainite

Phase transformation

Diffusion

Cahn–Hilliard

Finite elements

## ABSTRACT

Lower bainite is a steel microstructure composed of austenite, ferrite and carbides within the ferrite. The transformation of austenite to lower bainite is one of the most complex transformations in steel. The carbon concentration of bainitic ferrite is of major importance for the carbide precipitation. A phase-field model to simulate the transformation of lower bainite including carbon diffusion and carbide formation is presented in this work. The model is based on a classical phase-field approach coupled with a viscous Cahn–Hilliard equation to simulate the separation of the carbon. During the isothermal simulation a sheaf of bainitic ferrite grows. The carbon starts to diffuse within the supersaturated ferrite which can only contain a fraction of the carbon which was stored in the austenite. At the accumulations of the carbon concentration carbides are precipitated. The simulations show successfully the described growth characteristics of the lower bainite transformation including carbide formation.

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## 1. Introduction

Bainite is a microstructure of steel that can be formed by heat treating. It can be built by continuous cooling or isothermal between the temperatures of perlite and martensite (250–550 °C). In materials science a distinction between upper bainite and lower bainite is made. Upper bainite forms at higher temperatures whereas lower bainite forms at temperatures closer to the martensite start temperature. The transformation always starts from austenite. At first bainitic ferrite sheaves grow from the borders of the grain. These sheaves consists of smaller sub-units. Within the supersaturated ferritic sheaf the carbon starts to diffuse, because ferrite can contain much less carbon than austenite [1]. In upper bainite the majority of the carbon partitions into austenite and precipitates as carbides where the concentration is high enough. At lower temperatures the diffusion is slower and most of the carbon cannot partition out of the ferrite. It starts to build accumulations and precipitates as carbides within the sheaf. This movement of the carbon within bainitic ferrite can be denoted as uphill diffusion. The resulting microstructure is lower bainite.

Due to its advantageous balance of strength and ductility, bainite has applications in the automotive industry, in highly loaded parts of the railway and in other divisions of engineering. Models to describe the formation of bainite can be helpful tools

to accelerate the development of new applications, because the transformation is a very time-consuming process.

In materials science the phase-field method is widely used to model diffusive/reconstructive transformations as well as displacive ones [2,3]. It is based on a system of partial differential equations which describes the growth of phases and can be derived from the Ginzburg–Landau equation [2]. The evolution of the so called order-parameters is modeled. At the interfaces of the phases the parameters vary continuously. Therefore the solution does not show sharp interfaces, but diffuse ones which can be governed by a thickness parameter. The advantage of this approach is that it is not necessary to track the interfaces.

Especially for steel there are many approaches describing the transformations austenite-to-ferrite [4,5], austenite-to-perlite [6], Widmanstätten formation [7], austenite-to-martensite [8,9] and others. Phase-field models with coupled diffusion equations exist, too [10]. However there are few phase-field models for the bainitic transformation [11,12], because it is one of the most complex transformations in steel. Song et al. [12] simulate the growth of a bainitic sheaf with the phase-field method combined with a modified Fick's diffusion equation to model the partitioning of carbon at the interface between bainitic ferrite and austenite. This model is more relevant for upper bainite and it does not include the precipitation of carbides. They show high-quality HRTEM images. Arif and Qin [11] simulate the evolution of the subunits which arise on a lower scale than bainitic sheaf growth. Therefore they do not show a partitioning of carbon within the bainitic ferrite

\* Corresponding author.

E-mail address: [mahnken@itm.upb.de](mailto:mahnken@itm.upb.de) (R. Mahnken).

phase but a diffusion out of the phase. Remarkable is the three dimensional autocatalysis simulation. The formation of lower bainite, the partitioning of carbon within the bainitic ferrite and the precipitation of carbides have, up to our knowledge, not been considered until now.

There are other approaches simulating the evolution of bainite different to the phase-field method in the literature. For example Sidhu et al. [13] present a model describing the kinetics for an isothermal transformation. They calculate the volume fraction of bainite depending on the transformation time and the temperature. Another work [14] also focuses on the volume fraction growth and the incubation time of the bainitic transformation. Lambert-Perlade et al. [15] report about multi-scale crystallographic and metallographic investigations with analytical micromechanical models. Mahnken et al. [16] focus on the multi-scale simulation of the transformation. On the micro level it is based on an ordinary differential equation which considers the growth of different crystallographic variants. Another publication [17] discusses a macroscopic model with transformation plasticity.

In this work we present a model to simulate the bainitic transformation considering bainitic ferrite, austenite, carbide and the diffusion of carbon within a bainitic sheaf. The displacive transformation [1] between austenite and bainitic ferrite is described by a phase-field method. To simulate the complex diffusion behavior of the carbon within the bainitic ferrite the Cahn–Hilliard equation is used. This equation is central to materials science because it describes the movement of atoms between cells [2] and has been applied to simulate carbon diffusion before [7,11]. Fick's law cannot be applied here, because it does not describe uphill diffusion within one phase. The precipitation of carbides will be simulated with the phase-field method again. We do not consider crystallographic orientation, crystalline anisotropy or any kind of stress and strain.

An outline of this work is as follows: In Section 2 the governing equations of the coupled initial boundary value problem are presented. Firstly the multi-phase-field model based on the Ginzburg–Landau equation is derived from the local free energy. In a second step this model is extended by anisotropy. In Section 2.3 the diffusion equation is introduced. This equation is coupled to the phase propagation. The last subsection of Section 2 is about the precipitation of carbides. Section 3 provides a detailed insight into the implementation of the model. In Section 4 three numerical examples are presented showing the lower bainitic transformation. The last section is a summary and gives an outlook for further investigations.

## 2. The phase-field theory

### 2.1. Governing equations

The phase-field model is based on the Ginzburg–Landau equation [2]. It can be derived using a functional of the local free energy  $F$  which depends on the local phase-field order-parameters  $\phi_i$  and their spatial derivatives  $\nabla\phi_i$  [18,19,7]

$$F(\phi_1, \dots, \phi_n, \nabla\phi_1, \dots, \nabla\phi_n) = \int_V \sum_{i,j(i<j)}^{N_p} \left\{ f_{ij}^{intf}(\phi_i, \phi_j, \nabla\phi_i, \nabla\phi_j) + f_{ij}^{pot}(\phi_i, \phi_j) \right\} dV, \quad (1)$$

where  $N_p$  denotes the number of phases. The density of the local free energy functional is defined as the sum of an interfacial energy density  $f_{ij}^{intf}$  and a potential free energy density  $f_{ij}^{pot}$ . As a working solution we use the interfacial energy density [18] with the gradient energy coefficient  $\epsilon_{ij}$

$$f_{ij}^{intf} = \frac{1}{2} \epsilon_{ij} (\phi_i \nabla\phi_j - \phi_j \nabla\phi_i)^2. \quad (2)$$

For the potential energy term there are different approaches in the literature [3]. Fig. 1 illustrates two commonly used potentials, the double well potential and the double obstacle potential. We use the standard double well potential such that the potential free energy reads [18]

$$f_{ij}^{pot} = \frac{1}{4a_{ij}} \left[ \phi_i^2 \phi_j^2 - m_{ij} \left( \frac{1}{3} \phi_i^3 + \phi_i^2 \phi_j - \frac{1}{3} \phi_j^3 - \phi_j^2 \phi_i \right) \right], \quad (3)$$

where  $m_{ij}$  is the thermodynamic driving force and  $1/a_{ij}$  is the potential constant between the phases  $i$  and  $j$ .

By minimizing the local free energy the evolution equations of the phase-field order-parameters are derived [18,19]

$$\begin{aligned} \dot{\phi}_i &= \sum_{j=1, j \neq i}^{N_p} \frac{1}{\tau_{ij}} \left( \nabla \frac{\partial}{\partial \nabla \phi_i} - \frac{\partial}{\partial \phi_i} \right) (f_{ij}^{intf} + f_{ij}^{pot}) \\ &= \sum_{j=1, j \neq i}^{N_p} \frac{1}{\tau_{ij}} \left[ \epsilon_{ij} (\phi_j \nabla^2 \phi_i - \phi_i \nabla^2 \phi_j) - \frac{\phi_i \phi_j}{2a_{ij}} (\phi_j - \phi_i - 2m_{ij}) \right]. \end{aligned} \quad (4)$$

The parameters  $\epsilon_{ij}$ ,  $a_{ij}$ ,  $\tau_{ij}$ , and  $m_{ij}$  are now replaced by the physical material parameters, interface mobility  $\mu_{ij}$ , interface energy  $\sigma_{ij}$ , interface thickness  $\eta_{ij}$  and the change of Gibbs energy  $\Delta G_{ij}$ . Note that  $\mu_{ij} = \mu_{ji}$ ,  $\sigma_{ij} = \sigma_{ji}$  and  $\eta_{ij} = \eta_{ji}$  but  $\Delta G_{ij} = -\Delta G_{ji}$ .

$$\tau_{ij} = \frac{\eta_{ij}}{\mu_{ij}}, \quad a_{ij} = \frac{\eta_{ij}}{72\sigma_{ij}}, \quad \epsilon_{ij} = \sigma_{ij}\eta_{ij}, \quad m_{ij} = -6\Delta G_{ij}a_{ij}. \quad (5)$$

The derivation of the Eqs. (5) using the Gibbs–Thomson equation [20] can be found in the appendix. With these results the evolution equation of the phase parameters reads

$$\dot{\phi}_i = \sum_{j=1, j \neq i}^{N_p} \mu_{ij} \left[ \sigma_{ij} \left( (\phi_j \nabla^2 \phi_i - \phi_i \nabla^2 \phi_j) - \frac{36}{\eta_{ij}^2} \phi_i \phi_j (\phi_j - \phi_i) \right) - \frac{6 \cdot \Delta G_{ij}}{\eta_{ij}} \phi_i \phi_j \right]. \quad (6)$$

For the lower bainitic transformation considered in this work  $N_p = 3$  phases are involved:

1. bainitic ferrite ( $\phi_1$ ),
2. austenite ( $\phi_2$ ) and
3. carbide ( $\phi_3$ ).

### 2.2. Phase-field anisotropy

To simulate the typical slim form of bainite sheaves an anisotropic phase-field model as presented by [21,22] is used. The interface energy  $\sigma_{ij}$  is redefined as a function of the actual growth direction  $\theta$  and of a predefined main growth direction called  $\theta_0$

$$\sigma_{ij} = \sigma_{ij}(\theta, \theta_0). \quad (7)$$

To be specific we use

$$\sigma_{ij}(\theta, \theta_0) = \sigma_{ij}^0 \cdot (1 + s \cdot \cos(\theta - \theta_0)), \quad (8)$$

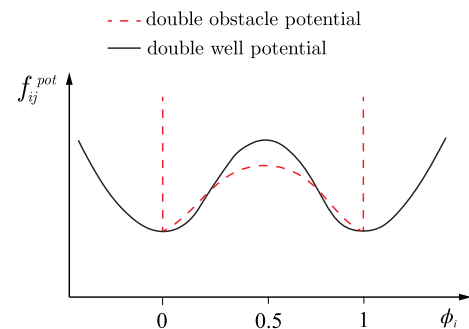


Fig. 1. Double well and double obstacle potential.

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