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Phase field modeling of the simultaneous formation of bainite and ferrite in TRIP steel

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ABSTRACT

In transformation-induced plasticity (TRIP) steels, Si and/or Al delay cementite precipitation during bainite transformation leading to a transformation product that is usually referred to as carbide-free bainite. The present work proposes an approach to calibrate the parameters of a multi-phase field model to simulate the austenite decomposition into ferrite and bainite in a TRIP steel. Ferrite nuclei are introduced at austenite grain boundaries and suitable interfacial mobilities are selected to reproduce experimental ferrite formation kinetics. Bainite nucleation occurs for a sufficiently high undercooling at available interface sites (i.e. austenite grain boundaries, austenite-ferrite interfaces) and/or within austenite grains. For simplicity, the formation of carbide-free bainite is considered and a suitable anisotropy approach is proposed for the austenite-bainite interface mobility. The proposed model is benchmarked and validated with experimental continuous cooling transformation data.

1. Introduction

Transformation Induced Plasticity (TRIP) steels are characterized by a complex microstructure consisting of ferrite, bainite, martensite and a considerable fraction of retained austenite (0.10–0.20). The presence of retained austenite in the final microstructure leads to an attractive combination of strength and elongation due to the TRIP effect resulting from the strain-induced transformation of retained austenite to martensite during deformation. In these steels, due to Si and/or Al addition, carbide precipitation is retarded during the bainite transformation stage such that so-called carbide-free bainite forms. Consequently, during bainite formation the remaining austenite is further enriched with carbon leading to high stability of austenite, which can be retained at room temperature.

There are a number of semi-empirical phase transformation models available for TRIP steels which are mainly based on the Johnson-Mehl-Avrami-Kolmogorov (JMAK) method [1-3]. In addition, analytical models for bainite formation were applied to TRIP steels [4,5]. These semi-empirical approaches are useful tools to describe the overall kinetics of ferritic and bainitic transformations, however, they are incapable of considering the morphological aspects of the complex microstructures.

In order to incorporate the morphological features of ferrite and bainite, meso-scale methods can be used that are now widely available for austenite decomposition including: Phase field modeling (PFM) [6], Monte Carlo (MC) methods [7] and Cellular Automata (CA) [8]. In particular, PFM is a powerful modeling tool for the simulation of microstructure evolution with complex morphological features, as it is not required to explicitly track the interfaces.

In PFM, the interface between the phases is treated as a region of finite width having gradual variation of the different state variables. Even though the interfacial width, η, is chosen to be much smaller than the scale of the microstructure, it is still significantly larger than the actual interface thickness of a few atomic distances. In order to perform meaningful quantitative calculations, the model has to be designed to become independent of the interfacial width, i.e. to capture the physics in the sharp interface limit. There are two main types of PFM. The first type, commonly known as physical order parameter model, originates from the work of Khachaturyan [9] that was applied in a continuum-field (CF) phase field formulation [10]. In this formulation, phase field variables are related to long-range order parameter fields. Here, one needs to have an interface thickness of 1 nm to replicate interface energies in the

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sharp interface limit. The second type of PFM at the mesoscopic scale which was developed by Langer et al. [11] is based on the work of Hohenberg and Halperin [12]. Steinbach et al. [13] and Garcke et al. [14] expanded this model to multi-phase systems. In Steinbach's model the microstructure is described with non-conserved field variables that represent, for example, the local structure and orientation. The model contains parameters that are related to physical properties of the system, such as interface energy and mobility [15]. The evolution of the phase field variables is described as the path that leads to the minimization of the total free energy based on kinetic principles. In this approach, as a modified finite difference method (FDM) can be introduced for diffuse interface problems that minimizes the discretization error associated with the FDM solution thereby decreasing the deviation from the sharp-interface limit [16].

A physical order parameter phase field model developed by Wheeler et al. [17] was used in the first PFM to simulate the isothermal austenite decomposition into ferrite in a Fe-C-Mn system [18]. However, perhaps because of its ease of relating model parameters to physical properties, multi-phase field modeling (MPFM) soon became the most widely used approach to simulate the austenite to ferrite transformation [19-22].

Coupling the single-phase field formulation presented by Loginova et al. [23] with proper anisotropy models, austenite decomposition into Widmanstätten ferrite has also been studied using PFM [24,25]. Loginova et al. [25] used a physical order parameter phase field model with an isotropic ferrite/austenite interface mobility and anisotropic ferrite/austenite interface energy and thickness for Widmanstätten ferrite.

There are many challenges in modeling the austenite decomposition into bainite because its underlying growth mechanism is controversially debated between two competing hypothesizes: military, displacive [26], or civilian, diffusional ledge-wise growth [27]. In addition, the bainite microstructure strongly depends on the temperature at which it forms, i.e. upper vs. lower bainite. Recently, attempts have been made to develop phase field models for bainite formation [28-31]. In particular, dedicated single phase field models were developed assuming displacive bainite formation [30,31]. On the other hand, Song et al. and Ramazani et al. use Steinbach's MPFM approach with a faceted growth mode to describe diffusional bainite formation. Detailed analysis of the bainite growth morphology is, however, not yet provided with MPFM. Further, no considerations have been made to use PFM to simulate the simultaneous formation of ferrite and bainite.

The present paper deals with MPFM of austenite decomposition into ferrite and upper bainite assuming diffusional bainite growth. The recent modeling work by Fazeli and Militzer [5] demonstrates that bainite formation in the present steel and cooling conditions can be described by a diffusional approach. Bainite forms in the investigated conditions in general between 500 and 600 °C which is consistent with the formation temperatures of upper bainite. Using a proper anisotropy model, the morphological complexity of bainite formation is described. The model is applied to continuous cooling austenite decomposition in a TRIP steel where, for simplicity, the formation of carbide-free bainite is assumed.

2. Model

2.1. Phase field formulation

For the MPFM of the austenite decomposition the commercial software MICRESS® is used as a numerically efficient phase field software. Here, the multi-phase field equations are formulated according to the approach of Steinbach et al. [13,32], i.e.:

$$\frac{d\phi_i}{dt} = \sum_{i \neq j} \mu_{ij} \left(\sigma_{ij} \left[\phi_j \nabla^2 \phi_i - \phi_i \nabla^2 \phi_j + \frac{\pi^2}{2\eta^2} (\phi_i - \phi_j) \right] + \frac{\pi}{\eta} \sqrt{\phi_i \phi_j}\, \Delta G_{ij} \right) \tag{1}$$

where ϕ_i , t, μ_{ij}, σ_{ij}, η and ΔG_{ij} represent the phase field parameters, time, interface mobilities, interface energies, interfacial width, and the chemical driving pressure between phases i and j.

The phase field equations are coupled with a diffusion model to calculate the evolution of the concentration field. Because of the low diffusion rate of substitutional atoms, it is assumed that only carbon can diffuse, i.e. para-equilibrium is used for thermodynamic calculations. Similar studies such as [5] show that para-equilibrium assumption leads to acceptable results as long as a mixed-mode character of the transformation is considered where the interface mobility is used as an adjustable parameter. The interface mobility is thus used as an effective parameter to account for the role of Mn and other substitutional alloying elements on the transformation kinetics.

The carbon concentration, c, is determined according to Tiaden et al. [32] by the following equations for a binary alloy with two phases

$$\frac{d\vec{c}}{dt} = \nabla\left[\phi_i D_i \nabla \vec{c}_i + \phi_j D_j \nabla \vec{c}_j\right] \tag{2}$$

where

$$c = (1 - \phi_j) c_i + \phi_j c_j \tag{3}$$

Here D_i and D_j are the diffusivities of carbon in phases i and j, respectively.

Thermodynamic parameters for the phase-field calculations, i.e. the quasi-binary para-equilibrium Fe-C phase diagram and chemical driving pressure, are calculated by Thermo-Calc®, using the TCFE-2000 database. The driving pressure is a function of both temperature and local carbon content. To avoid the computational cost of a full-coupling of the MICRESS® simulation with Thermo-Calc® the LinearTQ option is used which locally linearizes phase diagram and driving pressure [33]. At austenite/ferrite and austenite/bainite interfaces, the equilibrium partitioning ratio is maintained during carbon redistribution [32]. Numerical calculations are performed with the FD-correction method [16] that has been introduced into MICRESS® as a modified finite difference method (FDM) to reduce the deviation from the sharp-interface limit.

The numerical model consists of a set of adjustable parameters describing nucleation and growth of ferrite and bainite. Interface mobilities and nucleation conditions (nucleation temperatures, number of nuclei, and distribution of nuclei) are selected to fit the simulated transformation kinetics and resulting microstructure to experimental data available for two benchmark continuous cooling tests. Bainite grows in the form of sheaves that have a complex morphology consisting of many subunits. Within each sheaf the subunits are parallel with identical crystallographic orientation and habit plane [34]. Thus, for simplicity, bainite formation is considered in the present phase field simulations as nucleation and growth of sheaves. Suitable anisotropy factors are introduced into the interfacial mobility for bainite to reproduce the sheaf morphology in the simulations. All simulations are conducted in 2D with periodic boundary conditions.