



# Phase field modelling of microstructural evolution during the quenching and partitioning treatment in low-alloy steels



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## ABSTRACT

A multiphase-field model (PFM) was applied to study the microstructure development during rapid cooling from the austenitising temperature to the quenching temperature and the carbon distribution between martensite (described as supersaturated ferrite) and austenite during holding at a selected “partitioning” temperature.

Although the modelling does not really simulate martensitic transformations, the morphology of acicular ferrite/austenite microstructure developed during cooling resembles the experimental martensite/residual austenite microstructure at the quenching temperature quite well. The carbon partitioning between the carbon supersaturated martensite and the austenite is simulated for different partitioning conditions. Applying a criterion to calculate the fraction of retained austenite at room temperature from the local austenite carbon content before the final quenching, the phase field model predicts the fraction and distribution of the retained austenite in the final steel microstructure for varying processing conditions in the quenching and partitioning process.

The comparison between 2D and 3D simulations shows that 2D simulations predict a higher retained austenite fraction than the 3D ones. Despite the different carbon diffusion behaviour in 2D and 3D space, which mainly affects the retained austenite fraction, the morphology and distribution of the retained austenite in both 2D and 3D simulations are in good agreement with the experimental observations.

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## 1. Introduction

The Quenching & Partitioning (Q&P) process [1] opens up a new way to develop steel microstructures with exceptionally advantageous combinations of austenite/martensite phases at the industrial scale.

The Q&P process consists of the following steps:

1. heating to the austenitisation temperature to get a fully austenitic microstructure; intercritical annealing can be also chosen to get a dual ferrite/austenite microstructure;
2. quenching to a temperature below the martensite start ( $M_s$ ) temperature to allow a controlled fraction of austenite to transform to martensite; depending on the composition and on the microstructure formed at high temperature, bainite and pre-eutectoid ferrite may also form during quenching, although this is usually avoided in the Q&P process;

3. annealing at the quenching or higher temperature to allow the carbon partitioning between the martensite and austenite; during this stage bainite and carbides may also form;
4. quenching to room temperature; in this step part of the austenite is retained at room temperature and part of it is transformed to martensite.

At the end of the Q&P process the steel microstructure mainly consists of martensite formed in the first quench, martensite formed in the last quench and retained austenite; ferrite, if an initial intercritical annealing is chosen, bainite and carbides may be also present.

The final microstructure and properties of Q&P steels markedly depend on the stability of austenite during the final quench; this is influenced by the amount of carbon that can diffuse from martensite to austenite during the partitioning step, which is controlled by the time and temperature of the partitioning, but is also dependent on the martensite volume fraction formed at the quenching temperature. In the case of intercritical annealing the relative fraction of austenite and ferrite at high temperature also affects the carbon fraction in austenite and its stability during the first

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quench. Due to the complexity of metallurgical processes occurring during the entire Q&P process it is as yet not feasible to predict the final microstructure for given process setting parameters.

A physically-based model, able to describe all the relevant phase transformations occurring during the Q&P treatment, can identify the key parameters for the industrial processes and predict the final microstructure for varying composition and processing conditions.

In the literature different models are available for most of the transformation phenomena occurring in the annealing process. They are both empirical models [2–4], in which the experimental fractions of product phases were fitted with specific equations containing some adjustable parameters, and physically-based models [5–9], which, unlike the empirical models, are not restricted to a specific combination of composition and process schedule. The microstructure description of these modelling approaches is mostly limited to phase fractions and average grain sizes. Recently, the carbon diffusion from martensite to austenite during a Q&P process was described by assuming that the chemical potential of carbon in bcc and fcc is the same at the interface and that the interface migrates when a free-energy difference occurs [10]. However, both the carbon diffusion and the interface migration was described in one-dimension (1D) space and the effect of the morphology of the martensite and austenite was not considered.

Nowadays a number of mesoscale models, able to provide both the phase transformation kinetics and the microstructural evolution, have been developed. Among these, the phase field model (PFM) has recently emerged as a versatile tool to describe the microstructural evolution during material processing [11–14]. This technique can handle time-dependent growth geometries, and thus enables the prediction of complex microstructure morphologies, which makes it particularly suitable for modelling the phase transformations occurring in the Q&P process.

Recently a phenomenological multiphase field model was used to simulate the carbon diffusion from the carbon supersaturated martensite and austenite during the partitioning step of the Q&P process [15]. Since intercritical annealing was considered, the effect of the presence of ferrite formed at high temperature on the carbon partitioning process was also investigated. The authors showed that the carbon fraction within the austenite grains is strongly inhomogeneous with the carbon enrichment being stronger in the austenite close to the martensite phase. Although this study provided information about the effect of the partitioning time on the carbon distribution in the austenite and the stability of this phase during the final quench, details of the morphology of the martensite phase were not adequately represented. However, it is known that the morphology and orientation of the martensite laths affect the shape of untransformed austenite at the quenching temperature and a more realistic morphology of the austenite/martensite microstructure at the start of the partitioning step is important for the correct estimation of the carbon distribution between the martensite and ferrite before the final quench.

In the present paper the same phenomenological multiphase field modelling used in Ref. [15] is applied to simulate the microstructure development during rapid cooling to different quenching temperatures, starting from a fully austenitic microstructure. In order to develop the morphology of martensite laths formed during the first quench, the martensite phase is here represented as acicular ferrite supersaturated in carbon. Although not actually simulated as a martensite martensitic transformation, the appearance of the simulated austenite/acicular ferrite microstructure during the first quench is similar to that of the experimental austenite/martensite microstructure at the quenching temperature, overcoming the limitations of the model in describing the martensite transformation.

A single partitioning temperature is selected to simulate the carbon diffusion from the supersaturated ferrite to the austenite present at the quenching temperature. In this work the ferrite/austenite interface is set as immobile, and no nucleation and growth of new (bainitic) ferrite grains occurs during the partitioning step; therefore the fraction of austenite and ferrite remains constant while carbon diffuses. The effect of the fraction, size and morphology of austenite at the quenching temperature on the carbon distribution developed at the partitioning temperature is evaluated for different values of carbon diffusivity in austenite.

Applying a criterion to calculate the fraction of retained austenite at room temperature from the local austenite carbon content before the final quenching, it was possible to predict the fraction of retained austenite after the final quenching as a function of the quenching temperature and partitioning time and temperature.

As in Ref. [15], most of the simulations in this work are performed in two-dimensional (2D) space. However, previous work on phase field modelling of the austenite to ferrite transformation has shown that three-dimensional (3D) phase field simulations lead to a more realistic grain morphology than simulations in 2D [16]. Therefore a single set of quenching and partitioning temperatures is selected to perform a 3D phase field simulation of the quenching and partitioning step. The comparison between 2D and 3D simulations allows the analysis of the influence of different carbon diffusion behaviour in 2D and 3D space during the partitioning treatment on the retained austenite after the final quench.

## 2. Model

### 2.1. Basic description of the phase field model

In the present work, the multi-phase field formulation originally proposed by Steinbach et al. [11] and later extended to alloys by Eiken et al. [13] is employed to describe the phase transformation occurring during cooling and the carbon diffusion during holding at the partitioning temperature.

In the used phase field approach each grain  $i$  is identified by its own phase field parameter  $\phi_i(\vec{r}, t)$ , with  $\phi_i(\vec{r}, t) = 1$  if grain  $i$  is present at location  $\vec{r}$  and time  $t$  and  $\phi_i(\vec{r}, t) = 0$  if grain  $i$  is not present at  $\vec{r}$  and  $t$ . In the transition region of width  $\eta$ ,  $\phi_i(\vec{r}, t)$  changes continuously from 1 to 0: this region defines the diffuse interface. Each grain has a set of attributes, relevant for describing the transformation of interest: the lattice structure, body centre cubic (bcc) for ferrite grains and face centre cubic (fcc) for austenite grains, and the lattice orientation.

A concentration vector  $\phi_i(\vec{r}, t)$  is introduced to describe the local composition of the multicomponent system. The components  $x^{k=1\dots\xi}$  of the concentration vector denote the molar fraction of the solutes, while the component  $x^0$  denotes the molar fraction of the solvent (iron). Within the diffuse interface, the conservation of the total number of moles per unit volume is given by

$$x^k(\vec{r}, t) = \sum_{i=1}^v \phi_i x_i^k(\vec{r}, t) \quad (1)$$

where  $v$  is the number of coexisting grains in the diffuse interface and  $x_i^k$  is the concentration of solute  $k$  in the individual grain  $i$ . The kinetics of phase transformation is described by the time evolution of  $v$  field variables  $\phi_i(\vec{r}, t)$ , obtained by solving the following phase-field equations

$$\dot{\phi}_i = \sum_{j \neq i}^v M_{ij}^\phi(\vec{n}) \left[ b \Delta G_{ij}(\vec{x}_i, \vec{x}_j, T) - \sigma_{ij}(\vec{n}) K_{ij} + \sum_{i \neq j \neq k}^v J_{ijk} \right] \quad (2)$$

where  $M_{ij}^\phi(\vec{n})$  and  $\sigma_{ij}(\vec{n})$  are respectively the anisotropic phase field mobility and interface energy between grain  $i$  and  $j$ , with  $\vec{n}$  the nor-

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