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A REVIEW ON PHASE FIELD MODELING OF THE PHASE TRANSFORMATION (AUSTENITE–FERRITE) IN LOW CARBON STEELS

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Abstract*-The phase-field method has become an important and extremely versatile technique for simulating and predicting mesoscale morphological and microstructure evolution in materials. Phase Field method has been applied to solidification, martensitic transformations and grain growth, precipitate growth and coarsening and more recently to the other solid-state phase transformations like the austenite to ferrite transformation in steels, cracks propagation, nucleation and dislocation dynamics. It is designed to describe a microstructure with the conserved and without conserved field variables that are continuous across the interfacial regions. Based on Cahn-Hilliard nonlinear diffusion equation and the Allen-Cahn relaxation equation, the phase field method directs the temporal and spatial evolution of the field variables. It predicts the evolution of arbitrary morphologies and complex microstructures without explicitly tracking the positions of interfaces with the help of fundamental thermodynamic and kinetic information as the input This article presents an overview of the phase field methodology and its application to describe phase transformation in low carbon steel. Here we highlight the phase field modeling of austenite-ferrite transformation as the emerging active domain of research in the past few years. Practically as a metallurgical tool the austenite decomposition is the most extensively studied phase transformation for tailoring the properties of steels.*

Keywords: Phase field modeling (PFM); Steel; Austenite–Ferrite Transformation; Microstructure; Phase Transformation

1. INTRODUCTION

The phase field model (PFM) has become the significant computational technique for designing the processing paths for desired microstructure evolution during the phase transformation in steel. The influence behind the development of this model is the enormous progress in computer technology over the past decades. These models are increasingly applied for the features like sub-models that track the microstructure evolution according to a predefined process path and the sound physical principles. The most demanding application of steel, e.g. in the automotive industry [1] PFM has become a paramount importance for the production of low carbon steel. Compared to light weight metals and alloys (e.g. Al and Mg), steels are more advantageous as the austenite–ferrite transformation can easily be exploited to produce microstructures that are associated with significantly improved property profiles. Thus for the family of steel this paper emphasizes on the review of microstructure models. In the beginning, the PFMs were limited to solidification but now have spread to solid state phase transformation, deformation behavior, heat treatment, re-crystallization grain coarsening and grain growth etc. [2]. Primarily, the focus of this review is the austenite – ferrite transformation which includes austenite formation and austenite decomposition. Practically austenite decomposition is the most widely researched phase transformation as a metallurgical tool to tailor the properties of steels. Moreover, microstructure growth in the heat affected zone (HAZ) of welds are also getting attention to be simulated with PFM under the consideration of spatial constraints, which are due to the steep temperature gradients. A significant part of the simulation work in steels is conducted by the multi-phase field approach MICRESS (microstructure evolution simulation software) [3]. In the multi-phase field approach, the microstructure evolution of each grain and/or microstructure constituent is described by its own phase field parameter to predict the evolution throughout the simulation of an assembly of grains and phases. Though the application scope of PFMs is not restricted to MICRESS and alternative PFM approaches [4–7] are also proven to be potential for steels.

This review is an attempt to gauge the applications of the phase-field method in simulating the austenite–ferrite transformation involving in Steel. Such a review would however be incomplete without a prior brief survey of the phase field methodology and its application to steel.

Subsequently, the metallurgical phenomenon of austenite decomposition and austenite formation is deeply analyzed to examine the PFM application with the special attention is given to the microstructure evolution in the HAZ. Finally, the prospects and challenges are delineated to propose the focus areas of future investigation on the basis of this recent literature analysis.

2. GENERAL SURVEY

In order to evaluate the phase field methodology and applications to steels it is essential to know the basics of this process. The multi-phase equations are proposed in an earlier work by Steinbach et al. [8], which is used for describing the austenite (γ) – ferrite (α) transformation kinetics and the resulting ferrite grain size distribution.In this approach, a microstructure is described by means of a set of conserved and non-conserved phase-field variables that are continuous functions of spatial coordinates and time. The conserved phase- field variables are the typical example of molar fraction fields of the constituting components. Non-conserved phase-field variables, such as order parameter fields and phase-fields, contain information on the orientation and local structure. In this method, an easy correlation with physical parameters such as interface mobilities and energies are described such as$\phi_i$is phase field parameter which predicts the microstructure constituent grain *i*, where *i* = 1……N. Inside the grain *i* the value of $\phi_i$is 1 and 0 (zero) for other areas.This can be represented by, $\phi_i(r,t) = 1$ if the grain *i* is present at location *r* and time *t* and $\phi_i(r,t) = 0$ if the grain *i* is not present at *r* and *t*. In a transition region or interface $\phi_i(r,t)$ changes continuously from 1 to 0 such that$\sum_i^N \phi_i(r,t) = 1$, *r* is for each position and is the total number of grains. Then the differential equations unified with the rate of change phase field parameters [8],

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

Where$\mu_{ij}$is the interface mobility, $\sigma_{ij}$is the interfacial energy,η_{ij}isthe interface thickness and $\Delta G_{ij}$is the driving pressure. The minimization of the total free energy of the system influenced the evolution of the phase field parameters for describing microstructure evolution. The phase field equations can be unified with diffusion equations, which in turn help the carbon to describe the phase transformations in the Fe-C system and thermodynamic databases Thermo-Calc ®[9]. Further, the elastic strain energy due to transformation strains or an externally applied stress is formulated as a function of the phase-field variables and a temperature equation can be considered with the equations [2]. In the simulation each and every grain is considered with a number of attributes, e.g. its phase and crystallographic orientation. This leads to an obligation to provide interfacial properties (μ_{ij},σ_{ij},η_{ij}) as an input. The anisotropy of these interfacial properties is advantageous but the knowledge about the interfacial parameters potential anisotropy and mobilities is limited. Actually, the constituents of PFM are simulated as a growth model, where the nucleation of grains are acting as a quantified input in the new phase. Other adjustable factors as the inter interfacial mobilities, anisotropy factors and nucleation scenarios have to be specified as an input value in the form of density, nuclei distribution and the rate of nucleation. These phenomenological parameters are required to determine in order to simulate desired experimental observations. In PFM, it is complicated to quantify all the parameters, as there are large numbers of parameters and it is difficult to measure their properties. Furthermore, in phase field modelling interface treatment is a critical issue as for the diffusive nature of interface. For conserved and non-conserved phase-field variables, the interfaces have a finite width and the variations in properties at interfaces are continuous. This is called diffuse-interface description. So the interface thickness is taken larger than the actual thickness of the interface for reducing the computational cost. For lower undercooling larger interface widths can be used, but larger simulation domains are necessary which require efficient asymptotic analyses to evaluate the sharp interface limit. In phase transformation different assumptions are taken which is either for a mixture of solid-solid interface of two phases [10] or for a mixture of solid-liquid interface of two phases that are defined by a constant ratio for each element [11].

Even though these challenges, the PFMs has become a powerful technique to described the phase transformation for treating the interfaces without the explicit tracking of it. This methodology is perfectly suitable for phase transformations particularly in steels where austenite formation as well as austenite decomposition into Widmanstätten ferrite and bainite is common morphological complexities. It has the characteristics of handling growth geometries which are time-dependent and thus enables the prediction of complex microstructure morphologies easily.

At the beginning, Phase field modelling was limited to solidification process to explain the dendrite formation. Böttger et al. [2] presented a solidification model of steel including stainless steels and continuous casting and graphite nucleation in cast irons. Moreover, an overview of the simulation of peritectic solidification in Fe–C was explained by Tiaden [12].In the electric arc furnace (EAF) the scrap melting process involving liquid steel for steelmaking is another unique phase field application by Li et al. [4, 13]. The formation of dendrites during the Solid to liquid phase transformation is considered to be the classical example of phase field approach as a powerful computational materials science tool. Recently solid to solid transformations, i.e. austenite (γ) – ferrite (α) transformations has become the prime focus for the application of PFMs.

3. AUSTENITE (γ) DECOMPOSITION

3.1. Transformation models

Since the first work on phase field modelling about a decade ago many adjustments have been made to model austenite-to-ferrite transformation kinetics with PFMs [5,14]. In the early work the main focus of the study was to investigate the interfacial conditions and the transition between different transformation modes. For instance

some of the 1D simulations of these work were, local equilibrium conditions for a Fe–Cr–Ni alloy and para-equilibrium conditions for the Fe–C–Mn system by Yeon et al. [5]. Later, Loginova et al. [6] presented a PFM to evaluate the transition between diffusion controlled and massive transformation in Fe–C binary alloys. With the qualitative agreement of experimental observations they found that PFM traces a transition to the partition less massive transformation for sufficiently high undercooling. For example 1 nm interface thickness was considered for lower computational cost of 1D simulation in the work of Loginova et al.[6].Further, with the consideration of α - γ interfacial energy Loginova et al. [15] applied PFM 2Dsimulation where the interface thickness depends on the orientation of the growth direction. The magnitude of this anisotropy function expresses a relationship between $\alpha - \gamma$ interfacial energy. In this relation the amplitude of maximum and minimum energies are corresponds to mimic the high-energy incoherent and low-energy coherent interfaces, respectively. As shown in Figure. 1, the growth of Widmanstätten ferrite in a Fe–0.22 wt%C was possible to predict at 720 ℃ for a sufficiently large anisotropy amplitude is selected. Here the interface thickness decreases with the increase of critical amplitude and the extrapolation for realistic thickness suggests a higher value of 100 rather than 1 nm for the investigated condition but the authors indicated that a higher undercooling may lower this critical value. Recently, Yamanaka et al. [16] employed an alternative method, where the anisotropy extent is described by a strength factor of interfacial energy, which is similar to the investigation of Loginova et al. [15].

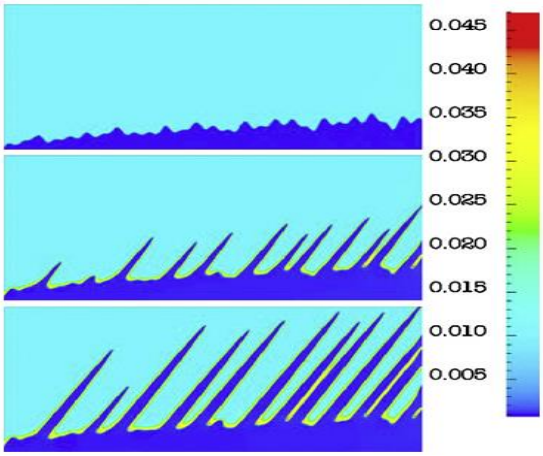

Figure 1. Widmanstätten ferrite growth 2D phase field simulations [15]. Colors (grey scale) indicate the carbon concentration level.

Isothermal austenite–ferrite transformation in Fe–C transition from allotriomorphic to Widmanstätten ferrite is simulated with respect to the increasing tendency of anisotropy strength, as shown in Figure. 2. In this 2D simulation further increase in anisotropy magnitude causes improved structure of Widmanstätten. Loginova et al. [15] and Yamanaka et al. [16] introduce the best examples of PFM to predict complex transformations from austenite into a number of transformation polygonal, massive and Widmanstättenferrite. In addition, Nakajima et al. [17] investigated the phase field modelling of supportive growth of pearlite from austenite in a Fe–C alloy. They studied the contribution of systematic inter lamellar spacing and undercooling on the transformation rate. During the simulation they

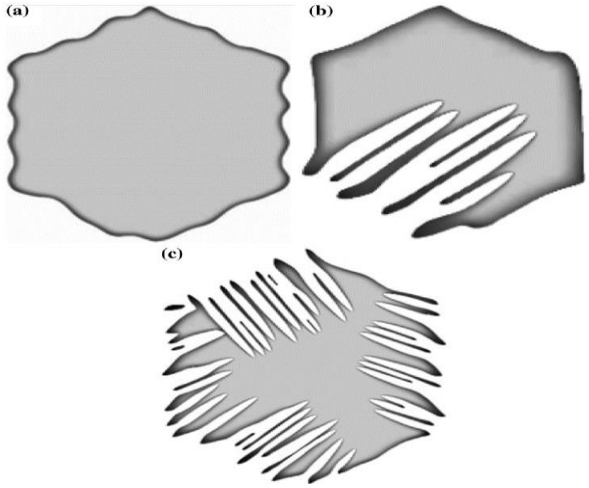

Figure. 2. 2D PFM simulations of ferrite growth into a hexagonal austenite grain surrounded by a ferrite matrix assuming (a) 0.1, (b) 0.35, and (c) 0.5 as different anisotropy factors [16]

controlled the formation of pearlite by carbon diffusion with sufficiently large interfacial mobilities. Examples of their 2D simulations for austenite-to-pearlite transformation with different range of inter lamellar spacing are shown in Figure. 3.

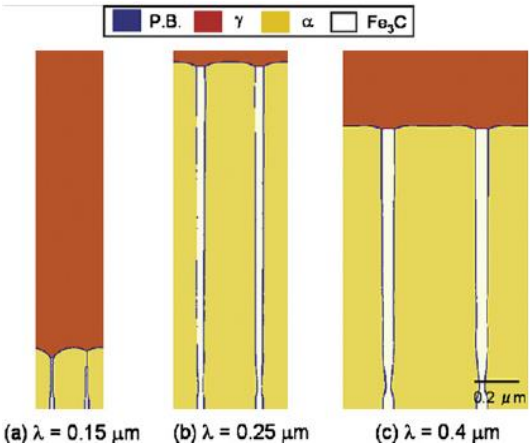

Figure 3. 2D PFM simulations of austenite-to-pearlite transformation in a Fe–C alloy with different inter lamellar spacing assuming that carbon diffusion occurs in austenite [17].

In the figure, the large curvature ferrite overgrows the cementite for a very fine spacing such that a lamellar structure cannot evolve. In the simulation, the highest growth rate was observed for Medium inter lamellar spacing's and for further progress the rate decreases with increasing spacing. Considering both the inter lamellar spacing and carbon diffusion the pearlite growth rates increased by a factor of 4. But it was still lower than the experimental observations. To eliminate this inconsistency with the experimental study, Steinbach and Apel [18] drawn-out the phase field simulations by taking the strain and stress effects on the pearlite formation kinetics in to consideration. In the analysis,

transformation strain brings the stability in growth rate of ferrite and cementite but also it provokes the needle like growth of cementite ahead of the ferrite front. This surprising growth of cementite platelets into austenite after ferrite within the expanse of cementite lamellae width. The experimental observations are in agreement with this resulting growth velocities.

Apart from these diffusional transformations, displacive martensitic transformation is also potential for PFMs though it has not been applied to steel so far. However, 3D simulations of martensite formation was employed for Fe–31%Ni[19].Thus the simulating opportunity of PFMs for all the product of austenite decomposition are reviewed here except bainitic transformation product. In this review, the simulations of ferrite and pearlite formations are performed in 1D and/or 2D without considering the nucleation stage. So for the further progress, one would have to include nucleation stage when simulating the overall transformation.

3.2. Overall transformation kinetics

Pariser et al. [14] were the first who conducted a 2D austenite-to-ferrite transformation simulation with the consideration of interfacial parameters i.e. mobility and Nucleation scenario which is influenced by the phases of the neighboring grains (α - α, α - γ, γ - γ). In this simulation they observed the practical conditions like experimentally observed continuous cooling transformation kinetics in two ultra-low-carbon content steels (22 and 33 wt ppm, respectively). To generate this kinetics in ultra-low carbon steel the interfacial parameters were adjusted to under cooling for nucleation and to suitable nucleation scenario at austenite grain boundaries. Similarly, Mecozzi et al. [20–22] simulated

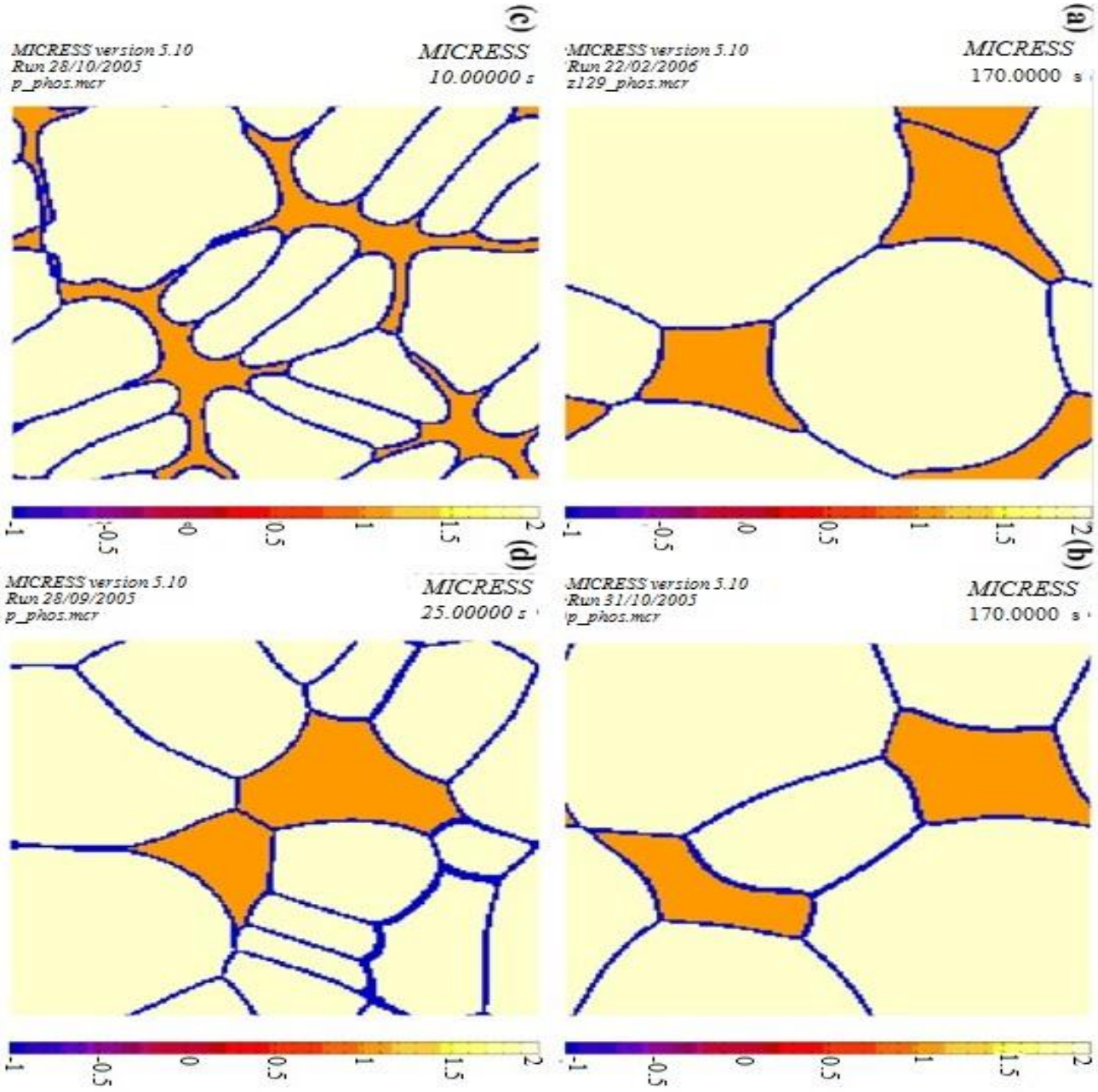

Figure 4. 2D (left) vs. 3D (right) Comparison of PFM simulated microstructures for continuous cooling transformation in a 0.1 wt% C–0.49 wt% Mn steel at 0.4 ℃/s (top) and 10 ℃/s (bottom); ferrite (white),

the 2D approach in low carbon steels including an Nbmicro alloyed grade. In this approach low-carbon steel transformation rates are also depended on long range diffusion of carbon and mixed-mode characteristics of transformation. In mixed mode, transformation changes gradually from interface to carbon diffusion controlled [23]. The simulation mimic the mixed-mode attribution with the presence of interfacial reaction and carbon diffusion. Here, para-equilibrium is largely emphasized for gauging the driving pressure for the transformation rather than slower redistribution of substitutional alloying elements.

2D simulations are the only shot coming of the austenite–ferrite phase field models. Militzer et al. [24] were the first who conducted the 3D simulations to describe the austenite-to-ferrite transformation, as shown in Figure 4. Compared to 2D simulations, 3D simulations are more realistic and from the morphological point of view realistic grain shapes are apparent in the 2D cuts from 3D simulations. Though the consequence of unrealistic grain shapes in 2D simulations are the long-elongated channels of austeniteremaining with a number of narrow inlet-type features between ferrite grains. These features are often appear as squished circles (see Figure 4c). Moreover, Militzer et al. [24] studied the detail of nucleation behaviour in this simulations. Initially they found the α - γ interface mobility, μ, was consistent with the experimentally observed transformation kinetics. However, the assumed nucleation scenario, i.e. nuclei density, spatial distribution of nuclei, nucleation temperature range were the key factors for selecting the mobility values. In simulations ofMecozzi et al. [25] all nuclei formation depends on the preferred nucleation sites as in the austenite grain boundary with triple lines. And each nucleus turns into ferrite grain in the final microstructure by considering the grain boundary mobilities sufficiently small. Other nucleation scenarios such as nuclei density and temperature range, δT, of nucleation determines the average grain size and the width of the grain size distribution respectively. This approach completely neglects the ferrite grain coarsening while conducting the simulations. Huang et al. [7, 26] modelled a 2D simulation of austenite-to-Ferrite transformation and ferrite growth in 0.17 wt%C–0.74 wt%Mn steel, while performing the simulation 50 pct of the nuclei have been consumed after the completion of ferrite grain coarsening of continuous cooling transformation [7].

Both grain growth and grain coalescence in the simulation was responsible for grain coarsening. To overcome the gap, an additional equation with a mobility of ferrite grain rotation was introduced to measure the coalescence. The hypothesis that not all the nuclei will transformed to a ferrite grain in the final microstructure is rational but further experimental justification of suitable mobility parameters for the ferrite grains would be necessary. Again, in the figure 5. Fast cooling of the nucleation sites near the grain interior are also active [7].A number of scenarios have been discussed with the reference of several literature about the transformation of ferrite nuclei into the simulation domain. There is a myriad of nucleation parameters in which partly are measured from the experimental data. Overall, the selection of the α-γ interface mobility requires further attention to solve more satisfactorily by fundamental studies may include atomistic simulations studies. Mecozzi et al. [20–22, 25] and Militzer et al. [24] assumed an Arrhenius relationship for temperature dependent mobility with a generally accepted activation energy of 140 kJ/mol in the PFM. Then an adjustable parameter, pre-exponential mobility factor was introduced which increases with cooling rate. Similarly for Arrhenius relationship of the interface mobility, Huang et al. [7,26] presented a correction term that decreases linearly with increasing temperature. So from the above discussion it is clear that the interface mobilities in the PEM are effective values.

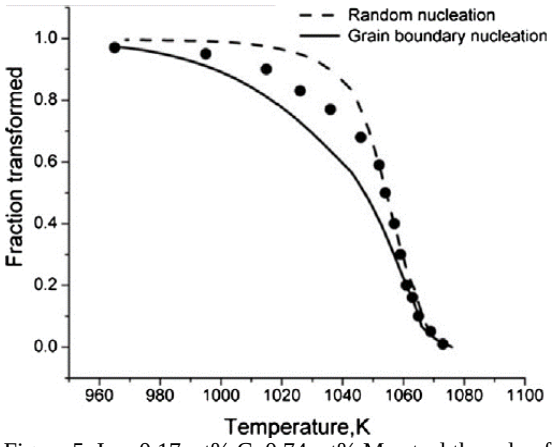

Figure 5. In a 0.17 wt% C–0.74 wt% Mn steel the role of nucleation site selection on PFM prediction of ferrite formation, cooled at 53 ℃/s [7].

4. AUSTENITE FORMATION

Reverse transformation or the austenite decomposition had been comparatively less studied. Only a few studies are reported on austenite formation [27, 28, 30–33]. Thiessen et al. [27, 28] studied the 2D phase field modelling of austenite formation from ferrite–pearlite and ferrite–martensite structures during heat treatment cycles that are similar to those in the weld HAZ. Further extension of this approach, Savran [31] employed PEMs to investigate the austenite formation during continuous heating of carbon steels (0.2–0.6 wt%C). The transformation kinetics was in agreement with experimental results due to the selective interface mobilities. In austenite formation these mobilities are consistent with a mixed-mode character. Azizi-Alizamini and Militzer [32, 33] simulated with more realistic values of interfacial energies for austenite formation in the Fe–C system. As an initial microstructures they used the ultrafine ferrite–cementite aggregates, pearlite and ferrite–pearlite. They predicted the preferential growth of austenite along cementite lamellae and sufficiently largeaustenite growth rates which is partially remain undissolved cementite particles within the austenite matrix. As illustrated in Figure 6, the resulting finger like morphology of inter critical austenite is in agreement with experimental observations [31]. Azizi-Alizamini and Militzerpresented a 3D simulationof austenite formation from spherical cementite particles [32]. The role of substitutional alloying elements is required to

unify with PFM to study the austenite formation in advanced high strength steels. Here the challenge is similar to the austenite decomposition.

It is anticipated that the effective mobility approach of adopting homogenized pearlite in austenite formation simulations of Thiessen et al. [27, 28] and Savran [31] will be utilised for future simulations with the lamellar pearlite structure. Thus the dependence relation between these mobility values and their temperature can be justified with more physically based models.

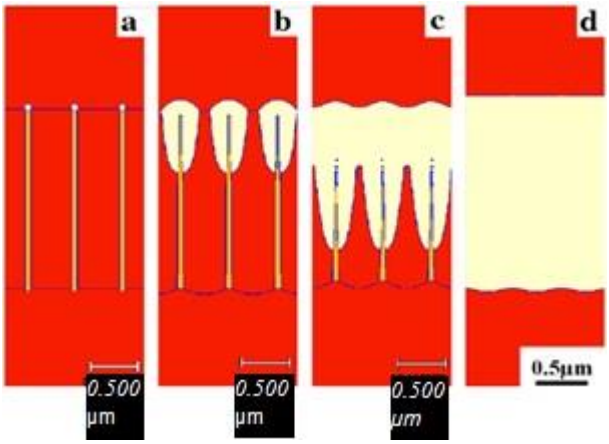

Figure 6. Phase field simulation in Fe–0.17 wt%C alloy (austenite formation) at 750 ℃ intercritical annealing temperature [33].'

5. CONCLUSIONS

Phase field modelling can be used to track the microstructure evolution in steels from casting to the final processing step and easily simulate the complex morphology like Widmanstätten ferrite.Bainite transformation is the only transformation product that has not been conducted yet with PFM. The application of phase field models to advanced high strength steels is the indication of the future prospect of bainite phase field simulations. Further, a particular advantage of PFM simulations can be employed to different microstructure processesduring annealing of cold-rolled steels that occur simultaneously. Here the different length scales of individual microstructure processes may be considered as the restriction. This potential gap can be overcome by describing pearlite as ferrite with eutectoid carbon concentration [27, 28, 31], instead of using more severe but computational expensive approach. The essential input information of PFM approach, i.e. Interfacial parameters and nucleation scenarios are applied empirically to fit the experimental observations are treated as the limitation. However, to analyse and understand the phase transformation mechanisms in steels with complex microstructural morphologiesPFM simulations can be a promising tool for predicting invaluable qualitative and semi-quantitative insight.

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