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A COMBINED MODEL FOR THE DESCRIPTION OF AUSTENITIZATION, HOMOGENIZATION AND GRAIN GROWTH IN HYPOEUTECTOID Fe-C STEELS DURING HEATING

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Abstract—A combined model which allows one to simulate all the steps of the reaustenitization process of ferrito-pearlitic plain carbon steel has been developed. The dissolution of pearlite, the transformation of ferrite into austenite and the homogenization of the carbon distribution is described with a finite volume method. The simulation is performed on a bidimensional domain where ferrite (α), pearlite (P) and austenite (γ) grains are represented. The dissolution of pearlite is described by the growth of spherical grains and simple nucleation and growth laws. The movement of α/γ interfaces is calculated by solving the diffusion equation for carbon in the α and γ phases and accounting for the solute flux balance at the interface using a pseudo-front tracking method. The diffusion model is coupled with a Monte Carlo simulation which describes the grain growth occurring in austenite at a later stage of austenitization. The evolution of the volume fractions of pearlite and ferrite, the maximum and minimum carbon concentrations in the domain and the mean austenite grain size are represented as a function of the temperature for a typical case of constant heating rate. The influence of the different steps of the austenitization process on the global kinetics is discussed. (\odot 1999 Acta Metallurgica Inc. Published by Elsevier Science Ltd. All rights reserved.

1. INTRODUCTION

Reaustenitization in hypoeutectoid steels in the ferrito-pearlitic condition occurs in several steps [1]. The first one is the transformation of pearlite into austenite. Nucleation of austenite grains takes place just above the eutectoid temperature and generally at the interfaces between pearlite colonies. The dissolution of pearlite is then very fast since the diffusion distances for carbon are relatively small (of the order of the interlamellar spacing). The second step is the transformation of proeutectoid ferrite into austenite. This transformation occurs at higher temperatures and is only completed above the $(\alpha + \gamma)/\gamma$ line in the phase diagram (the Ac_1 line). The formation of austenite is followed by homogenization of the carbon distribution and finally grain growth which is predominant at high temperature or long austenitization times.

Different models have been proposed for the description of reaustenitization [2, 3], homogenization [4] and grain growth [5–12]. However, these models are generally restricted to one or two steps of the process. Recently, the present authors have proposed a bidimensional model that describes

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the transformation of ferrite into austenite and homogenization [13]. In this model, it was assumed that the kinetics of pearlite dissolution was much faster than the dissolution of ferrite. Therefore, the first step of reaustenitization was not described, and the initial microstructure was composed of ferrite and austenite zones, the latter corresponding to the former carbon-rich pearlitic regions. This model has been refined in order to account for the formation of austenite from pearlite as well. The present contribution describes the modifications that have been carried out in the finite volume model of Ref. [13] in order to account for the dissolution of pearlite. It also contains a short description of a Monte Carlo (MC) model that has been used to simulate the grain growth in austenite. Finally, a typical result obtained with the diffusion model coupled with the MC model is shown.

2. DIFFUSION MODEL

The model is mainly based on the two-dimensional finite volume method presented in Ref. [13] for the resolution of the diffusion equation in the presence of two phases. The calculation domain is subdivided into hexagonal cells that can have five different states: ferrite (α), pearlite (P), austenite (γ), ferrite/pearlite interface (α /P) or ferrite/austenite interface (α / γ), as illustrated in Fig. 1. There is no

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need to introduce γ/P interfacial cells, due to the simple algorithm used for the transformation of P cells into γ cells (see below). The initial microstructure is composed of ferrite and pearlite zones only. Consequently, at the beginning of the calculation all the cells are of the type (α), (P) or (α/P). This initial condition can be achieved numerically by making grains grow over the domain as described in Ref. [13] or by digitizing a real micrograph. In the latter case, the lamellae of the pearlite colonies are not resolved and thus belong to the same (P) region.

Upon heating, the nucleation of austenite is described by simultaneously creating a given number of grains at the eutectoid temperature. The total number of grains of austenite in the calculation domain is obtained with the following relation:

$$N_{\text{grains}} = N_{\text{A}} w_x w_y (1 - f_\alpha) \tag{1}$$

where w_x and w_y are the dimensions of the domain, $N_{\rm A}$ the density of nuclei in a fully pearlitic microstructure and f_{α} the initial volume fraction of ferrite. The coordinates of the nucleation sites are obtained by randomly choosing a cell inside the pearlitic domain that is among the (P) and (α/P) cells only. In order to account for the more frequent occurrence of austenite grains on the ferrite/ pearlite boundaries, a higher probability is used for the cells of the (α/P) type. Although this probability factor has been arbitrarily set to 10 in the present calculation, it could be estimated from experimental observations. In a section micrograph, if $N_{\alpha/P}$ is the number of grains that have nucleated at α/P interfaces per unit length of interface and $N_{\rm P}$ is the number of grains per unit area that have nucleated within pearlite colonies, this probability factor would be simply given by $N_{\alpha/P}/(a \times N_P)$, where a is the width of the hexagonal cells.

Austenite grains are grown into the pearlitic matrix at a uniform velocity v(T), which is calculated



Fig. 1. Illustration of the hexagonal mesh used to describe the formation of austenite in a ferrito-pearlitic microstructure.

as a function of the temperature, the latter being given as a thermal history T(t). The kinetics law v(T)must correspond to the interlamellar spacing of the pearlite. It can be obtained experimentally or it can be calculated using the numerical model presented in Ref. [14]. The radius of the grains at time t is obtained using the following relation:

$$R_t = R_{t-\Delta t} + v(T(t))\Delta t \tag{2}$$

where Δt is the time step and $R_{t-\Delta t}$ the radius at the previous step.

At each time step, all the pearlitic cells that fall within a distance R_t from a given nucleation centre are captured. These cells are assigned the state (γ) or (α/γ) according to the previous state [(P) or (α/P), respectively]. The (α) or (α/γ) cells falling within these different circles are not affected by the procedure. The initial concentration of the austenite cells is set to the eutectoid composition.

The growth of austenite into ferrite is then calculated by solving the diffusion equation in the α and γ domains following the finite volume technique described in Ref. [13]. The calculation starts at the eutectoid temperature at the same time as the nucleation of austenite grains. It is performed on the domain composed by cells of the (α), (γ) and (α/γ) types only. In other words, the domain over which carbon diffusion is calculated grows with the number of (γ) and (α/γ) cells transformed from (P) and (α/P) cells, respectively. The calculation is stopped when the domain is entirely austenitic and the distribution of carbon satisfies a given homogenization criterion.

The finite volume method provides a variation of carbon concentration in each cell at every time step. For the (α/γ) cells, these variations correspond to an average over the α and γ phases. Since the thermodynamic equilibrium must be satisfied at the interface, the variation of the average concentration in each of these cells is converted into a variation of the fraction of ferrite using the lever rule approximation. Once an (α/γ) cell is fully austenitic, it becomes a (γ) cell and new interfacial (α/γ) cells are created around it [i.e. (α) neighbor cells become (α/γ) interfacial ones]. It was shown that such a procedure numerically diffuses the interface over one mesh element but satisfies the solute-flux balance and the equilibrium condition at the interface. Further details can be found in Ref. [13].

It should be pointed out that a hexagonal grid is used in the diffusion calculation in order to have the same grid topology as in the Monte Carlo simulation of grain growth.

3. GRAIN GROWTH MODEL

A Monte Carlo (MC) model has been developed in order to simulate normal grain growth in austenite. The model is based upon a hexagonal mesh of cells that can undergo various transitions. The topology of the mesh is the same as that used in the



Fig. 2. Microstructure used as an initial condition in the simulation (Ck45 steel).

diffusion model. The Monte Carlo algorithm will not be described here, since it follows the classical approach of Anderson and coworkers [5–9]. The details can be found in Ref. [15].

The size of the MC domain is generally taken to be much larger than that used in the diffusion model in order to have a sufficiently large number of grains. The size of the hexagonal Monte Carlo cell, a, is adapted accordingly in order to obtain a mean grain size (or a grain density) equivalent to the value used in the diffusion model, i.e.

$$\frac{N_{\text{grains}}}{w_x w_y} = \frac{N_{\text{grains}}^{\text{MC}}}{N_{\text{a}}^{\text{MC}} a^2} \text{ or } a = \sqrt{\frac{w_x w_y N_{\text{grains}}^{\text{MC}}}{N_{\text{a}}^{\text{MC}} N_{\text{grains}}}}$$
(3)

where $N_{\rm a}^{\rm MC}$ and $N_{\rm grains}^{\rm MC}$ are the total number of cells and the initial number of grains in the Monte Carlo model, respectively, whereas $N_{\rm grains}$ is the number of grains in the diffusion calculation [see equation (1)]. The initial grain structure is generated according to the procedure described in Ref. [13]. Periodic boundary conditions are used.

The time unit in a Monte Carlo simulation or Monte Carlo time step (MCS) corresponds to N_a^{MC} random attempts of transitions (see Ref. [5]). The MCS is converted into a real time step, Δt , according to a relation proposed by Radhakrishnan [16]

$$1 \text{ MCS} = K_{\text{MCS}} e^{-\frac{Q_{\text{MCS}}}{RT}} \Delta t$$
 (4)

where K_{MCS} and Q_{MCS} are parameters to be adjusted. They have been determined in the present case for a Ck45 steel according to various measurements and numerical simulations [15]. The following values were obtained:

$$K_{\rm MCS} = 3.07 \times 10^{13} / {\rm s}$$

 $Q_{\rm MCS} = 288595 \, {\rm J/mol}$ (5)

4. RESULTS

The microstructure of a ferrito-pearlitic Ck45 steel presented in Fig. 2 has been used to generate the initial microstructure of the simulation. The result of the digitizing procedure is shown in Fig. 3(a). This $100 \,\mu\text{m} \times 100 \,\mu\text{m}$ domain is enmeshed with 43 200 hexagonal cells. The light yellow zones correspond to pearlite and the ones in dark red to ferrite.

The calculations were performed with a density of austenite grains of $5 \times 10^9/\text{m}^2$, which corresponds to 29 grains for the simulation domain of Fig. 3, assuming an initial volume fraction of ferrite $f_{\alpha} = 0.41$. The nucleation cells were chosen randomly from among the pearlitic regions. An arbitrary ratio of 10 was used for the nucleation probability in (α/P) cells as compared with the probability in (P) cells in order to account for the preferential nucleation at the α/P interface. The growth kinetics was calculated with the v(T) curve presented in Fig. 4 (continuous line). These data were determined experimentally by Roberts [17] for a pearlitic microstructure having an interlamellar spacing of 0.5 µm. Values predicted with a front-tracking finite element model [14] are also shown on this figure for the sake of comparison. The heating rate used in the simulation was 1°C/s. The diffusion coefficient of carbon in austenite was calculated as a function of temperature and local carbon content. the Bhadeshia's approach [18] has been followed to account for these dependencies.

The results of the calculation are presented in Fig. 3 where micrographs of the simulated microstructure are shown at six points during heating. The various colors depict the carbon content in austenite (light yellow/dark red: high/low carbon concentrations, respectively). As can be seen in Fig. 3(a), which shows the microstructure at the beginning of the transformation, nucleation preferentially takes place on ferrite/pearlite boundaries, which is a direct consequence of the higher nucleation probability used for (α/P) cells as compared with the (P) cells. The austenite grains then grow rapidly into the pearlitic areas [Figs 3(b)-(d)] and into ferritic areas at longer times [Figs 3(d)-(f)]. After 130 s [Fig. 3(f)], the domain is fully austenitic and the carbon concentration is within 0.39% and 0.5%.

The austenitization and homogenization kinetics obtained with the model can be analyzed in more detail in Fig. 5 where the volume fractions of pearlite and ferrite are plotted as a function of temperature. It can be noticed that pearlite transforms into austenite much faster than ferrite; at 750°C pearlite has totally disappeared, whereas the dissolution of ferrite has just started. The phase transformation is completed at 830°C and the temperature for a homogeneous concentration of carbon in austenite is about 1000°C.



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Fig. 3. Microstructure evolution during reaustenitization of an Fe–0.45% C alloy as calculated with the finite volume model. Pearlitic zones (P) (in light yellow) and ferritic zones (α) (in dark red) are progressively dissolved into austenite grains (γ). The corresponding temperatures are: (a) 732°C; (b) 737°C; (c) 742°C; (d) 747°C; (e) 779°C; (f) 857°C. Other parameters are 100 × 100 µm² domain size, 43 200 cells, $N_{\text{grains}} = 29$ (grain density 5 × 10⁹ grains/m²), heating rate of 1°C/s, pearlite lamellar spacing of 0.5 µm.

A simulation with the former model (see Ref. [13]) in which the dissolution of pearlite was assumed to be instantaneous has been performed using the same conditions. This allows one to estimate the influence of pearlite dissolution on the global austenitization time. The evolution of the volume fraction of ferrite obtained under such conditions has been represented in Fig. 5 with a dotted line. This curve



Fig. 4. Steady-state dissolution rate of a pearlitic microstructure with an interlamellar spacing of 0.5 µm. Values measured by Roberts [17] and calculated with a finite element model [14]. The β angle imposed in the numerical calculation corresponds to the angle in the austenite phase at the triple point $\gamma/\alpha/Fe_3C$ (see Ref. [14]).

is almost superimposed on the continuous line of the new model. It can be deduced that under the present conditions, the dissolution of pearlite can be neglected in the overall austenitization process, since it only slightly delays the transformation at the beginning, but has no influence on the temperature at which the transformation ends.

The Monte Carlo simulation has been performed on a 780 μ m × 780 μ m domain. These dimensions were adjusted in order to start with a microstructure containing about 2000 grains and a mean grain size equal to the value used in the diffusion model. The evolution of the microstructure is shown in Fig. 6. The mean austenite grain size obtained as a function of the temperature has also been represented in Fig. 5. As can be seen, grain growth is very slow at the temperature at which the phase transformations occur. It becomes substantial only above 950°C when the mobility of the grain boundaries is sufficiently large.

The results obtained with the diffusion and Monte Carlo models tend to validate the assumption that austenitization of ferrito-pearlitic steels can be subdivided into three steps: (i) dissolution of pearlite; (ii) transformation of ferrite into austenite and carbon homogenization; and (iii) grain growth of austenite. Using different models for the description of each individual step may thus be a fairly good and simple approach. However, it should be pointed out that the present results have been obtained under particular conditions. Nucleation of austenite has been described with a very simple law which does not account for overheating and con-



Fig. 5. Kinetics of austenitization, homogenization and grain growth in an Fe–0.45% C steel as calculated with the two-dimensional finite volume and Monte Carlo models for a heating rate of 1°C/s. The volume fraction of ferrite, represented by a dotted line, was obtained with the assumption of instantaneous dissolution of pearlite at the eutectoid temperature. Homogenization is described with the maximum (c_{max}) and minimum concentrations (c_{min}) observed in the calculation domain.



Fig. 6. Evolution of the grain structure as calculated with the Monte Carlo model for a heating rate of 1°C/s. The Monte Carlo step and the temperature corresponding to the micrographs are: (a) MCS = 0, $T = 850^{\circ}$ C; (b) MCS = 1480, $T = 1010^{\circ}$ C; (c) MCS = 5000, $T = 1045^{\circ}$ C; (d) MCS = 19 500, $T = 1100^{\circ}$ C. The numbers of grains in the domain are, respectively, 1841, 993, 438 and 137.

tinuous nucleation. Moreover, at lower heating rates or in the presence of a coarser pearlite microstructure, the growth velocity of austenite into pearlite colonies would be smaller. In such cases, the dissolution kinetics of pearlite might have an influence on the total transformation time. The present model can be a very useful tool to investigate such effects.

5. CONCLUSION

For the first time, a model which combines all the steps of the reaustenitization process of ferritopearlitic plain carbon steel has been developed. The dissolution of pearlite, the transformation of ferrite into austenite and the homogenization of the carbon distribution have been described in a single model. The simulation of grain growth has been performed separately, but using the mean austenite grain size coming from the diffusion model as an initial condition. It has been shown that the previous assumption of subdividing the austenitization process into several individual steps is fairly good. Merging the phase transformation and grain growth models could be envisaged, since both finite volume and Monte Carlo methods use a similar hexagonal grid. However, the length scales associated with these two phenomena would create an unnecessarily large number of cells for the solution of the diffusion equation. Moreover, grain growth plays an important role only at high temperature or very long austenitization time and does not significantly influence the growth kinetics of austenite.

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