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A microstructure model for recrystallisation and phase transformation during the dual-phase steel annealing cycle

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ABSTRACT

A three-dimensional cellular automata model is developed for the description of the relevant metallurgical mechanisms occurring in the annealing stage of dual-phase steels: ferrite recrystallisation, pearlite-to-austenite and ferrite-to-austenite transformation on heating and austenite-to-ferrite transformation on cooling. Based on the local grain-boundary and interface velocity, the latter controlled by both interface mobility and carbon diffusivity, the model is able to simulate the microstructure development throughout the annealing stage. The model also provides information on the carbon gradient in austenite at the end of the cycle, which is relevant for the prediction of martensite formation during the subsequent quenching. The simulated structure thus provides a realistic representation of many microstructural aspects.

1. Introduction

Due to the combination of high strength and good formability dual-phase (DP) steels are increasingly popular in the automotive industry. DP-steel is often produced by intercritical annealing of cold rolled strip. The structure of the steel at the beginning of the annealing process usually is a deformed ferrite/pearlite mixture. Upon heating to the intercritical annealing temperature the ferrite recrystallises. Depending on the strain energy in the deformed ferrite grains and on the heating rate, recrystallisation of ferrite can evolve to a significant degree before the pearlite, *P*, and ferrite, α, start to transform to austenite, γ. During the isothermal holding (generally not longer than a few minutes) a two-phase microstructure of ferrite and austenite is obtained. At the end of the isothermal holding period there can be a short period of slow cooling before the final quench. In this slow-cooling period (typical cooling rates between 1 and 20 K/s) part of the austenite transforms back to ferrite. In the subsequent quench any remaining austenite is expected to transform to martensite, resulting in the characteristic ferrite/martensite dual-phase steel microstructure.

The final microstructure will have a pronounced effect on the mechanical properties of the steel. The transformation processes occurring during the annealing cycle, i.e. ferrite recrystallisation, pearlite-to-austenite, ferrite-to-austenite, austenite-to-ferrite and austenite-to-martensite phase transformations, have an influence on the final microstructure. In the literature a number of different models are available for all the mentioned transformation processes ranging from simple (empirical) Johnson–Mehl–Avrami–Kolmogorov (JMAK) [1–5] to sophisticated phase-field models [6–11]. With phase-field-modelling detailed microstructure descriptions can be obtained. Unfortunately, phase-field modelling is associated with a high computational cost, especially for three-dimensional systems. Multiple JMAK models for the different transformations coupled together can provide a process model that is much faster to calculate [12,13]; however the microstructure description of these models is limited to phase fractions and average grain sizes.

The physical basis for JMAK models is formed by descriptions of the nucleation and growth behaviour of grains, i.e. by combining a nucleation-rate equation with a growth-rate equation, phase fractions can be obtained by correcting for impingement [14]. When the growth-rate equation is set to be dependent on the solute-element diffusion in a grid microstructure, descriptions similar to those from phase-field modelling can be obtained [15,16]. In this type of computer models nucleation and growth are described per grain and no local information from the grid is used in the calculation of the growth rate of a grain. By including local information from the grid in the growth model of the grains a type of model is obtained which is probably best described as a Cellular Automata (CA) model. An important advantage of a CA-model is the option to start from any realistic microstructure; this is an

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essential feature for the microstructure simulation of the DP annealing cycle, since aspects of the initial microstructure are maintained during intercritical annealing.

In this work a CA-model will be presented that describes all transformation processes in the DP-steel annealing cycle. In the CA-model growth is primarily described per grain but where possible local information of the situation at the interface is also used in the growth sub-models. By following this grain-based formalism a highly efficient process model is obtained that can handle three-dimensional systems within a reasonable simulation time, while maintaining a satisfactorily accurate description of all transformation processes involved. Such a model inevitably contains a number of assumptions and simplifications. In the presentation of the different model components the assumptions and simplifications will be discussed. After definition of the simulation settings, the capabilities of the CA-model are demonstrated for a (model) Fe–C–Mn steel.

2. Theory

2.1. Cellular automata model

In the CA-model used in the present work the simulated polycrystalline system is discretised in a three-dimensional grid of cubic cells of dimension δ. Each cell in this system has 26 neighbouring cells, at distances $\delta, \sqrt{2}\delta, \sqrt{3}\delta$. Periodic boundary conditions are applied. While in typical CA-models the state of each cell depends on the state of the neighbouring cells through particular transformation rules, the present model works differently: the transformation takes place at grain-boundary cells according to the sub-models described later in this section.

At each time, t, each cell has the following properties:

1. The grain to which the cell belongs. The setting of this property for each cell of the system identifies univocally the *grain-boundary cells*, which have neighbours that belong to a different grain. Note that each cell belongs to only one grain and therefore this is a sharp-interface model.
2. The growth length, l^i_{cell}, for each grain-boundary cell, i. This property is updated every time step, Δt, by Euler time integration of the grain-boundary velocity, i.e.

$$l^i_{cell}(t+\Delta t) = l^i_{cell}(t) + v^i_{cell}\Delta t, \tag{1}$$

where the velocity v^i_{cell} is equal to the grain-boundary velocity, v, which is calculated according to the relevant sub-model (see Sections 2.2–2.4).

When the growth length of a cell, l^i_{cell}, has reached the grid spacing, δ, the nearest neighbour cells are transformed into interface cells and their growth length starts to evolve according to Eq. (1). Next-nearest neighbours are transformed when l^i_{cell} exceeds the face diagonal of the cubic cell, i.e. $l^i_{cell} \geqslant \delta\sqrt{2}$, and the last neighbours are transformed when l^i_{cell} exceeds the body diagonal of the cubic cell, i.e. $l^i_{cell} \geqslant \delta\sqrt{3}$. When all its neighbour cells have been transformed, a cell is no longer a grain-boundary cell and its growth length l^i_{cell} looses its meaning. When cells of different grains grow simultaneously into a shared neighbour cell, the first cell that reaches the critical length determines to which grain the shared neighbour cell transforms.

To ensure that every change in the grain volume and surface area is directly reflected in the transformation kinetics, the maximum time step size, Δt, is subjected to the criterion

$$\Delta t < \left(\sqrt{3}-\sqrt{2}\right)\delta / v \tag{2}$$

in the present cubic cell configuration. On the basis of Eq. (2) the time step is selected dynamically during a simulation.

Eq. (2) shows that the maximum allowed time step depends on the grid spacing (δ) used in the simulation. The optimal value for the grid spacing depends on the details of the simulation system. If a large grid spacing relative to the grain size is chosen, the volume and surface area of the grains will occasionally change abruptly (because they are discretised in cells). Especially for the austenite-to-ferrite transformation it is important that grain volume and surface area changes are accurately described as they play an important role in the transformation kinetics (see Section 2.4.2). This usually limits the grid spacing to a few tenths of a micron. Of course smaller grid sizes increase the computation time.

As stated above, the cells in the CA-model form grains. Grains have a number of properties (besides the collection of cells that belong to them):

(i) The phase of the grain (ferrite, austenite or pearlite).
(ii) Strain energy.
(iii) Average carbon concentration.
(iv) Carbon concentration at the interface.

For all growing grains the grain-boundary velocity, v, is determined according to the classical equation

$$v = M\Delta G \tag{3}$$

where M is the interface mobility and ΔG the driving force for the transformation [17].

For the different metallurgical processes (ferrite recrystallisation and phase transformations) that occur during the DP-steel annealing cycle different sub-models are used for the calculation of the driving force ΔG in Eq. (3). These processes, which will be simulated by the CA-model and will control the growth of the interface cells through Eq. (1), are presented in Sections 2.2–2.5.

2.2. Ferrite recrystallisation

2.2.1. Nucleation

In the present application of the model the nucleation of recrystallised grains is described as site-saturation. Site-saturation can be interpreted as a collection of pre-existing nuclei that start to grow when a certain temperature is reached. In the CA-model this is implemented as a nucleation density n_{RX} and a nucleation temperature T^{nucl}_{RX}, which are input parameters. The number of nuclei formed, N_{RX}, is given by

$$N_{RX} = n_{RX}V_\alpha, \tag{4}$$

where V_α is the volume of non-recrystallised ferrite. In the present application of the model the number of nuclei is calculated for each ferrite grain, i, and the total number of recrystallised nuclei is given by $N_{RX} = \sum_i n_{RX}V^i_\alpha$, where V^i_α is the volume of the single grain i. This approach allows relating the nucleus density to the local strain energy. In the present simulation, the positions of the nuclei in the grains are chosen randomly. It is possible in the model to limit nucleation at specific sites like grain-boundary cells.

2.2.2. Growth

During ferrite recrystallisation the grain-boundary velocity, v, can be described by

$$v = M^{\alpha\alpha}_0 \exp\left(-Q^{\alpha\alpha}_g/RT\right)\Delta G_{RX} \tag{5}$$

where $M^{\alpha\alpha}_0$ and $Q^{\alpha\alpha}_g$ are respectively the pre-exponential factor and the activation energy for the grain-boundary mobility and ΔG_{RX} is the strain energy of the non-recrystallised grains. The newly nucleated grain is assumed to have zero strain energy. The growth velocity depends on the strain energy of the neighbouring grains and is calculated locally. If all deformed grains have the same strain