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Prediction of post-dynamic austenite-to-ferrite transformation and reverse transformation in a low-carbon steel by cellular automaton modeling

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Abstract

The post-dynamic transformation that takes place during the subsequent isothermal holding for the case when dynamic strain-induced transformation (DSIT) from austenite to ferrite occurs during hot deformation is investigated by cellular automaton modeling. The simulation provides a better understanding of carbon diffusion in retained austenite and the resulting microstructure evolution during the post-dynamic transformation. The predictions reveal that continuing transformation from retained austenite to ferrite and the reverse transformation can occur simultaneously in the same microstructure during post-deformation isothermal holding owing to the locally acting chemical equilibrium conditions. Competition between forward and reverse transformation exists during the early stage of post-dynamic heat treatment. It is also revealed that increasing the final strain of DSIT might promote the reverse transformation, whereas the continuous austenite-to-ferrite transformation yields a diminishing effect. The influence of the DSIT final strain on the grain size of ferrite and the characteristics of the resultant microstructure is also discussed.

Keywords: Strain-induced transformation; Post-dynamic transformation; Cellular automaton; Modeling; Low-carbon steel

1. Introduction

A primary goal in steel design is to refine the ferrite grain size, as this is a mechanism that can simultaneously improve strength and toughness. Hence, specific emphasis has been placed on the large-scale design of ultrafine-grained steels [1–3]. In recent years, a number of techniques and methods have been developed to produce ultrafine-grained steels with a ferrite grain size of around 1 μm [4–11]. Among the various approaches, the novel technique of dynamic strain-induced transformation (DSIT) [1,12] from austenite to ferrite has received much attention owing to its capability of producing ultrafine ferrite (UFF) microstructures with grain sizes that typically fall into the 1–3 μm range [11–21]. In DSIT, the UFF microstructure is achieved by heavy deformation of the undercooled, metastable austenite just above the transformation start temperature (Ar3) without using high levels of alloying. In general, the concurrent deformation and phase transformation is believed to be necessary for UFF microstructure production in the DSIT process. Owing to its conceptual simplicity and efficiency for grain refinement, and the associated improvement in strength and toughness, the DSIT mechanism has been the subject of extensive investigations [11–26].

Commonly, a typical DSIT schedule consists of a reheating step to form a desired austenite grain size and subsequent cooling to a deformation temperature between the Ae3 and Ar3 temperatures (the equilibrium and empirical austenite to ferrite transformation temperature, respectively). Specific deformation (e.g. deformation mode and

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level) is then applied to achieve UFF. Suitable post-deformation treatment (e.g. controlled cooling) is also generally included to preserve the UFF microstructure obtained via DSIT when the deformation is interrupted. During the DSIT process, the time available for phase transformation is usually insufficient to fully complete the transformation from austenite to DSIT ferrite. The unstable retained austenite can continue transforming into ferrite. Such post-dynamic transformation (post-DT) influences the final microstructure of the product significantly. Just like the metadynamic recrystallization [27], post-DT can start immediately after deformation without any incubation period as ferrite nuclei are already present in the material. The transformation kinetics can also differ from that of conventional γ–α transformation or DSIT.

Despite the considerable importance of UFF design strategies, only a few investigations have focused on post-DT. Recently, Sun et al. [28] investigated the microstructural evolution and kinetics of the isothermal post-DT after compression deformation in a low-carbon steel using both dilatometry and optical microscopy. However, the focus was centered on the development of a quantitative dilatometric method for the measurement of the DSIT ferrite fraction [29]. Due to the limitations of the experimental methods they used, Sun et al. were unable to improve their understanding of the post-DT mechanism significantly. It still remains unclear how ferrite growth were controlled through the post-deformation process.

With the recent development of mesoscale microstructure-based transformation models [30], simulations can now provide deeper insight into the mechanism of the austenite–ferrite transformation and its morphological complexity. Various mesoscopic methods are conceivable, e.g. the cellular automaton (CA) [31–36], the Monte Carlo [37,38] and the phase field models [39–42].

Recently, the present authors developed an integrated CA model to simulate DSIT in low-carbon steels [43,44]. In that work the nucleation of DSIT ferrite and the associated carbon diffusion behavior during DSIT were addressed. The refinement mechanism of the DSIT ferrite can also be studied. The present work is built on the previous work of DSIT modeling, focusing on the numerical simulation of microstructure evolution during post-DT after DSIT. In this work, a modified CA model is developed to jointly predict the metallurgical mechanisms of solute diffusion, interface migration and grain coarsening which pertain to the post-DT mechanism. In modeling this transformation, the simulated results of DSIT, including the morphology of grains, distribution of phases and solute concentration field, are input as the initial conditions for the following post-DT simulation. Specifically, this model takes into account the effect of local solute redistribution on the migration of the γ/α interfaces, which allows both the continuing transformation from austenite to ferrite and the reverse transformation to be studied. The influence of the DSIT final strain on the transformation kinetics and microstructure evolution is also obtained by the model.

2. Model concept

2.1. Growth of ferrite grains

When deformation is interrupted after DSIT, the strain-induced ferrite grains can grow continuously during the subsequent post-deformation holding period. Different from conventional grain-coarsening, this mechanism of the movement of the γ/α interface can be referred to as "transformation growth". The driving force comes from the difference in free energy between the two phases. In our model, the kinetics of ferrite growth during post-DT is described as a mixed-mode process governed both by carbon diffusion and by the γ/α interface mobility. The transformation associated with the γ/α interface motion is described by a free boundary problem for carbon diffusion in austenite and the dynamics of the moving interface. The kinetics of the γ/α interface is determined by

$$V_{\alpha\gamma} = M_{\alpha\gamma}F \tag{1}$$

where $V_{\alpha\gamma}$ is the velocity of γ/α interface and $M_{\alpha\gamma}$ is the effective mobility of γ/α interface, which includes the structural influence on the interface mobility, such as incoherence, the set-up of stresses and solute drags. It can be described, as per Loginova et al. [45], as:

$$M_{\alpha\gamma} = M_0 \exp\left(-\frac{Q_{\alpha\gamma}}{RT}\right) \tag{2}$$

where M_0 is the pre-exponential factor of the interface mobility, $Q_{\alpha\gamma}$ is the activation energy for boundary migration, R is the universal gas constant (8.314 J mol^{-1} K^{-1}) and T is the absolute temperature (in K).In DSIT, the driving force for interface migration, F is provided both by the chemical driving force, F_{chem}, that is associated with the transformation and by the stored deformation energy, E_d,

$$F = F_{chem} + E_{\mathrm{d}} \tag{3}$$

The chemical driving force for the γ/α interface migration, F_{chem}, can be derived from Svoboda et al. [46]:

$$F_{chem} = \mu_{Fe}^{\gamma} - \mu_{Fe}^{\alpha} \tag{4}$$

where μ_{Fe}^{γ} and μ_{Fe}^{α} are the chemical potentials of iron in austenite and ferrite, respectively, determined by the local carbon concentration on either side of the γ/α interface. The chemical potentials of iron in austenite and ferrite phases are calculated using the regular solute sublattice model [47] in the simulation.

During the post-dynamic holding, the stored deformation energy E_d is released dramatically due to recovery. The evolution of the stored energy $E_d(t)$ with soaking time t is given as following [48],

$$E_d(t) = \left[E_d(t_0)^{1/2} - C_0\mu_i^{-1/2}kT\ln\left(1+\frac{t}{\tau_0}\right)\right]^2 \tag{5}$$

where $E_d(t_0)$ is the initial stored energy of deformation which comes from the previous DSIT simulation [44], t_0 is the time when recovery starts, C_0 is a combined fitting