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Modelling discontinuous dynamic recrystallization using a quantitative multi-order-parameter phase-field method

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ABSTRACT

A multi-order-parameter phase-field model was built by coupling a phase-field model with a physically-based statistical nucleation model to predict the microstructure evolution and flow stress responses of discontinuous dynamic recrystallization in 304L stainless steel. Individual growth kinetics simulations of recrystallized nucleus showed that the critical nuclei size was determined by balance between the local stored energy difference and grain boundary energy. This was different from the widely-used semi-analytical Roberts-Alhblom model of nucleation criterion and showed good agreement with Bailey-Hirsch model. The migration rate of the recrystallization interface did not follow the monotone change but strongly depended on the deformation conditions. The overall simulations of dynamic recrystallization agreed well with experimental observation. The characteristic features such as effect of deformation conditions on the peak stress, critical strains and grain size were quantitatively captured by the model. The sensitivity of grain boundary mobility to both temperature and strain rate was found from simulation. If the initial grain size decreased to a critically small value, the enhanced work hardening effect due to grain refinement maybe results in the dramatic increase of nucleation density, and hence finer steady-state grain size. The transition from single peak flow behaviors to multiple peak implies the change of dominating recrystallization behavior from nucleation to interface migration.

1. Introduction

During the thermo-mechanical processing in the metallic materials, dynamic recrystallization (DRX) is one of the most important restoration mechanisms accompanied with plastic deformation. Investigating the microstructural mechanisms and constructing the quantitative description of DRX kinetics are extremely important to controlling final microstructure as well as the macroscopic mechanical behavior. In the past decades, many researchers endeavored to carry out extensive experimental and modeling studies on the fundamental understanding of DRX [1,2].

For materials with high stacking fault energy, e.g. aluminum, the dynamic recovery is fast and DRX can occur in a slow and continuous manner, and this is know as continuous dynamic recrystallization (CDRX). In CDRX, the recrystallized microstructure forms through the progressive transformation of subgrains into new grains, within the deformed original grains [3]. On the other hand, the mechanism for DRX of metallic materials with low or medium stacking fault energy, e.g. copper or austenitic steel, involves the formation of nuclei and the movement of grain boundaries. The process of nucleation and grain growth are clearly distinguished and exhibits a cyclic behavior, and therefore is called discontinuous dynamic recrystallization (DDRX) [1]. In this paper, our discussion pays more attentions to DDRX.

In the past decades, many physically-based models and microstructural simulation methods have been developed for describing the process of nucleation and grain growth kinetics of DDRX at coarse-grain scale [4]. These models were designed to involve some characteristic features, such as stored energy evolution by the competition between the accumulation and elimination of dislocations, the critical conditions for the onset of nucleation and the overall nucleation rate and interface migration kinetics of recrystallized grains. In the topic of nucleation, for example, a semi-analytical model of nucleation criterion proposed by Robert et al. has been widely adopted to get the critical strains of DDRX [5], while the overall nucleation rate is described by a purely

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phenomenological model in which some parameters show little physical meaning and had to be fitted by experiments [6]. Zurob et al. developed a model based on the Bailey-Hirsch bulging mechanism and the subgrain size distribution to describe the nucleation step of recrystallization [7]. Cram and Hutchinson et al. then extended this model to DDRX by coupling to grain growth and polyphase plasticity descriptions [8]. In the topic of grain growth of recrystallization, many models with a mean field concept have been able to successfully predict the flow stress response, kinetics and grain size of DDRX, e.g. the inverse power-law relationship between the steady-state flow stress and the average steady-state grain size, as shown in the studies of Montheillet et al. [9] and Huang et al. [10]. In contrast to the static recrystallization case, the interaction between the continuous deformation and recrystallization during DRX brings the difficulty to find the analytical solution of interface migration rate of DRX front. More recently, some numerical mesoscopic models, such as cellular automaton [6,11–13], Monte Carlo [14], level-set [15] and phase-field method [16–21], have been developed to simulate the interface migration kinetics. These models provide both the prediction of overall DRX behaviors and the spacial morphology of microstructure. For example, most of these models exhibited the ability of capturing qualitatively or quantitatively the relationship between grain evolution behaviors and transition from single-peak to multi-peak flow curves. Other microstructure-related features, such as necklace formation, topological deformation and recrystallization textures, have also been describe by those mesoscopic models. Moreover, the principles inside these microstructural models are generally universal and easily extended to simulate the processes which many microstructure evolutions mechanisms occur simultaneously, such as the grain coarsening after recrystallization or phase transformation [22] and the combination of phase transformation and recrystallization [23]. Totally speaking, most of the above models tried to build a computational framework to explain the common well-established characteristics by experiments and also provide an alternative tool of predicting microstructure evolution during hot processing. We should perceive that the robustness and accuracy of computational models has the great promotion space to describe the physical essence of recrystallization better.

In present study, a multi-order-parameter phase-field method was adopted to describe quantitatively the influence of stored energy on the interface migration on polycrystalline materials. The phase-field method provided a thermodynamically-based framework to simulate the interface movement without the explicit calculation and tracking of interface velocity. The relation between plastic flow and stored energy was obtained from a concise dislocation evolution model for work-hardening and dynamic recovery, as it has been shown to apply at large strains in the hot working range, in particular for austenitic steels. The individual growth of nuclei during DRX was then investigated for revealing complex interface migration behaviors of recrystallized front and evaluating the rationality of the existing nucleation models. Then a physically-based nucleation model based on Bailey-Hirsch bulging mechanism and a statistical distribution of subgrains was integrated with phase-field model to simulate the stress induced bulging nucleation of recrystallization. The overall simulations of DRX were performed using this integrated model to study the effect of deformation temperature, strain rate and initial grain size on the microstructure evolution and stress-strain responses. 304L austenitic stainless steel, which does not undergo phase transformation over a wide temperature range, was used as model alloy of low stacking-fault energy material. Its hot torsion test provides the experimental data of both the mechanical and microstructural aspects for the parameter evaluation of work hardening model and comparative analysis with simulations.

2. Numerical Model

2.1. Dislocation evolution and flow stress

During the plastic deformation at high temperature, two processes, work hardening and recovery, will coexist. Generally, the total dislocation density as well as the flow stress will be in a dynamically equilibrium state during deformation only if dynamic recovery exists. There are many pioneer works about the dislocation evolution models during hot deformation [24,25]. In these models, the evolution of dislocation density ρ can be described by two concurrent terms: storage and recovery. If the mean free path is assumed as constant, Estrin-Mecking relationship [26,27] can be built as following concise expression, namely:

$$\frac{d\rho}{d\epsilon} = h - r\rho \tag{1}$$

where ϵ is equivalent plastic strain, h and r represent the work hardening and recovery term respectively. EM model has been shown to apply at large strains in the hot working range, in particular for austenitic steels [9,27]. Generally, the work-hardening term h and the dynamic recovery term r in Eq. (1) is the function of temperature and strain rate. J.J. Jonas deduced the relationship of h and r with experimental stress-strain curves and found the following descriptions [28]:

$$\sigma\theta = 0.5r(\sigma_{sat}^2 - \sigma^2) \tag{2}$$

$$h = r\frac{\sigma_{sat}^2}{(M_t\alpha\mu b)^2} \tag{3}$$

where σ is the equivalent flow stress, $\theta = d\sigma/d\epsilon$ is the work hardening rate, σ_{sat} is the saturation stress when the dislocation evolution reaches the dynamic equilibrium at the asymptotic stress curves. α a constant, M_t the average Taylor factor, μ the shear modulus and b is Burgers vector. Clearly the recovery term r can be retrieved from the slope of $\sigma\theta$ vs σ^2 curves. σ_{sat} is defined by the extrapolation of the θ vs σ plot to $\theta = 0$. Both θ vs σ and $\sigma\theta$ vs σ^2 plots can be derived from the fitted experimental stress-strain curves. The detailed description about the fitting of parameters in EM model can be found from [28]. It is well-known that these featured variables are usually shown as the function of Zener–Hollomon parameter ($Z = \dot{\epsilon}\, exp\left(\frac{Q_{act}}{RT}\right)$). This parameter encompasses two of the most important hot deformation variables (T and $\dot{\epsilon}$), which relates the equivalence of temperature and strain rate to the microstructure development during hot working.

The deformation induced stored energy G_s then can be calculated as $G_s = 0.5\mu b^2\rho$, while the macroscopic stress is related to the average dislocation density $\bar{\rho}$ using Taylor equation $\sigma = \sigma_0 + M_t\alpha\mu b\sqrt{\bar{\rho}}$.

2.2. Nucleation model

During DDRX, two significant features of nucleation should be considered in the models, namely the critical conditions for onset of nucleation and the overall nucleation rate. Roberts and Ahlblom developed a nucleation criterion based on the bulging mechanism [5]. In this model, the net free energy change equation is built by involving the dislocation evolution at the recrystallization front. If the dynamic recovery is ignored in dislocation evolution model, the critical dislocation density ρ_c and critical nuclei size d_c can be deduced from the turning point of free energy equation using semi-analytical method:

$$\rho_c = \left(\frac{20\gamma_{gb}\,\dot{\epsilon}}{3blM_{gb}\tau^2}\right)^{1/3} \tag{4}$$

$$d_c = \frac{6blM_{gb}\tau\rho_c^2}{5\,\dot{\epsilon}} \tag{5}$$

where M_{gb}, γ_{gb}, l and τ are grain boundary mobility, grain boundary