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Phase-field simulation of static recrystallization considering nucleation from subgrains and nucleus growth with incubation period

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ABSTRACT

In this paper, a computational method for static recrystallization that simultaneously predicts nucleation and nucleus growth is newly proposed. We employ the Kobayashi–Warren–Carter (KWC) phase-field model to express nucleation due to the coalescence of subgrains. The completion of nucleation is judged according to the mean value of the order parameter and the standard deviation of the crystal orientation. We decide whether or not the nucleus grows by virtue of the nucleus size. In addition, some restrictions are set on the nucleus boundaries to represent the absorption of phantom nuclei. A static recrystallization simulation is carried out for a deformed FCC crystal with a large number of subgrains using the present method. The results show that nuclei start to grow after their nucleation incubation periods and that the growing nuclei absorb phantom nuclei. To verify the proposed simulation method, we compare the results obtained from this simulation with some experimental data, i.e., histograms of the nucleation rate and the misorientation on grain boundaries.

1. Introduction

The mechanical properties of metals are strongly affected by the microstructures that are mainly produced in the final stage of processing. In case of cold rolling, the final process is annealing, in which static recrystallization occurs [1,2]. During cold rolling, subgrains are formed and the mean dislocation density becomes high due to the large deformation. Here, a subgrain is defined as a grain that is smaller than a usual grain, e.g., 1–10 μm, and whose difference in crystal orientation from adjacent grains is also smaller than that of a usual grain, e.g., 2–5°. The recrystallization process is classified into nucleation and nucleus growth (Fig. 1). In the first stage, a group of subgrains surrounded by high-angle grain boundaries turns into a new nucleus [1]. In the second stage, the stored dislocation energy acts as a driving force allowing the nuclei to grow, and the growing nuclei cover the entire domain. The produced structure is more stable and has a lower dislocation density than the deformed structure. In particular, the mechanism of nucleation is important in static recrystallization. Nucleation can be classified into two types, i.e., the bulging and coalescence of subgrains. The nucleation based on bulging occurs as a result of stored strain energy in the case of comparatively small deformations [3]. The nucleation due to coalescence is induced by the rotation of subgrains in the case of large deformations [4,5]. It is said that the former occurs frequently during dynamic recrystallization that proceeds simultaneously with deformation [6–8], and the latter is mostly observed during static recrystallization [9,10]. The coalescence of subgrains was discussed by Li [11]. Humphreys and Chan showed by in situ high-voltage electron microscopy observation that a clear difference between the orientations of two subgrains disappeared during annealing [12]. This behavior is evidence of the rotation of subgrains.

Recently, it has been highly expected that microstructure formation due to such recrystallization can be clarified by computational approaches. To pursue this aim, many computational simulations of static recrystallization have been reported [13–20]. The numerical models often used to simulate static recrystallization are the Monte Carlo model [13], cellular automaton models [13,14] and phase-field models [15–20]. These models are used for reproducing not only static recrystallization but also dynamic recrystallization. The phase-field model is attracting increasing attention because it was developed in the framework of continuum mechanics [21], while the Monte Carlo model and cellular automaton model are discrete models using probability theories and local rules, respectively. Since the phase-field model is often used as a

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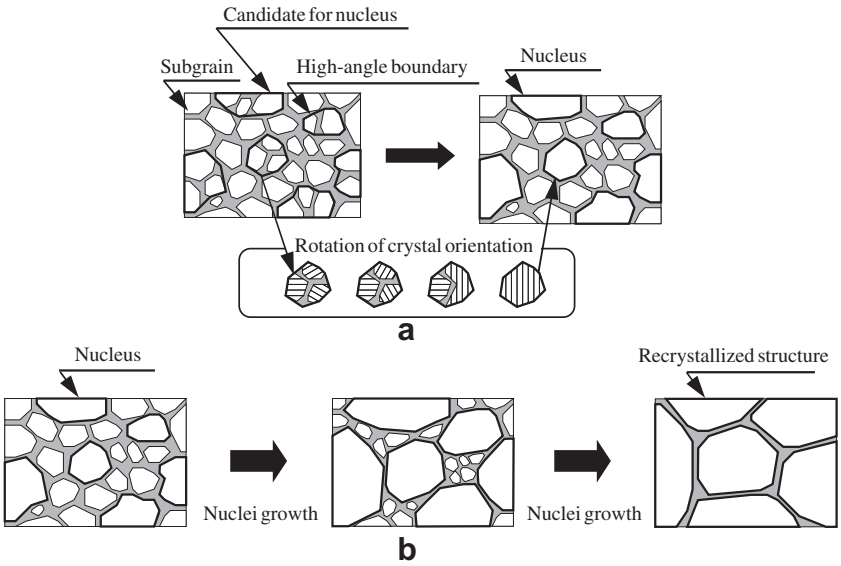

Fig. 1. Schematic process of static recrystallization: (a) nucleation stage and (b) nucleus growth stage.

powerful tool to reproduce the formation of microstructures in the framework of continuous theory, we adopt the phase-field model in this study. On the other hand, to reproduce dynamic recrystallization in the future, it will be necessary to couple a microstructure evolution model with a dislocation-based crystal plasticity model [22] belonging to continuum mechanics. In such a case, it will be preferable to adopt the phase-field model, which is also one of the continuum models used for the calculation of microstructure evolution. Therefore, here we use the phase-field model even for static recrystallization. In particular, the KWC phase-field model [23,24] and a multi-phase-field model [25–27] are suitable for expressing recrystallization phenomena. The KWC phase-field model has only two continuous variables, i.e., order parameter ϕ and crystal orientation θ. The order parameter ϕ satisfies $\phi = 1$ in the recrystallized phase, $\phi = 0$ in the matrix and $0 < \phi < 1$ in the interface, while the crystal orientation θ has the form $\theta = \theta_r$ in the recrystallized phase, $\theta = \theta_m$ in the matrix and $\theta_m < \theta < \theta_r$ or $\theta_r < \theta < \theta_m$ in the interface. Note that the KWC phase-field model is more useful for reproducing nucleation than the multi-phase-field model because the continuity of crystal orientation makes it possible to describe the changes in crystal orientation. The multi-phase-field model has as many identical order parameters as the number of grains. Numerous studies on the use of the phase-field model for static recrystallization have been reported as mentioned below. For example, an essential discussion about the application of the phase-field model to recrystallization was provided by Lask [15]. Takaki et al. simulated static recrystallization using the KWC model [16] and a multi-phase-field model [17] based on the microstructure in deformed metals. Wang et al. conducted a phase-field simulation of industrial-scale recrystallization for an alloy [18]. Suwa et al. discussed subgrain growth using the multi-phase-field model [19]. The relationship between the discrete atomic model and KWC model was discussed by Bishop and Carter [20]. Although various phenomena have been reproduced using the conventional phase-field models, static recrystallization including nucleation has never been simulated using the phase-field model.

In our previous work [28], we developed a calculation method based on the KWC phase-field model for nucleus growth phenomena considering nucleation from subgrains existing in plastically deformed structures. However, a problem with our previous procedure is that it consists of two steps. The first step is a calculation for all candidates for nucleus to obtain the incubation periods of all nucleations. After the completion of this step, the second step is to compute nucleus growth, in which nuclei start to grow when the pre-calculated incubation periods have elapsed. Therefore, temporal continuity between the nucleation and nucleus growth is not achieved, even though nucleus growth should start immediately after the completion of nucleation. In addition, grain sizes were not taken into account in our previous simulation although only nuclei with radii larger than critical nucleus radius grow in the actual recrystallization.

In this study, a method of simulating static recrystallization, in which both the nucleation incubation period and the critical nucleus radius are considered simultaneously, is developed on the basis of the KWC phase-field model to reproduce that nuclei whose radii are larger than the critical radius start to grow after the completion of nucleation and that the small nuclei are absorbed by the growing nuclei. Also, the numerical results obtained by this calculation are shown to confirm that the above scheme works effectively. As a result, recrystallization including nucleation can be reproduced using the KWC phase-field model, which shows its usefulness for simulating static recrystallization with nucleation due to the coalescence of subgrains. In addition, the results are compared with experimental data in terms of the nucleation rate and misorientation on grain boundaries to qualitatively evaluate the developed simulation method.

2. KWC phase-field model

In this section, we briefly explain the KWC phase-field model [20], which is uniquely characterized by the existence of an evolution equation for the crystal orientation θ. The evolution equations for ϕ and θ in the KWC phase-field model are derived from a Ginzburg–Landau-type free energy, which is extended to a more general energy including the grain boundary energy. The extended free energy is expressed in terms of the order parameter and crystal misorientation as

$$F = \int_V \left\{ \frac{\alpha^2}{2} (\nabla\phi)^2 + f(\phi) + E_{gb}(\phi, \nabla\theta) \right\} dv, \tag{1}$$

where f denotes the free energy of the bulk, E_{gb} the grain boundary energy and α is the gradient coefficient related to the interface energy. Expanding E_{gb} in a Maclaurin series about $\nabla\theta$ and neglect-