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# Multiscale modeling of hot-working with dynamic recrystallization by coupling microstructure evolution and macroscopic mechanical behavior

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ABSTRACT

Dynamic recrystallization (DRX) occurs during the hot-working of a metallic material with low-to-medium stacking-fault energy. The macroscopic mechanical behavior during hot-working is largely affected by the microstructure evolution due to DRX. In this study, a novel multiscale hot-working model was developed by coupling the multi-phase-field dynamic recrystallization (MPF-DRX) model and large deformation elastic–plastic finite element (FE) method using J2 flow theory to evaluate the microstructure evolution and macroscopic mechanical behavior, respectively. We call this model the multi-phase-field and finite element dynamic recrystallization (MPFFE-DRX) model. Compression simulations with nonuniform deformation of a cylinder confirmed that the newly developed MPFFE-DRX model can be used to evaluate the macroscopic mechanical behavior during hot-working by considering the DRX microstructure evolution, which differs depending on the area. We also confirmed that the MPFFE-DRX model can be used to simulate macroscopic mechanical behavior depending on the initial microstructure by varying the initial grain size.

## 1. Introduction

Hot-working is a process in which a metallic material is plastically deformed at an elevated temperature higher than the recrystallization temperature (Humphreys and Hatherly, 1995). Because hot-working is performed under such high temperatures, dynamic recovery (DRV) due to a thermally activated process actively occurs in addition to the dislocation accumulation due to plastic deformation. In particular, for a metallic material with low-to-medium stacking-fault energy, dynamic recrystallization (DRX) also occurs, in which the recrystallized grains having low dislocation density are nucleated when the dislocation density exceeds a critical value and grow to the deformed materials driven by the stored energy difference between the plastically deformed grain and the recrystallized grain. For DRX materials, the macroscopic mechanical behavior during hot-working is largely affected by the microstructure evolution due to DRX (Roberts and Ahlblom, 1978; Sakai and Jonas, 1984; Humphreys and Hatherly, 1995). Therefore, predicting and evaluating the macroscopic mechanical behavior during hot-working with high accuracy requires considering the DRX microstructure evolution.

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Finite element (FE) computation is widely used in numerical simulations of hot-working with DRX. The DRX volume fraction, average diameter of DRX grain, and so on that are used to express the DRX microstructure evolution are incorporated into the constitutive equations as internal state variables (Göbel, 1991; Busso, 1998; Yanagimoto et al., 1998; Manonukul and Dunne, 1999; Davenport et al., 2000; Cho et al., 2005; Yeom et al., 2005; Fan and Yang, 2011; Brown and Bammann, 2012; Momeni et al., 2012). In these cases, we must model the changes of such internal state variables depending on the histories of plastic deformation and temperature. However, models that precisely express the complicated histories of deformation and temperature during actual hot-working are very difficult to develop. In addition, we cannot obtain the microstructure itself from these simulations.

Ding and Guo (2001) developed a cellular automaton dynamic recrystallization (CA-DRX) model that allows the average mechanical behavior of the computational domain to be investigated based on changes in the DRX microstructure. In this model, the DRX grain growth, changes in dislocation density due to plastic deformation and DRV, and average stress of the entire computational region are computed by the cellular automaton (CA) method, Kocks–Mecking model (Mecking and Kocks, 1981), and Bailey and Hirsch's equation (1960), respectively. This CA-DRX model is widely applicable and has already been applied to various materials and problems (Ding and Guo, 2004; Qian and Guo, 2004; Kugler and Turk, 2004; Goetz, 2005; Xiao et al., 2008; Zheng et al., 2008). Takaki et al. (2008, 2009) proposed a multi-phase-field dynamic recrystallization (MPF-DRX) model in which the multi-phase-field (MPF) method (Steinbach and Pezzolla, 1999), which can be used to accurately simulate the grain growth process, is used instead of the CA method in the CA-DRX model. The MPF-DRX model can also be used to express transient deformation (Sakai et al., 1983; Tanner and McDowell, 1999; Tanner et al., 1999; Frommert and Gottstein, 2009), where the strain rate and temperature change during deformation (Takaki et al., 2011). Although the CA-DRX and MPF-DRX models can express the microstructure evolution during DRX and calculate the mechanical behavior of the domain based on the computed microstructure, these models are limited to uniform deformation. Because the deformations in actual hot-working are nonuniform, these models cannot be used to evaluate the macroscopic mechanical behavior of hot-working processes such as hot-rolling, extrusion, and drawing.

Recently, multiscale models using the FE method for the macroscopic hot-working process and a model for the DRX grain growth and phase transformation microstructure evolution have been investigated (Qiang and Esche, 2005; Gawad et al., 2008; Won and Im, 2010; Svyetlichnyy, 2012). However, in these computations, the FE simulations are performed by using a constitutive equation that depends on the internal state variables, which are independent of the microstructure evolution. The grain growth and phase transformation of the microstructure are simulated based on the FE simulation results. Therefore, these multiscale models are not a complete coupling model.

Many multiscale models have been developed for cold-working, as reviewed by McDowell (2010) and Horstemeyer and Bammann (2010). For example, Groh et al. (2009) developed three different length scale models that use molecular dynamics, discrete dislocation dynamics, and crystal plasticity; Ohashi et al. (2007) expressed scale-dependent mechanical properties using discrete dislocation dynamics and crystal plasticity finite elements; and Sundararaghavan and Zabaras (2006) proposed FE homogenization based on microstructure evolution. However, because grain boundary migration is not active in the cold-working process, no multiscale models are available that consider grain boundary migration.

In this study, a novel multiscale hot-working model was developed by coupling the MPF-DRX model and a large deformation elastic–plastic FE method to evaluate the microstructure evolution and macroscopic mechanical behavior, respectively, during hot-working. In this model, the micro and macro fields interfere with each other, and the model acts as a complete coupling model as a homogenization method (Terada and Kikuchi, 1997; Terada et al., 1997). We call this model the multi-phase-field and finite element dynamic recrystallization (MPFFE-DRX) model. To the best of our knowledge, this is the first attempt at using multiscale modeling to completely couple microstructure evolution and macroscopic mechanical behavior. After deriving the MPFFE-DRX model, we confirmed its validity by simulating compression of cylinders with nonuniform deformation. We confirmed that the MPFFE-DRX model can be used to simulate macroscopic mechanical behavior depending on the initial microstructure by varying the initial grain size.

## 2. MPFFE-DRX model

In our developed MPFFE-DRX model, the microstructure evolution during DRX is evaluated by the MPF-DRX model, and the macroscopic mechanical behavior during hot-working is calculated by the FE method. The DRX microstructure evolution is computed by a finite difference (FD) method, and the FD computations are performed for every element used in the macroscopic FE simulation. The concept is very similar to that of the homogenization method (Terada et al., 1997; Terada and Kikuchi, 1997). The tangent modulus of the equivalent stress–strain curve is transferred from the micro field to the macro field, and the equivalent strain rate and temperature are transferred from the macro field to the micro field.

### 2.1. Micro field model

In the MPF-DRX model (Takaki et al., 2008, 2009), the polycrystalline structure and growth are expressed by the MPF model proposed by Steinbach and Pezzolla (1999). In the MPF model, the *i*th grain out of *N* grains in the polycrystal is indicated by the phase-field variable $\phi_i$. $\phi_i$ takes the value of 1 in the *i*th grain and 0 in the other grains; it smoothly changes at the grain boundary between the *i*th grain and other grains. The time evolution equation of $\phi_i$ is derived as the total free