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Monte Carlo simulation of primary recrystallization and annealing twinning

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Abstract

The formation of annealing twins has been studied from the beginning of the 20th century and a variety of mechanisms have been suggested. Molecular dynamics simulations on the atomic scale have also been performed. This paper reports a microscale simulation of primary recrystallization and twinning of a nickel alloy based on the Monte Carlo approach. Different twin morphologies were simulated. A possible dependence of grain growth direction on twin formation during annealing was demonstrated. The formation of incoherent Σ3 and Σ9 boundaries is verified as the indirect outcome after coherent Σ3 formation.
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Keywords: Monte Carlo simulation; Primary recrystallization; Twinning; Nickel alloy

1. Introduction

The first observation of annealing twins can be traced back to the beginning of the 20th century [1]. As technology and material developed, this phenomenon was largely observed during the annealing of face-centered cubic materials with low stacking fault energy (SFE). The related mechanisms have also been studied for decades. By considering a combination of the proposed mechanisms [2–4], annealing twin formation has been defined as a nucleation of partial Shockley loops at the {1 1 1} ledges (or emission of partial dislocations) from the migrating grain boundaries (GBs) [5,6], including the formation of 5-fold twins in nanocrystalline materials [7]. This has been supported by molecular dynamics simulations [8,9].

According to Gleiter's theory [3], the twinning probability depends both on the annealing temperature and on the difference in the Gibbs' free energy between the growing and the shrinking grains [3]. Pande et al. [10] found that the number of twins per grain depends on the grain size (not directly on temperature), and on the driving force. However, in these theories, the Gibbs' free energy gradient or the driving force was only related to the GB energy. They were then modified by Cahoon et al. [11] and Li et al. [12], who introduced the stored energy effect.

Moreover, in Gleiter's model [3] the annealing twin was formed by accident when the migrating GB was parallel to a {1 1 1} plane of a growing grain. This theory was verified by a recent study based on transmission electron microscopy (TEM) observations [13], which showed that the twin formation depends on the direction of grain growth. All of these studies show that annealing twinning is an important mechanism in terms of primary recrystallization.

As a statistical and stochastic approach, Monte Carlo (MC) simulations are widely used for primary recrystallization and grain growth. However, twin formation has not yet been introduced into this type of simulation, especially using orientation imaging microscopy (OIM) maps as

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input data, which contain the microstructure, the position of each pixel and their orientation.

Before the development of field emission gun-scanning electron microscopy (FEG-SEM), it was difficult to obtain an OIM map of the deformed state due to the resolution limit. Despite this problem, Caleyo et al. [14] attempted to simulate primary recrystallization from an OIM map measured by SEM; non-defined pixels were attributed to orientations based on the global texture of the deformed material. Baudin et al. [15] performed simulations using TEM data. Note that the input data could also be obtained from finite-element modeling of a deformed state [16]. After the development of FEG-SEM, performing MC simulations directly from OIM maps became feasible [17,18].

The present paper reports a microscopic simulation of primary recrystallization through a MC approach. Experimental data for a deformed material, obtained by an electron backscatter diffraction (EBSD) system installed on a FEG-SEM, will be used as input data. Multiple twinning will also be introduced, taking into consideration the variation of stored energy and the direction of grain growth.

2. Material and initial structure

A nickel alloy that had been hot forged and homogenized was employed [19]. After these treatments, this material presents a recrystallized and homogenous microstructure. The mean grain size is ~17 μm, ignoring twins.

A sample cut from this material was deformed by cold rolling to 60% reduction. Its deformed microstructure was analyzed by an EBSD system installed on a FEG-SEM. This analysis was carried out on the transverse plane, i.e. rolling direction (RD)–normal direction, (ND). The acquisition step was 200 nm based on a hexagonal grid. An EBSD map of $50 \times 50\ \mu m^2$ was chosen as the initial microstructure for simulation, whose texture is in good agreement with the bulk texture (Fig. 1). The main texture components are Copper {1 1 2} ⟨1 1 1⟩ and the α-fiber (from Goss {0 1 1} ⟨1 0 0⟩ to Brass {0 1 1}⟨2 1 1⟩). This global texture was analyzed by neutron diffraction at the Laboratoire Léon Brillouin (CEA Saclay, France) on the diffractometer 6T1.

The distribution of stored energy within this chosen microstructure was obtained with the help of line-broadening measurements of the neutron diffraction peaks [20,21] and by calculating the kernel average misorientation (KAM) [22,23].

Firstly, using the neutron diffraction, the stored energy (per unit volume) after deformation was determined as a function of grain orientation $H(\varphi_1, \phi, \varphi_2)$, and these energies of the three main components are shown in Fig. 2. Taking the measurement errors into consideration, the stored energy is almost identical for every component. Therefore, in this simulation, the stored energy was considered as a parameter independent of the grain orientation. Hence, instead of considering different $H(\varphi_1, \phi, \varphi_2)$ as the maximum stored energy which depends on grain orientation, a mean value H_{max} was calculated (Eq. (1)) as the maximum stored energy density of the whole deformed material. This mean value is independent of grain orientation, and allows us to have a global vision of the stored energy in this deformed material.

$$H_{max} = \sum_{i=1}^{n} F(\varphi_{1i}, \phi_i, \varphi_{2i}) \bullet H(\varphi_1, \phi, \varphi_2) \quad (1)$$

Here n is the number of main orientations existing after deformation. The volume fraction $F(\varphi_{1i}, \phi_i, \varphi_{2i})$ of every main orientation was calculated from the orientation distribution function (ODF) by LaboTex software. The ODF is determined by using the discrete ADC method [24]. These fractions were then normalized before calculation of H_{max}.

The minimum stored energy (H_{min}) is chosen arbitrarily as 10% of H_{max}. This minimum value is not set to zero since zero is reserved for the recrystallized pixels that will appear during the simulation of the recrystallization.

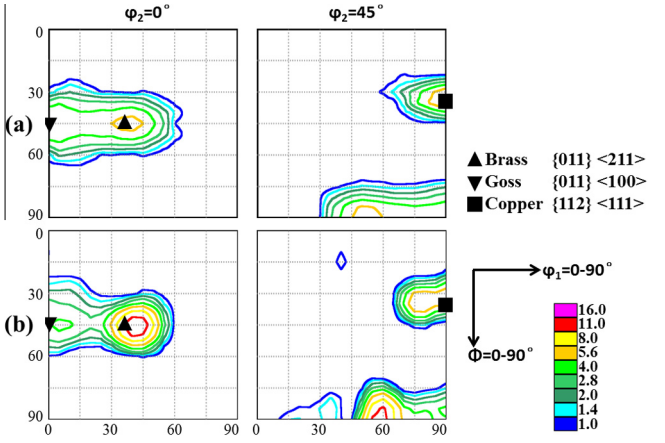

Fig. 1. (a) Bulk texture (neutron diffraction) of the deformed sample after 60% cold rolling, and (b) local texture (OIM) of the initial microstructure for the simulation. Three main texture components (Copper, Brass and Goss) after deformation are indicated with different black symbols.

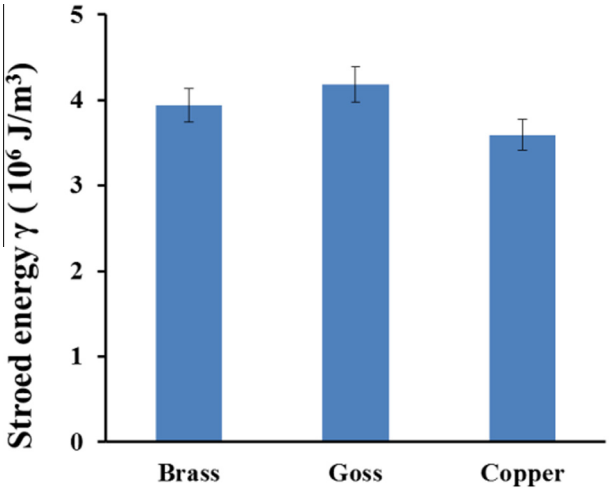

Fig. 2. Stored energy (per unit volume) of the three main components formed after cold rolling to 60% reduction.

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