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Development a dislocation density based model considering the effect of stacking fault energy: Severe plastic deformation

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ABSTRACT

Considering the effect of an intrinsic material parameter, stacking fault energy (SFE), a model based on dislocation density is developed to investigate the evolutions of dislocation density, cell size and flow stress during severe plastic deformation of aluminum and nickel. In fact a model is presented considering the work hardening and different annihilation mechanisms for dislocation densities in cell interiors and cell walls. Annihilation terms are developed on the basis of SFE through the model. The calculations show that the total dislocation density, dislocation density in cell interiors, dislocation density in cell walls and flow stress are decreased with increasing SFE. To verify the model results, they are compared with the experimental data and a good agreement is observed.

1. Introduction

In recent years, favorable physical and mechanical properties for metals are achieved through grain refinement processes [1,2]. Severe plastic deformation (SPD) technique is one of the most efficient ways to produce ultrafine-grained or nanostructured materials through the top-down approach [3–5]. Constrained groove pressing (CGP) is one of these techniques which has appropriate ability for grain refinement [6,7]. The principle of CGP is subjecting a material to large amount of plastic shear deformation with asymmetrically grooved and flat dies, alternatively [8].

There are many dislocation density based models to describe the flow stress evolution of material during plastic deformation [9–19]. In these models, dislocation density is considered as an internal variable of material and the development of dislocation density as a function of strain can be determined. Considering the Taylor theory [20], these models can predict the stress–strain curve of materials during plastic deformation. In addition, for the cell forming materials, the evolution of cell size can be calculated [11,12]. One of the most essential approaches to evaluate the deformation of materials is Kocks–Mecking model (K–M) [9,10]. The K–M model describes the deformation in term of total dislocation density. This approach has been developed in recent years [21,22] and some SPD processes have been analyzed on the basis of this model [23,24]. However, an adequate description for large strains related to SPD requires a more detailed representation of dislocation population in dislocation cell forming materials [25]. It has been shown that the collective tendency of dislocations is increased with increasing the strain value and as a result, a distinct dislocation structure consisted of two parts of cell interiors and cell walls is achieved at large strains [7,26,27]. The K–M model has not considered this point. Therefore, the K–M model cannot be appropriate for large strains [25]. Considering this limitation in the K–M model, Estrin et al. [11] proposed a two-dimensional dislocation model which considers large deformations and is based on evolutions of dislocations in cell walls and cell interiors. Toth et al. [12] extended the model to a three-dimensional model, which is known as ETMB (Y. Estrin, L.S. Toth, A. Molinari, Y. Brechet) model. In some investigations, the cell wall dislocation density is divided into two distinct groups of statistical dislocation density and geometrically necessary dislocation density [13,14]. Moreover, in some other studies plastic behavior of material is described through the evolutions of the mobile and forest dislocations [15–17], the evolutions of the polar and non-polar dislocations [18] or in terms of three types of dislocations [19] (the average mobile dislocation density, and the average immobile dislocation densities in the cell interiors and in the cell walls). Although some of these models consider more types of dislocations, their simplicity is less than others.

Among different models of plastic deformation, ETMB has been usually used in modeling of severely deformed metals [28–34]. Since 2002 to 2013, the model describes the behavior of different materials during SPD processes [28–34]. This model considers dislocation densities in cells (ρ_c) and walls (ρ_w) and assumes that the dislocations evolutions in each of cells or walls consist of: dislocation generation, migration of the dislocations from the cell interi-

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ors to the cell walls and dislocations annihilation called recovery [11]. Although the model gives results that are in good agreement with the experimental data, there are some problems in the model, especially in the annihilation description [35]. The annihilation of dislocations is dependent on the inherent characteristics of material, such as the degree of dislocation dissociation and the rate of self-diffusion [36–38]. However, ETMB model is based on mathematical expressions which are not dependent on the real material properties. Stacking fault energy (SFE) is the important intrinsic parameter of material which determines the extent of dislocation dissociation and influences on the configuration of dislocations [39]. It has been shown that a decrease in SFE reduces the dislocation annihilation rate during severe plastic deformation of metals [40]. However, this physical parameter has not yet been considered in the model. Besides the SFE, other physical parameters such as temperature are also important and should be considered [35,37]. In addition to above imperfections, ETMB model does not distinguish between the dislocations annihilation processes in the cell interiors and cell walls. However, the cell interiors and cell walls are two distinguish regions with different population of dislocation and should have different behaviors. Following the idea in Refs. [41–43], the softening is not similar in these parts for FCC materials. Annihilation in cell walls, where the average dislocation density is higher, is controlled by climb, while cross-slip processes are responsible for that in cell interiors [30]. Therefore, these two different mechanisms require distinguish expressions. Based on this fact, in some researches, different constants for cell interiors and walls are invoked in the coefficient and exponent parts of recovery terms [30,35,44]. These coefficients and exponents should be selected in accordance with the characteristics of materials. However, due to disregarding of material characteristics in the original formulation of ETMB model, the effect of SFE has been related to the constants. For example, in some researches it is declared that the recovery exponent of cell interiors is proportional to the stacking fault energy of the material and inversely proportional to the absolute temperature of deformation [30]. This assumption has been cited in different papers [12,45]. However, the validity of this assumption has not been examined in Ref. [30]. Verification of this assumption requires a comparison between materials with different SFE values, which has not been presented in Ref. [30]. On the other hand, some investigations have shown that this assumption is not correct and can be inconsistent with physical metallurgy [35]. Although Ref. [30] considered that the SFE of materials and the process temperature have not the same effects on the dynamic recovery kinetics, physical metallurgy describes that both parameters have similar effects on the dynamic recovery kinetics [35]. In Ref. [35], considering the application of model on two different materials, it is empirically assumed that SFE can be attributed to recovery coefficient of the cell interiors and temperature is related to recovery coefficient of the cell walls [35] which is in contrast to Ref. [30]. Therefore, it seems that disregarding of the influences of inherent material characteristics such as SFE through a physical metallurgy based approach and usage of empirical relations has led to contradiction with physical concepts or lack of solidarity in usage of ETMB annihilation terms in investigations. An improvement of model to a physical based model considering SFE, in addition to introducing solidarity in applications of model, make this chance to evaluate the effect of inherent parameters on model. Therefore, the aim of this paper is development of ETMB model to a material based model which considers intrinsic material parameters such as SFE.

2. Model development

The increase of dislocations in the cell walls consists of:

(a) Dislocation generation due to Frank-Read sources [12]:

$$\left(\frac{d\rho_w}{d\gamma}\right)^{+} = \frac{\sqrt{3}\beta^*(1-f)\sqrt{\rho_w}}{bf} \tag{1}$$

where b is the magnitude of Burgers vector, γ is the value of accumulated resolved shear strain, β^* is a constant and f is the volume fraction of cell walls [11,12]:

$$f = f_\infty + (f_0 - f_\infty)\exp(-\eta\gamma) \tag{2}$$

where f_∞, f_0 and η are the model parameters.

(b) Fraction (β^*) of dislocations of cell interiors which migrates to the cell walls during deformation [12]:

$$\left(\frac{d\rho_w}{d\gamma}\right)^{+} = \frac{6\beta^*(1-f)^{2/3}}{bdf} \tag{3}$$

where d is the cell size [45]:

$$d = \frac{K}{\sqrt{f\rho_w + (1-f)\rho_c}} \tag{4}$$

$$K = K_0 + K_1\exp(-\gamma/\kappa) \tag{5}$$

where K_0, K_1 and κ are the constants.

On the other hand, recovery reduces the density of dislocations within walls:

$$\left(\frac{d\rho_w}{d\gamma}\right)^{-} = -\frac{1}{\dot{\gamma}}\left(\frac{d\rho_w}{dt}\right)^{-} \tag{6}$$

where $\dot{\gamma}$ is the resolved shear strain rate and $\left(\frac{d\rho_w}{dt}\right)^{-}$ is the rate of annihilation in the walls. In the present work, it is assumed that the annihilation of dislocations in the cell walls occurs by the time dependent dissolution of dislocation dipoles through climb. The rate of decrease in dislocation density due to climb can be calculated as [46]:

$$\left(\frac{d\rho_w}{dt}\right)^{-} = 2\rho_w v^* \tag{7}$$

The factor 2 accounts for two dislocations which annihilate simultaneously at one single annihilation event. v^* is the frequency of process and represents the time required for a pair of edge dislocations to climb a distance $h/2$ in the cell walls:

$$v^* = \frac{2v_c}{h} \tag{8}$$

v_c is the climb velocity. The distance h can be estimated as [47]:

$$h = \frac{\delta Gb}{\tau_w} \tag{9}$$

where G is the shear modulus, δ is a constant and τ_w is the shear strength in the cell walls [48]:

$$\tau_w = \alpha Gb\sqrt{\rho_w} \tag{10}$$

where α is a material constant.

Climb is a diffusional based process which is controlled by net velocity of jogs along dislocations [46]:

$$v_c = c_j b v_j \tag{11}$$

Here, c_j is the jog concentration along the dislocation lines and can be estimated as [49]:

$$c_j = \sqrt{\rho_w} \tag{12}$$

v_j is the velocity of jogs and according to hard ball model can be expressed as [36]:

$$v_j = 2bvn_c\left(\frac{b}{D}\right)^2\exp\left(\frac{-U}{RT}\right)\left[\exp\left(\frac{\Omega\tau^*}{kT}\right) - 1\right] \tag{13}$$

where n_c is the number of nearest neighbor sites for diffusion and is approximately 11 in FCC metals [36]. v is the Debye frequency, k is