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Effects of grain size and initial immobile dislocation density on fatigue behavior of polycrystalline metals

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ABSTRACT

Grain size and initial dislocation density introduced by different mechanical processing methods may have a strong influence on fatigue behavior of polycrystalline metals. Using the reaction-diffusion model developed by Walgraef and Aifantis, we examined the ability of fatigue dislocation patterning and the evolution of dislocation density in the materials with different grain sizes (100 nm–10 μm) and initial immobile dislocation densities (IIDD, $1\times10^{12}\,m^{-2}$–$1.58\times10^{15}\,m^{-2}$). The results show that there is a clear relation among the necessary length scale for dislocation patterning, the grain size and the IIDD. Furthermore, the nominal life for fatigue damage initiation of these materials was evaluated based on the evolution of dislocation density and the ability of the dislocation patterning, showing good consistency with the experimental findings.

1. Introduction

In recent years, severe plastic deformation (SPD) techniques, such as accumulative roll bonding (ARB) [1], equal channel angular pressing (ECAP) [2,3], and high-pressure torsion (HPT) [4], have been developed to enhance tensile strength of metals through reducing grain size to submicron scales and introducing a high density of immobile dislocations in the form of dislocation tangles, cells, low-angle grain boundaries and/or geometrically necessary boundaries as well as pileups at the grain boundaries (GBs) [5]. Such variations in both the grain size and the initial defect density may influence fatigue behaviors of the materials, such as fatigue properties of the ultrafine-grained metals are not always satisfied in low cycle fatigue (LCF) regime [6–10], and ultrafine-grain Cu produced by SPD exhibited cyclic softening similar to that observed previously in moderately predeformed Cu [9].

It is well known that fatigue damage always preferentially originates from cyclic strain localization sites, where fatigue extrusions/intrusions corresponding to the formation of persistent slip bands (PSBs) (typical dislocation wall structure) have formed extensively [11]. Thus, the ability of dislocation patterning from randomly-distributed dislocations to veins, walls and cells [12–14] and the evolution of dislocation density strongly affect fatigue cycles needing for the formation of fatigue damage and cyclic deformation (hardening/softening) behavior [15–17]. Experimental results have revealed that there are no dislocation walls in the materials as the grain size or the geometrical scale becomes too small (less than ~1 μm)[13,14,18,19]. Dislocation patterning behavior i.e. the formation of PSBs, in fatigued materials as a cooperative phenomenon for dislocation populations has been simulated by the reaction-diffusion model developed by Walgraef and Aifantis [20] and Schiller and Walgraef [21]. Following the Walgrael–Aifantis(W–A) model, fatigue size effects on dislocation patterning behavior were investigated subsequently by Glazov and Laird [22] even though there are some limitations in the model [23]. In this paper, we will present a systematic examination on effects of grain size and initial immobile dislocation density (IIDD) on dislocation patterning and fatigue damage life of polycrystalline metals using the W–A model. Evolution of dislocation structures in the materials during cyclic loading was discussed.

2. Reaction-diffusion model and simulation method

In this study, we setup an one-dimensional system with grain size (L) ranging from 0.1 μm to 10 μm, and the system has different initial immobile dislocation density (ρ_{IIDD}) ranging from $1\times10^{12}\,m^{-2}$ to $1.58\times10^{15}\,m^{-2}$, and no initial mobile dislocations. These systems correspond to coarse-grained (CG), fine-grained (FG) and ultrafine-grained (UFG) materials with different processing states (i.e., annealing cold-worked or SPD). For example, a system with smaller L and higher ρ_{IIDD} refers to UFG materials produced by SPD, while the system with larger L and lower ρ_{IIDD} refers to annealed CG metal. In the case of $\rho_{IIDD}=1\times10^{12}\,m^{-2}$, there are no dislocations existing inside the

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$L < 1$ μm system, but in the subsequent simulation processes the dislocation will form inside the system. Thus, the value of the selected ρ_{IIDD} should be reasonable.

Similar to the self-organization phenomena in other systems, the dislocation patterns (dislocation walls) forming within the PSBs are the result of the dynamic equilibrium of different processes, such as dislocation nucleation, annihilation, pinning, and diffusion. Thus, dislocation patterning in the systems can be simulated by considering the fact that dislocation patterns result from the "reaction+diffusion" system of the mobile and the immobile dislocations [24]. This process can be described by the following differential equations [24]:

$$\begin{aligned} \frac{\partial X}{\partial t} &= D_x \nabla^2 X - bX + \gamma X^2 Y + g(X) \\ \frac{\partial Y}{\partial t} &= D_y \nabla^2 Y + bX - \gamma X^2 Y \end{aligned}, \quad (1)$$

where X and Y stand for densities of the immobile and the mobile dislocations, respectively. In fact, the edge dislocation dipoles in the dislocation walls and the matrix veins can be regarded as the immobile dislocations, while the screw dislocations between the walls in the PSB ladders and in the matrix veins as the mobile dislocations. The diffusion term ($D_x \nabla^2 X$ and $D_y \nabla^2 Y$) in Eq. (1) was formulated like the second Fick's law. The diffusion-like coefficients, D_x and D_y, were introduced to represent the ability of dislocation diffusion. The value of D_x is much larger than that of D_y. In the reaction term (bX and bY), the coefficient b mainly depends on the stress, strain and their rates.

The dislocation patterning behavior inside the grain was simulated using no-flux(close) boundary conditions as follows:

$$\begin{aligned} \frac{\partial X(0)}{\partial x} &= \frac{\partial X(L)}{\partial x} = 0 \\ \frac{\partial Y(0)}{\partial x} &= \frac{\partial Y(L)}{\partial x} = 0 \end{aligned}, \quad (2)$$

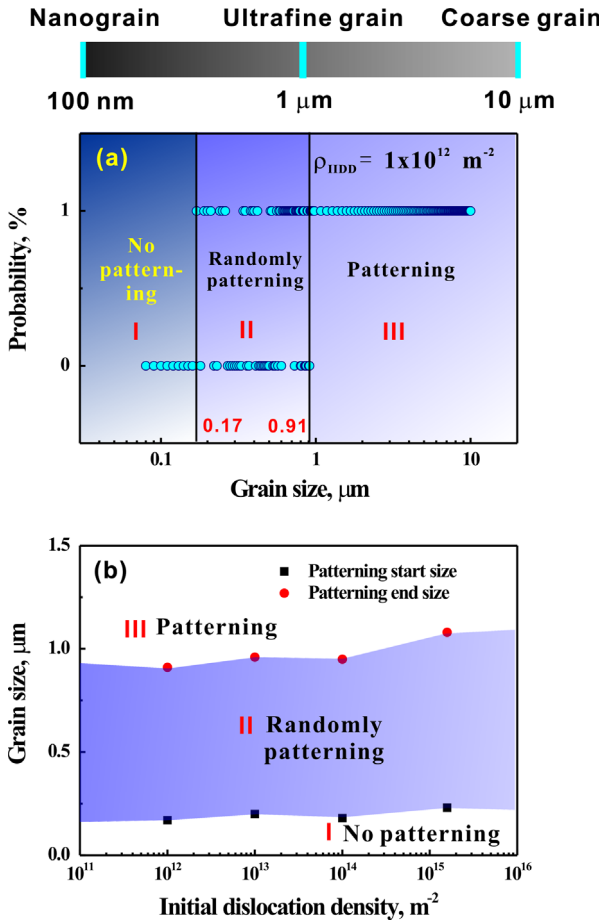

Fig. 2. (a) Possibility of dislocation patterning as a function of grain size with $\rho_{IIDD} = 1 \times 10^{12}$ m^{-2}, (b) relationship between the dislocation patterning-needed (DPN) grain size and the initial immobile dislocation density.

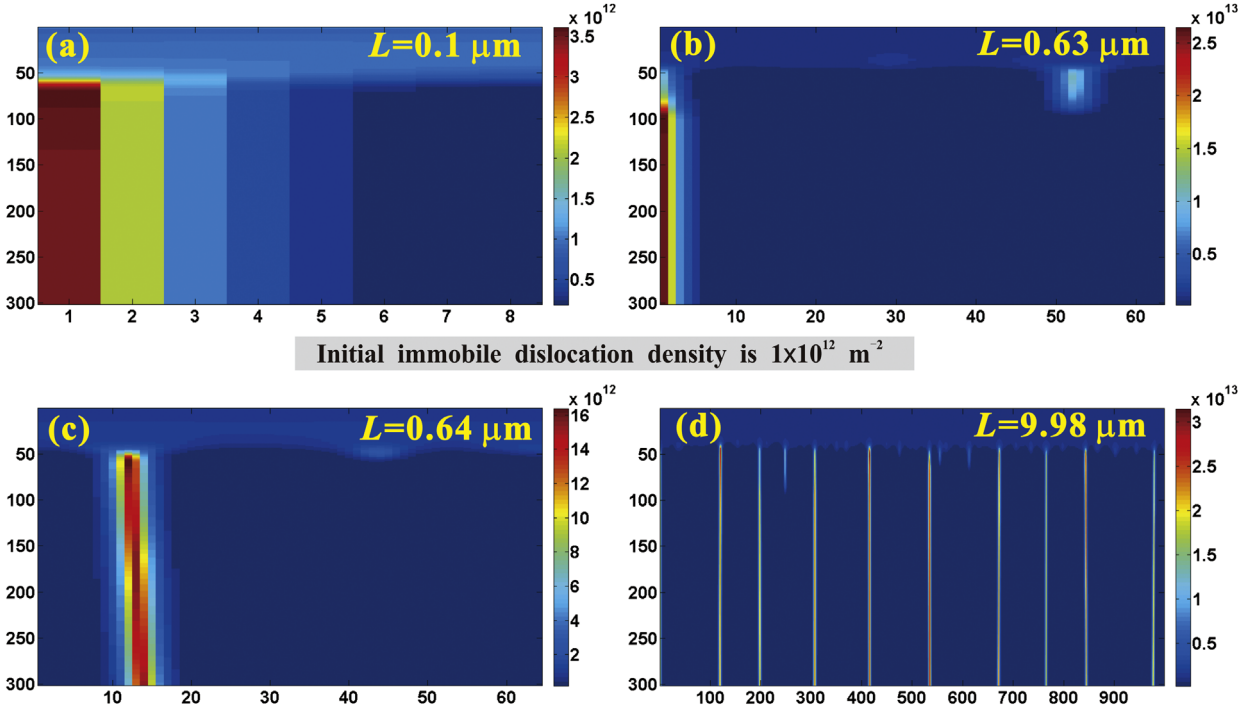

Fig. 1. Dislocation patterning behavior inside the grains with a size of L=(a) 0.08, (b) 0.63, (c) 0.64, and (d) 9.98 μm for a given $\rho_{IIDD} = 1 \times 10^{12}$ m^{-2}, respectively. The Y axis indicates nominal fatigue cycles and the X axis refers to the location for dislocation patterning.