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Multiscale constitutive modeling for plastic deformation of nanocrystalline materials

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ABSTRACT

Macroscopic and microscopic constitutive modeling that can display large plastic deformation with shear band were presented for nanocrystalline materials subjected to uniaxial load over a wide strain rate range. The macroscopic model implemented with parameters microscopic meaning was established based on the theory of plastic dissipation energy. The microscopic model based on deformation mechanisms was composed of two parts: hardening and softening stages. In the hardening stage, the phase mixture model was used and a shear band deformation mechanism was proposed in the softening stage. Numerical simulations shown that the predications were in good agreement with experimental data. Finally, a parameter of normalized softening rate was proposed and its characteristics were evaluated quantitatively. It can be concluded that the failure strain could be prolonged when the normalized softening rate decrease through changing the softening path.

1. Introduction

Nanocrystalline materials, because of their distinctive mechanical and physical properties, have attracted a great deal of attention from material science community [1,2]. Novel varieties of nanocrystalline materials and newly synthesis methods come forth continuously. Studies on their properties, one of which is concerning to the plastic deformation, have been deep into the microscopic field [3–7]. The mechanisms of plastic deformation for nanocrystalline materials are very complicated. Many researchers have tried to reveal the relations between experimental observations and essence based on the microstructure. There are four major deformation mechanisms have been proposed to deal with small uniform plastic deformation. These mechanisms contain grain-boundary diffusion, grain-boundary sliding, dislocation and lattice diffusion [8–12]. In real process of deformation, the effective mechanisms acted on the grains maybe not only one but two or more combined. Kim and Estrin [13] presented a phase mixture model to simulate the deformation behavior of nanocrystalline materials. They considered that the deformation in grain interior phase was controlled by dislocation and diffusion mechanism and grain boundary phase was governed by boundary diffusion mechanism. Zhou et al. [14] proposed a constitutive model based on phase mixture model to simulate deformation behavior of bcc and fcc nanocrystalline materials, respectively. However, none of these models have treated softening behavior as part of considerations. Gutkin et al. [15] gave a model holding that deformation-induced migration of grain boundaries and their triple junctions caused local softening in nanocrystalline samples under superplastic deformation. A grain rotation based geometric softening mechanism was presented by Joshi and Ramesh [16] for predicting the development of shear band in nanocrystalline materials under quasi-static loading rates. Nevertheless, they still cannot evaluate the failure strain of nanocrystalline materials with obvious plastic deformation quantitatively. In this paper, a mechanism with respect to the generation and development of shear band will be proposed, and the corresponding microscopic model based on the deformation mechanism will be derived. Further, a macroscopic constitutive model, where the parameters have the microscopic meaning, will be established.

2. Constitutive model

2.1. Macroscopic constitutive model

For nanocrystalline materials with macroscopic softening plastic deformation, the theory of plastic dissipation energy presented by Li and Howard [17] can be employed here. The increment of the plastic dissipation energy in the process of deformation is:

$$dW^{(p)} = \sigma_{ij} d\varepsilon_{ij}^{(p)} \tag{1}$$

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