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A constitutive model for the mechanical behaviors of bcc and fcc nanocrystalline metals over a wide strain rate range

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Abstract

A new constitutive model based on the deformation mechanisms was developed for both bcc and fcc nanocrystalline metals over a wide strain rate range. Nanocrystalline metals were treated as composites consisting of grain interior and grain boundary phases, and the deformation mechanisms and physically based constitutive relations of grain interior and grain boundary phases over a wide strain rate range were analyzed and determined for both fcc and bcc nanocrystalline metals. Based on our recently established phase mixture method, a new mechanical model was built to calculate the stress–strain relations of nanocrystalline metals over a wide strain rate range; and the grain size and porosity effect was considered in the developed model, the predictions keep in good agreements with various experimental data in small plastic strain range, where uniform deformation can be assumed. Further discussion was presented for calculation results and relative experimental observations.

Keywords: Nanocrystalline materials; Deformation mechanism; Constitutive model; Strain rate sensitivity

1. Introduction

Nanocrystalline materials, defined as polycrystalline materials with average grain size less than 100 nm, have been a source of great interest currently due to their unusual mechanical and physical properties. Many results have shown that nanocrystalline materials exhibit the grain size and strain rate dependent mechanical behaviors, the most recent relative review can be seen in Ref. [1]. To understand this sort of mechanical behavior, several models have been proposed recently using the concept of a two-phase composite. Capolungo et al. [2] used a homogenization method to describe the grain size and strain rate effects on the stress–strain relations. However, they assumed that grain boundary phase has an elastic perfect-plastic behavior, which could be refined as mentioned in their paper. Meanwhile, diffusion controlled plastic flow has been omitted in their model. Jiang and Weng [3] proposed a generalized self-consistent polycrystal model to simulate the grain size dependent mechanical behavior of nanocrystalline materials, but rate-independent case was assumed in their model. Zhu et al. [4] developed a polycrystalline constitutive theory based on the model [5] of Asaro, Krysl, and Kad (AKK) for deformation mechanisms in nanocrystalline metals and the extended aggregate Taylor model [6] of Asaro and Needleman (AN). Their work presented a thoroughly description of the dislocation mechanism for nanocrystalline materials, but they didn't include diffusion mechanism. Kim and Estrin [7] proposed a phase mixture model to simulate the deformation behavior of nanocrystalline material, which was treated as a mixture of two phases: grain interior material whose plastic deformation was governed by dislocation and diffusion mechanism and grain boundary phase whose plastic flow is controlled by a boundary diffusion mechanism. Using a simple rule of mixtures, the grain size and strain rate dependence of the overall plastic deformation behavior of nanocrystalline materials was described. But it should be noted that the *iso*-strain assumption applied in their model is only one of extreme assumptions for composite materials (the other extreme assumption is *iso*-stress). Despite the successes provided by these models, the effects of grain size and strain rate (especially in a wide strain rate range) on the mechanical behavior of nanocrystalline materials are not well described in term of their main deformation mechanisms as yet, and none of them mentioned the difference between the mechanical behaviors of fcc and bcc nanocrystalline materials in a numerical way.

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The deformation mechanism of the nanocrystalline material is very complicated. Even for a same material, the deformation mechanism will also change with the further deformation. For example, shear band evolution phenomena during the plastic deformation process have been observed in the tension and compression tests [8,9], this indicates that the deformation will become non-uniform in the plastic deformation and this will be further analyzed in the discussion. As a first step, we will be focused on the mechanical behavior of the nanocrystalline metals in small plastic strain range where uniform deformation can be assumed. The grain interior and grain boundary deformation mechanisms and physically based constitutive relations over s wide strain rate range will be firstly analyzed and determined for both fcc and bcc nanocrystalline metals, then a new mechanical model based on our recently established phase mixture approach will be built to calculate the stress–strain relations of nanocrystalline metals over a wide strain rate range, and the grain size and porosity effect will be considered in the developed model. The developed model will be used to simulate the grain size and strain rate dependent mechanical behavior of both bcc and fcc nanocrystalline materials, and the simulation results will be compared with various experimental data. Finally, further discussion will be presented for the different stress–strain response, shear localization behaviors and strain rate sensitivity of bcc and fcc nanocrystalline metals.

2. Time-dependent mechanical modeling for nanocrystalline materials

2.1. A new phase mixture model

Nanocrystalline materials were usually treated as composite materials with grain interior phase and inter-grain phases such as grain boundary and triple junctions. Since the volume fraction of triple junctions becomes significant only when $d < 10$ nm [2]. In this paper, triple junctions were incorporated in grain boundary phase. This simplification should not have a major influence on the results for materials with a grain size greater than 10 nm. Recently, we have proposed a new phase mixture model [10] to describe the intermediate mechanical behavior between two extreme status (*iso*-strain and *iso*-stress assumption) status, nanocrystalline metals were assumed to be composed of an array of repeating unit cubic cells, each cell consists of two phases: grain interior phase and grain boundary phase, and grain boundary phase has two parts: part I includes four side layers around the cubic grain; part II contains two layers (upper layer and lower layer), as shown in Fig. 1. Thus the strain of part I, denoted as $\varepsilon_{\mathrm{GBI}}$, is same with that of the grain interior, $\varepsilon_{\mathrm{GI}}$; meanwhile, the stress of part II, denoted as σ_{GB1}, equals to the total stress of grain interior and part I of grain boundary, σ_{t}. Given the grain size d and grain boundary thickness δ, one can get volume fraction of grain interior phase, part I and part II of grain boundary phase, denoted as f_{GB1}, f_{GB2} and f_{GB2}, by their geometrical definitions as follows:

$$f_{\mathrm{GI}} = \frac{(d-\delta)^3}{d^3}, \tag{1}$$

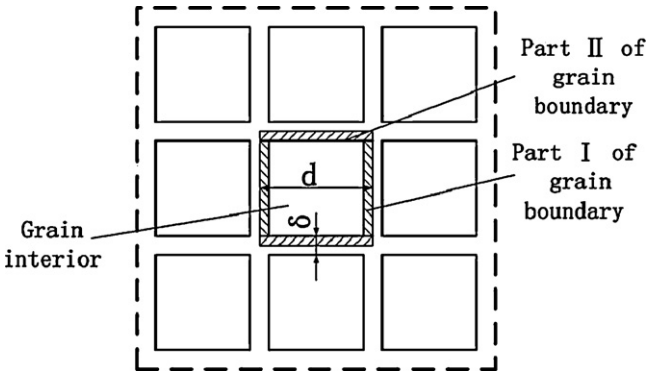

Fig. 1. The structure of unit cubic cell.

$$f_{\mathrm{GB1}} = 1 - \frac{\delta}{d} - \frac{(d-\delta)^3}{d^3}, \tag{2}$$

$$f_{\mathrm{GB2}} = \frac{\delta}{d}, \tag{3}$$

It should be noted that Eqs. (2) and (3) are only exactly right for the cubic unit cell case. Here, we can give a definition of 'equivalent' *iso*-strain part (part I) and *iso*-stress part (part II) by adjusting the value of f_{GB1} (the total volume fractions ($f_{\mathrm{GB1}} + f_{\mathrm{GB2}}$) of the grain boundary phase keep constant). Thus, the volume fractions of 'equivalent' *iso*-strain part (part I) and *iso*-stress part (part II), denoted as f'_{GB1} and f'_{GB2}, can be expressed as

$$f'_{\mathrm{GB1}} = 1 - \xi\frac{\delta}{d} - \frac{(d-\delta)^3}{d^3}, \tag{4}$$

$$f'_{\mathrm{GB2}} = \xi\frac{\delta}{d}, \tag{5}$$

where ξ is a modification factor and can be determined by experimental results finally. Further, the macroscopic stress and strain of nanocrystalline materials, denoted as σ and ε, can be expressed as

$$\sigma = \sigma_{\mathrm{t}} = \sigma_{\mathrm{GB2}} = \sigma_{\mathrm{GI}}\frac{f_{\mathrm{GI}}}{f_{\mathrm{GI}} + f'_{\mathrm{GB1}}} + \sigma_{\mathrm{GB1}}\frac{f'_{\mathrm{GB1}}}{f_{\mathrm{GI}} + f'_{\mathrm{GB1}}}, \tag{6}$$

$$\varepsilon = \varepsilon_{\mathrm{t}}(f_{\mathrm{GI}} + f'_{\mathrm{GB1}}) + \varepsilon_{\mathrm{GB2}} f'_{\mathrm{GB2}}, \tag{7}$$

In above equations, σ_{t} is the total stress of grain interior and part I of grain boundary. σ_{GI}, σ_{GBI} and σ_{GBI2} are the stresses of grain interior phase, part I and part II of grain boundary phase respectively;$\varepsilon_{\mathrm{GI}}$,$\varepsilon_{\mathrm{GBI}}$ and $\varepsilon_{\mathrm{GB2}}$ represent the strains of grain interior phase, part I and part II of grain boundary phase respectively. With the determination of constitutive relations of grain interior and grain boundary phase in term of their main deformation mechanisms (presented in Section 2.2), the macroscopic stress–strain relation of nanocrystalline materials can be built by combining the mechanical behaviors of grain interior, part I and part II of grain boundary based on the above model.