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Prediction of mechanical properties in bimodal nanotwinned metals with a composite structure

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ABSTRACT

Nanostructured face-centered cubic (fcc) metals with nanoscale twin lamellae and multiple distribution of microstructural size are proved to possess higher yield strength and good ductility. In this paper, a mechanism-based theoretical model is developed to simulate the yield strength, strain hardening, and uniform elongation of the nanotwinned composite metals with bimodal distribution of microstructural size. The mechanisms of strengthening and the failure in such bimodal nanotwinned metals are studied for evaluating the strength and ductility. A modified mean-field approach is adopted here to calculate the total stress-strain response of this kind of nanotwinned composite structures. The contribution of microcracks generated during plastic deformation has been taken into account to predict strain hardening and uniform elongation. Our simulation results indicate that the proposed model can successfully describe the mechanical properties of bimodal nanotwinned metals with a composite structure, including the yield strength and ductility. We further demonstrate that the yield strength and elongation are both sensitive to the twin spacing and the volume fraction of components. The calculations based on the proposed model agree well with the experimental results. These findings suggest that the high yield strength and high ductility can be achieved by optimizing the grain size and the twin spacings in the nanotwinned composite structures.

1. Introduction

Nanostructured metals have stimulated vast interests due to their distinctive mechanical properties, for example, the superior mechanical strength compared to those of corresponding coarse-grained counterparts [1–7], which make these materials play the essential role in designing lighter and stronger structures of technological applications. Unfortunately, the improved strength in nanostructured metals is always achieved with the loss of ductility and work-hardening capability [3,4,8–13], which is similar to the traditional strengthening methods such as refining grain size, solid solution alloying and phase transformation. Therefore, how to achieve the simultaneously higher strength and ductility in metals and alloys is the essentially challenging issue in the application of the nanostructured metals. In the past ten years a great number of endeavors have been made to explore how to improve the strength with keeping good ductility and toughness. Mixing the various sizes of microstructures in nanostructured metals have been proved as an effective approach for a superior synergy in strength and ductility. For example, the nanostructured metallic materials with bi/multi-modal grain size distribution perform higher yield strength with a good ductility [14–23]. Generating the intrinsic twin boundaries in polycrystalline metals is also an alternative method to improve the tensile ductility in higher-strength nanostructured metals, such as the nanotwinned polycrystalline coppers and nanotwinned stainless steels [24–28]. More recently, a novel strategy is developed to strengthen the metallic materials by means of dynamic plastic deformation to embed the nanotwinned grains into the matrix of nano-sized grains or coarse-grains. Such nanotwinned composites with bimodal distribution of microstructural size exhibit the excellent combination of strength and ductility [29–32].

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After discovering the effective methodologies in experiments for enhancing the strength-ductility synergy, a plenty of theoretical studies have been carried out to investigate the deformation mechanisms and then to predict the corresponding mechanical properties. In general, micromechanical models and finite element methods are widely utilized to simulate the stress-strain response in the composite nanomaterials such as the particle reinforced metals matrix composites and nanograins/nanotwins strengthened composite metallic materials [20–23,33–38]. For the nanotructured metals with a bimodal grain size distribution, the secant Mori-Tanaka (M-T) mean-field approach [20,21,39] and the visco-plastic self-consistent scheme [40,41] are often applied to simulate the yield strength and ductility of such composite structure, which are sensitive to the grain size distribution and volume fraction of component. For the nanotwinned polycrystalline metals, the molecular dynamic (MD) simulations are performed usually in the atomic scale to quantify the contributions of the twin boundaries (TBs) to the strength, strain hardening and toughness [42–47]. The mechanism-based theoretical models with a continuum description are presented to describe the mechanical behaviors in the nanotwinned metal. For example, the crystal plasticity models for nanotwinned copper were developed to simulate the stress-strain response as well as the fracture behaviors by finite element method [38,48–50]. The dislocation density-based plasticity models were developed to describe the variation of strength, strain hardening and the ductility of nanotwinned metals with the twin spacing, and a scale law of the maximum strength in nanotwinned metals was explored [51–54]. However, for the nanotwinned composite metals, it remains unclear how to predict the mechanical properties as the functions of grain size, twin spacing, and volume fraction of each component. The explicit theoretical model that enables to describe the experimental results is still in lack.

In this work, a micromechanical composite model is developed to study the mechanical properties of nanotwinned composites with a bimodal distribution of microstructural size. The mechanism-based plastic model for nanotwinned metals is adopted to describe the constitutive relation of nanotwinned phase. The strain-gradient plastic model is also presented to simulate the stress-strain relation of nano/ultrafine grained phase. In the framework of composite model, the contribution of microcracks generating during plastic deformation is taken into account in the mechanical properties of the bimodal nanotwinned composite. The calculations demonstrate that our proposed theoretical model can completely characterize the mechanical properties such as the yield strength, strain hardening, and elongation in such kind bimodal nanotwinned metal. These properties are sensitive to the microstructural size such as the twin spacing and grain size, as well as the volume fraction of each component.

2. Theoretical description

2.1. Composite model

Experiments have demonstrated that the bulk nanostructured austenitic stainless steel contains nano-sized/coarse grains with the nanoscale nanotwins embeded in micro-size grains by means of dynamic plastic deformation [30,32]. This complex microstructure can be characterized by a composite structure with a bimodal distribution of microstructures. This nanotwinned composite metal consists of polycrystalline phase and nanotwinned phase, as shown in Fig. 1. Motivated by this observation, we can consider the grain size in polycrystalline phase and twin spacing in nanotwinned phase as the bimodal size distribution in such nanotwinned composite metals. As a consequence, a modified mean-field approach is applied to simulate the stress-strain response of the bimodal nanotwinned metals, and the influence of bimodal size distribution must be taken into account. From the micromechanical model developed by Weng [55,56], the relationship between the hydrostatic and deviatoric strains of the constituent phases and those of the composite follows

$$\begin{aligned}\varepsilon_{kk}^{(0)} &= \frac{\alpha_0^s(\kappa_1-\kappa_0)+\kappa_0}{c_0\alpha_0^s(\kappa_1-\kappa_0)+\kappa_0}\bar{\varepsilon}_{kk},\ \varepsilon_{ij}^{(0)'} = \frac{\beta_0^s(\mu_1-\mu_0^s)}{c_0\beta_0^s(\mu_1-\mu_0^s)+\mu_0^s}\bar{\varepsilon}'_{ij} - \frac{c_1\beta_0^s\mu_1}{c_0\beta_0^s(\mu_1-\mu_0^s)+\mu_0^s}\varepsilon_{ij}^{p(1)} \\ \varepsilon_{kk}^{(1)} &= \frac{\kappa_0}{c_0\alpha_0^s(\kappa_1-\kappa_0)+\kappa_0}\bar{\varepsilon}_{kk},\ \varepsilon_{ij}^{(1)'} = \frac{\mu_0^s}{c_0\beta_0^s(\mu_1-\mu_0^s)+\mu_0^s}\bar{\varepsilon}'_{ij} + \frac{c_0\beta_0^s\mu_1}{c_0\beta_0^s(\mu_1-\mu_0^s)+\mu_0^s}\varepsilon_{ij}^{p(1)},\end{aligned} \tag{1}$$

and the mean stress components of polycrystalline phase and nanotwinned phase are given by

$$\begin{aligned}\sigma_{kk}^{(1)} &= 3\kappa_0\frac{\kappa_1}{c_0\alpha_0^s(\kappa_1-\kappa_0)+\kappa_0}\bar{\varepsilon}_{kk},\ \sigma_{ij}^{(1)'} = \frac{2\mu_0^s\mu_1\left[\bar{\varepsilon}'_{ij}-(1-c_0\beta_0^s)\varepsilon_{ij}^{p(1)}\right]}{c_0\beta_0^s(\mu_1-\mu_0^s)+\mu_0^s} \\ \sigma_{kk}^{(0)} &= 3\kappa_0\frac{\alpha_0^s(\kappa_1-\kappa_0)+\kappa_0}{c_0\alpha_0^s(\kappa_1-\kappa_0)+\kappa_0}\bar{\varepsilon}_{kk},\ \sigma_{ij}^{(0)'} = \frac{2\mu_0^s\left\{\left[\beta_0^s(\mu_1-\mu_0^s)+\mu_0^s\right]\bar{\varepsilon}'_{ij}-c_1\beta_0^s\mu_1\varepsilon_{ij}^{p(1)}\right\}}{c_0\beta_0^s(\mu_1-\mu_0^s)+\mu_0^s}.\end{aligned} \tag{2}$$

Therefore, the dilatational and deviatoric stresses and strains of the composite are connected by

$$\begin{aligned}\bar{\sigma}_{kk} &= 3\kappa_0\left[1+\frac{c_1(\kappa_1-\kappa_0)}{c_0\alpha_0^s(\kappa_1-\kappa_0)+\kappa_0}\right]\bar{\varepsilon}_{kk}, \\ \bar{\sigma}'_{ij} &= 2\mu_0^s\left\{\left[1+\frac{c_1(\mu_1-\mu_0^s)}{c_0\beta_0^s(\mu_1-\mu_0^s)+\mu_0^s}\right]\bar{\varepsilon}'_{ij}-\frac{c_1\mu_1}{c_0\beta_0^s(\mu_1-\mu_0^s)+\mu_0^s}\varepsilon_{ij}^{p(1)}\right\}.\end{aligned} \tag{3}$$