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DEFORMATION MECHANISM OF BIMODAL METAL-GRAPHENE COMPOSITES WITH NANOTWINNED STRUCTURE

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Abstract. The theoretical model is suggested which describes micromechanisms of plastic deformation in bimodal metal-graphene composite consisting of large grains embedded into nanocrystalline/ultrafine-grained metal-matrix reinforced by graphene inclusions. In the framework of the model, lattice dislocation slip and grain boundary sliding has occurred in nanocrystalline/ultrafine-grained matrix, and lattice dislocation slip and migration of twin boundaries are realized in large grains with a nanotwinned structure providing the plastic deformation of bimodal metal-graphene composite. With this assumption, the yield stress of nanotwinned bimodal metal-graphene composite was calculated.
Keywords: metal-graphene composite, bimodal structure, nanotwins, twin boundaries, yield stress

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1. Introduction

It is well known that suppression of the lattice dislocation slip by graphene inclusions is the main mechanism of the hardening of metal-graphene composites [1-3]. It leads to a significant decrease in the ductility of the metal-graphene nanocomposites in comparison with the initial nanocrystalline/ultrafine-grained (NC/UFG) materials without graphene inclusions. For example, the experiments [2] on measuring the microhardness and elongation to failure of the copper-graphene composite show an increase in microhardness by 39% and a decrease in elongation to failure by more than 3 times, as compared to pure copper.

At the same time, a new class of materials with a bimodal structure (materials consisting of large (micrometer-size) grains embedded into a NC/UFG matrix) has been presented. According to the experimental papers [4-6] and computer simulations [7-9], the presence of the large (micrometer-size) grains into a NC/UFG matrix reinforced by graphene inclusions can significantly increase the ductility of the metal-graphene composite.

Thus, the main aim of this paper is to suggest a theoretical model which describes peculiarities of the plastic deformation and the yield stress of the bimodal metal graphene composites with nanotwinned structure.

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2. Model

Consider a two-dimensional model of a bimodal composite solid that consists of an NC/UFG metallic matrix with the inclusions in the form of graphene platelets and large grains with nanotwinned structure, loaded by an uniaxial tensile load σ (Fig. 1). Suppose that graphene platelets are mostly located along the grain boundaries in the metal matrix, and assume that graphene platelets adhere well to the matrix and do not contain pores. In the model, graphene platelets are presented by discs of diameter L and thickness H. Following model [10], we also assume that large grains do not contain graphene platelets and include $N+1$ identical nanotwins of the same thickness λ and length d_{CG} distributed periodically (Fig. 1).

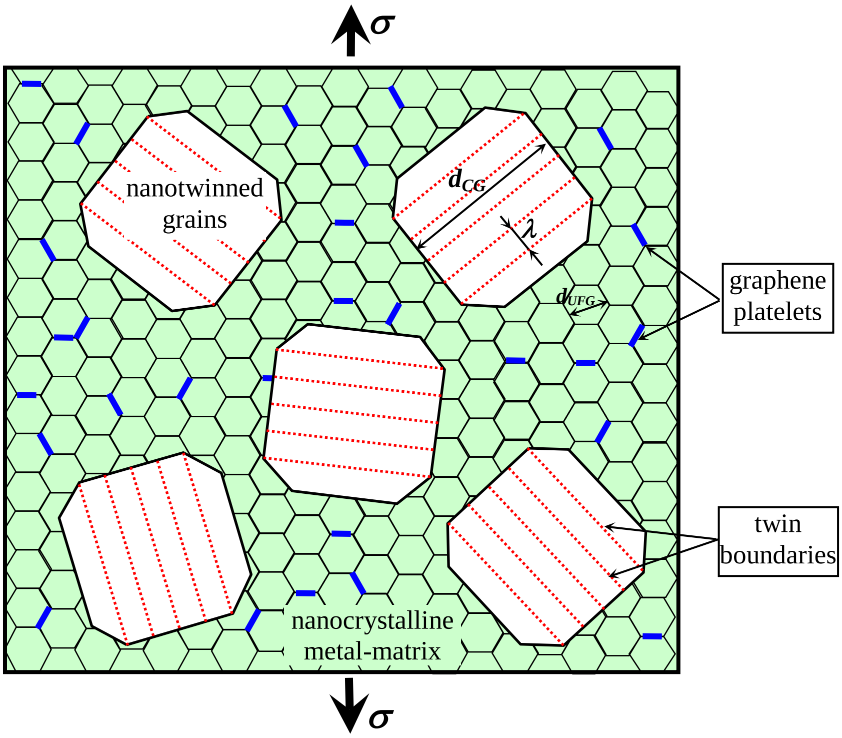

Fig. 1. Model of the bimodal metal-graphene composite consisting of large grains with nanotwinned structure embedded into NC/UFG metal matrix reinforced by graphene inclusions

Therefore, these nanotwins are divided by N twin boundaries, with the same distance λ between them (Fig. 1). The action of external tensile stress σ causes shear stress τ along the twin boundaries. For our model, the action of shear stress τ causes slip of the partial dislocations with Burgers vectors b (partial b-dislocations) along the planes parallel to the twin boundaries. At the same time, the slip of the partial dislocations (for FCC materials – the Shockley dislocations) along the planes parallel to the twin boundaries serves as the primary mechanism of migration of the twin boundaries in the direction normal to the twin plane by one interplane distance $\delta = a/\sqrt{3}$, where a is the crystal lattice parameter.

Along with twin boundary migration, other deformation mechanisms can act in nanotwinned grains. For example, these mechanisms are the emission of partial dislocation from grain boundaries and the motion of jogged dislocations. However, according to experimental data [11,12] and theoretical model [10], two principal deformation mechanisms act in the nanotwinned materials: twin boundary migration and dislocation motion across twins.

At the same time, according to paper [13], plastic deformation of NC/UFG metallic matrix with graphene inclusions can be realized through two mechanisms: the emission of lattice dislocations from GBs and their sliding through the grain, and grain boundary sliding.

Further, calculate the yield stress of bimodal metal-graphene composites with nanotwinned structure.

3. Yield stress of bimodal metal-graphene composites with nanotwinned structure

Following the theoretical model [10], the yield stress of nanotwinned solid has the form

$$\sigma_y^{NT} = \begin{cases} \sigma_{TBM}, & \lambda < \lambda_*, \\ \alpha\sigma_{TBM} + (1-\alpha)\sigma_{HP}^{NT}, & \lambda \geq \lambda_*. \end{cases} \quad (1)$$

where σ_{TMB} is yield stress associated with twin boundary migration (see [10], for details), $\sigma_{HP}^{NT} = \sigma_0 + K\lambda^{-1/2}$ is the classical Hall–Petch law, σ_0 and K are the materials parameters, α is the volume fraction of the large grains where the yield stress is equal to the σ_{TBM}.

According to the theoretical model [13], the yield stress of the UFG metal-graphene composite with graphene inclusions is given as

$$\sigma_y^{UFG} = f_{gr}\min(\sigma_{c1}, \sigma_{c2}) + (1 - f_{gr})\sigma_{c1}, \quad (2)$$

where $\sigma_{c1} = \sigma_{c0} + \sigma_{em}^{GB}$ is critical stress for emitting lattice dislocations from grain boundaries, $\sigma_{c0} = \sigma_0 + Kd_{UFG}{}^{-1/2}$, d_{UFG} is mean grain size of UFG matrix, $\sigma_{c2} = M_1\tau_{c2}$, $\tau_{c2} = 140$ MPa [14] is the critical shear stress for slipping graphite monolayers, M_1 is the geometric factor, f_{gr} is the fraction of grain boundaries containing graphene (see [13], for details) and σ_{em}^{GB} is the stress necessary to free a dislocation segment pinned by obstacles lying at a distance l from each other which has the following form [15]

$$\sigma_{em}^{GB} = \frac{MGb}{4\pi(1-\nu)l}\left\{\left[2 - \nu\left(3 - 4\cos^2\gamma_0\right)\right]\ln\frac{l}{b} - 2 + \nu\right\}, \quad (3)$$

where $M = 3.06$ is the Taylor factor for face-centered cubic crystals [16], and γ_0 is the angle between the Burgers vector of a rectilinear dislocation and its line, $l = L(\pi^2 - 8f_{GB})/4\pi f_{GB}$ [17] is the distance between the nearest points of neighboring graphene platelets lying in one GB, $f_{GB} = f_v d_{UFG}/(3H)$ is the fraction of grain boundary area in the UFG phase occupied by graphene, f_v is the volume fraction of graphene.

Formulas (1)-(3) allow to express the yield stress of bimodal metal graphene composites with nanotwinned structure as follows:

$$\sigma_y = \beta\sigma_y^{NT} + (1-\beta)\sigma_y^{UFG}, \quad (4)$$

where β is the volume fraction of the large grains with nanotwinned structure.

4. Results and Discussion

Using formulas (1)-(4), calculate the dependence of the yield stress σ_y on the twin thickness λ for the case of bimodal Cu-graphene composite characterized by the following parameter values: $G = 44$ GPa, $\nu = 0.38$, $b = 0.25$ nm, $a = 0.352$ nm [15], $\sigma_0 = 200$ MPa and $K_{HP} = 1750$ MPa [18]. We also put $d_{CG} = 1000$nm, $\alpha = 0.4$, $\lambda_* = 15$ nm [11,12], $d_{UFG} = 200$ nm, $\gamma_0 = 60°$, $M_1 = M$, $L = 100$ nm, $H = 3.5$ nm, $N = 2N'$, $N' = \lfloor d/2\lambda \rfloor$, where $\lfloor X \rfloor$ means an integer part of a rational number X. The calculated dependence $\sigma_y(\lambda)$ (the solid lines 1, 2 and 3) is shown in Fig. 2 for various values of the volume fraction β (0.3, 0.5 and 0.7, respectively) of large grains. The dashed line 4 in Fig. 2 depicts the theoretical dependence of the yield stress on the twin thickness for UFG nanotwinned Cu obtained in paper [10]. The horizontal dashed line 5 defines the yield stress σ_y^{UFG} of UFG metal-graphene matrix without nanotwinned grains. The dependences $\sigma_y(\lambda)$ (curves 1-3) in Fig. 2 show the transition from softening to hardening at $\lambda = 15\,\text{nm}$ and define that optimum twin thickness λ is equal to 15 nm as well as in the case of UFG nanotwinned Cu (curve 4). The dependencies in Fig. 2 also demonstrate that the yield stress σ_y of bimodal metal-graphene composite with nanotwinned structure is higher than the yield stress σ_y^{UFG} of the UFG metal-graphene composite without nanotwinned grains in the range of the twin thickness $10\text{nm} < \lambda < 40\text{nm}$.

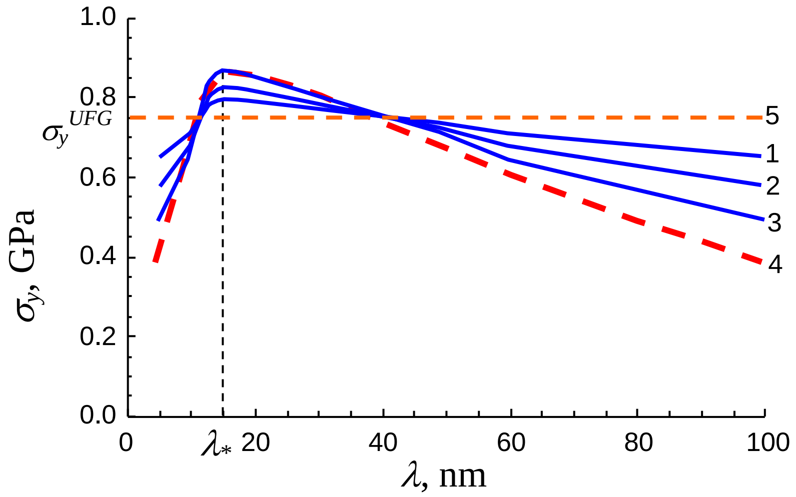

Fig. 2. The dependences of the yield stress σ_y on the twin thickness λ for bimodal nanotwinned Cu-graphene composite (curves 1-3), for UFG nanotwinned Cu (curves 4) and for NC/UFG metal-graphene composite (curve 5)

5. Calculation

Thus, the theoretical model which describes the plastic deformation mechanisms of the bimodal metal-graphene composite with nanotwinned structure has been developed. Within the model, the principal deformation mechanisms represent the twin boundary migration and the dislocation motion across the twins in the nanotwinned grains, and the lattice dislocation slip and the grain boundary sliding in the UFG metal-graphene matrix. The dependence of the yield stress of the bimodal Cu-graphene composite with the nanotwinned structure on the twin thickness has been calculated. The results of the calculations demonstrate the transition from the strengthening to the softening of the composite at a critical twin thickness λ_* (Fig. 2) and the strong dependence of the yield stress of the bimodal metal-graphene composites on the volume fraction of the large grains with nanotwinned structure and the twin thickness. Also, it was shown that the yield stress of the bimodal metal-graphene composite with large nanotwinned grains exceeds the yield stress of the UFG metal-graphene composite without nanotwinned grains in a wide range of the twin thickness. Besides, it is well known that the presence of the large grains with nanotwinned structure embedded into the UFG metal-matrix reinforced by graphene inclusions significantly increases the ductility of the metal-graphene composites. Thus, the bimodal metal-graphene composite with large nanotwinned grains exhibits simultaneously high strength and ductility exceeding those of the conventional metal-graphene composites.

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