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Mechanism of fracture toughness enhancement in bimodal metal-graphene composites with nanotwinned structure

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Abstract. A theoretical model is suggested which describes a mechanism of the fracture toughness in a bimodal nanotwinned metal-graphene composite consisting of large grains with nanotwinned structure embedded into ultrafine-grained/nanocrystalline metal-matrix reinforced by graphene inclusions. In the framework of the model, the migration of nanotwin boundaries in the large grains releases in part local stresses near crack tips and provides the enhancement of the plastic deformation of the bimodal nanotwinned metal-graphene composites. At the same time, the presence of the graphene inclusions induces the crack bridging effect which also increases the fracture toughness of the metal-graphene composites. In exemplary case of aluminum-graphene composite, it was shown that the formation of the bimodal nanotwinned structure in ultrafine-grained/nanocrystalline matrix and account for the crack bridging by the graphene inclusions leads to a significant increase in the fracture toughness of the bimodal nanotwinned metal-graphene composites.

Keywords: fracture toughness, microcracks, plastic deformation, metal-graphene composites, bimodal nanotwinned structure, nanotwin boundaries

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Introduction

Recent experimental [1,2] and theoretical studies [3–6] demonstrate that metals, alloys and composites with a bimodal structure (materials with large grains embedded in an ultrafine-grained/nanocrystalline (UFG/NC) matrix) simultaneously exhibit high strength and ductility. In addition, according to [5–8], the formation of a nanotwinned structure in the large grains is accompanied by an additional increase in the strength and the plasticity of such materials. It should be noted that, in most cases, the addition of graphene inclusions to the UFG/NC matrix leads to a significant increase in the strength of such composites but is often accompanied by a decrease in their plasticity and fracture toughness. The main reason for the decrease in the fracture toughness of the UFG/NC metal-graphene composites is considered to be the hamper of the dislocation slip due to the presence of the graphene inclusions, which act as obstacles to

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the dislocation slip [9-13]. As a result, hindered dislocation pile-ups are formed at the graphene inclusions. These pile-ups of the dislocations are strong stress concentrators that stimulate the formation of microcracks. Thus, the development of mechanisms for increasing the plasticity and the fracture toughness of the UFG/NC metal-graphene composites is relevant and important for their practical application. One of the ways to increase the fracture toughness of the UFG/NC metal-graphene composites can be the formation of a bimodal nanotwinned structure in the UFG/NC matrix with the graphene inclusions. In particular, in the theoretical work [6], a significant increase in the strength and the ductility of the UFG/NC metal-graphene composite due to the formation of the large grains with a nanotwinned structure was shown. According to these data, a theoretical model is suggested that describes the mechanism of increasing plasticity and the fracture toughness in the UFG/NC Al-graphene composite due to the formation of a bimodal nanotwinned structure.

Model

Consider a two-dimensional model of a bimodal composite consisting of an UFG/NC metal matrix with inclusions in the form of graphene platelets and large grains with a nanotwinned structure under a uniform tensile stress σ_0 (Fig. 1). Assume that graphene plates are mainly located along grain boundaries in the metal matrix and do not contain pores, while the large nanotwinned grains do not contain the graphene inclusions. Also, it is assumed that under the action of the external load a straight semi-infinite crack of type I evolutes in the UFG/NC matrix approaching the boundary of a large grain with the nanotwinned structure consisting of periodically distributed nanotwin boundaries (Fig. 1).

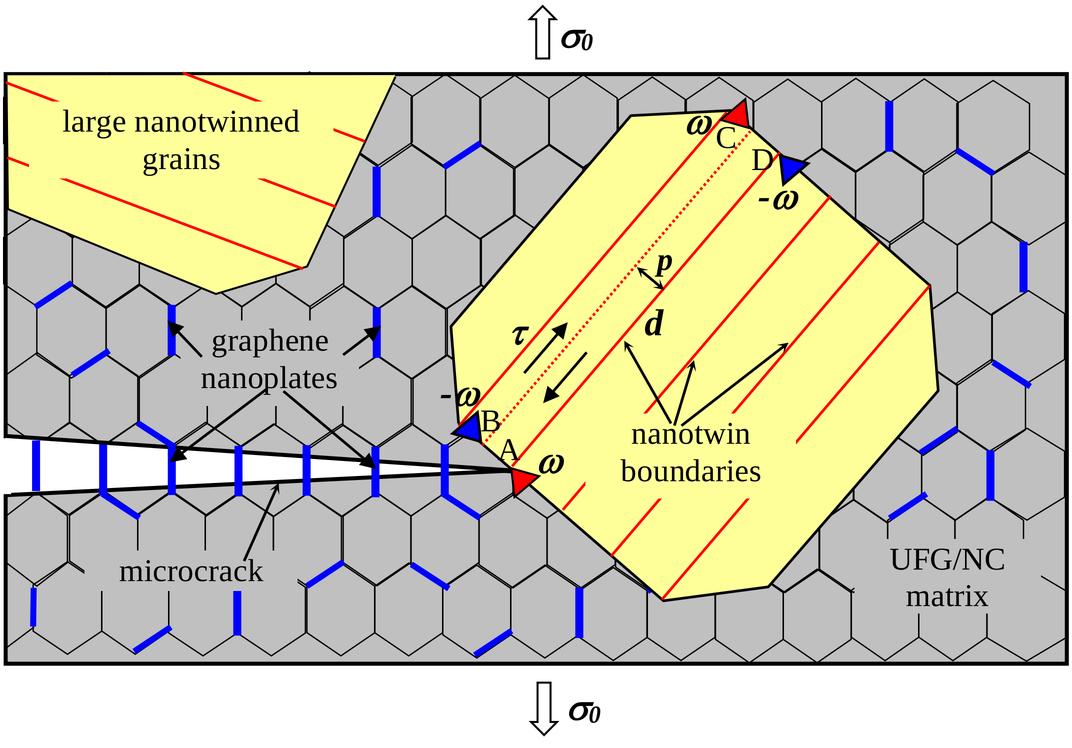

Fig. 1. Model of a bimodal metal-graphene composite consisting of large grains with nanotwinned structure embedded into UFG/NC metal matrix with microcracks reinforced by graphene inclusions

The crack intersects the configuration of identical graphene inclusions (which are nanoplatelets with length L and thickness H) oriented perpendicularly to the crack plane. In the region, where the distance between the crack edges is less than the length of the graphene nanoplatelets, bridges appear between the crack surfaces forming a zone of so-called crack bridging. Friction between the graphene nanoplatelets and the UFG/NC matrix creates forces that prevent crack opening, thereby increasing the fracture toughness of the composite.

Within the model, the microcrack concentrates the external stress σ_0 near the crack tip and the resulting local stress induces the migration of a nanotwin boundary to a distance p (Fig. 1). Action of the concentrated external stress σ_0 causes shear stress τ along the nanotwin boundaries. In turn, action of the shear stress τ causes slip of the partial dislocations with Burgers vectors b (partial b-dislocations) along the planes parallel to the nanotwin boundaries. At the same time, the slip of the partial dislocations along the planes parallel to the twin boundaries serves as the primary mechanism of the 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. As a result of the successive migration of the twin boundary, two walls of the partial dislocations with Burgers vectors b and $-b$ are formed on the opposite boundaries of the large grain. According to the theory of disclinations [14], such finite walls of edge dislocations are modeled by dipoles of wedge disclination dipoles with strengths $\pm\omega$ (hereinafter called $\pm\omega$-disclinations) whose magnitudes are equal to $\omega = 2\arctan(b/2\delta)$ (Fig. 1). Finally, a quadrupole ABCD of the wedge $\pm\omega$-disclinations is formed (Fig. 1). The disclination quadrupole ABCD is supposed to have a rectangular shape with the sizes d and p (Fig. 1), where d is an average grain size of the large nanotwinned grains. Thus, stress-induced migration of the nanotwin boundary causes the plastic deformation near the crack tip accompanied by the formation of the quadrupole of $\pm\omega$-disclinations whose stress field influences the microcrack growth.

Effect of nanotwin boundaries migration near microcrack tips on the fracture toughness of bimodal nanotwinned metal-graphene composites

Consider an individual quadrupole of the $\pm\omega$-disclinations ABCD formed near the tip of a flat mode I crack due to the successive migration of a nanotwin boundary to the distance p in a bimodal metal-graphene composite with nanotwinned structure (Fig. 1). In order to examine the effect of the disclination quadrupole on crack propagation, we use the energy criterion of crack growth. In the considered case of the plane strain state, this criterion has the following form [15,16]:

$$\frac{1-\nu}{2G}(K_I^2 + K_{II}^2) = 2\gamma, \qquad (1)$$

where K_I and K_{II} are the stress intensity factors, γ is the specific surface energy, G is the shear modulus and ν is Poisson's ratio. In our case (see Fig. 1), the stress intensity K_I and K_{II} are given by the following expressions [15,16]:

$$K_I = K_I^\sigma + k_I^q, \quad K_{II} = k_{II}^q, \qquad (2)$$

where K_I^σ is the stress intensity factor associated with the applied stress σ_0, while k_I^q and k_{II}^q are the stress intensity factors associated with the stress field of the $\pm\omega$-disclination quadrupole ABCD (Fig. 1).

The influence of the formation of the disclination quadrupole ABCD near crack tip on the crack advance can be accounted for through the introduction of the critical stress intensity factor K_{IC}. In this case, the formation of the disclination quadrupole changes the value of K_{IC} compared to the case without the disclination quadrupole. As a result, the critical condition for the crack growth can be written as follows [16]:

$$K_I^\sigma = K_{IC}\,. \tag{3}$$

Substitution of (2) to (1) and account for formula (3) allow us to obtain an expression for the fracture toughness of the composite, which accounts for the toughness effect of the plastic deformation due to the twin boundary migration near the crack tip [16]:

$$K_{IC} = \sqrt{(K_{IC}^\sigma)^2 - (k_{IIC}^q)^2} - k_{IC}^q, \tag{4}$$

where $k_{IC}^q = k_I^q\big|_{K_I^\sigma = K_{IC}}$, $k_{IIC}^q = k_{II}^q\big|_{K_I^\sigma = K_{IC}}$ and $K_{IC}^\sigma = \sqrt{4G\gamma/(1-\nu)}$ is the fracture toughness of the composite in the situation when the disclination quadrupole and the graphene platelets are absent.

In the examined case of a semi-infinite crack, the disclination located at the crack tip (at the point A) turns out at the surface of the composite and disappears. As a result, the disclination configuration consists of three individual disclinations (at the points B, C and D). For this disclination configuration (Fig. 1), the stress intensity factors k_I^q and k_{II}^q are calculated as follows [16]:

$$\begin{aligned}
&k_I^q = G\omega\sqrt{d}\, f_1(\alpha,t)/(2\sqrt{2\pi}(1-\nu)),\\
&k_{II}^q = G\omega\sqrt{d}\, f_2(\alpha,t)/(2\sqrt{2\pi}(1-\nu)),\\
&f_1(\alpha,t) = \sum_{k=1}^{3}(-1)^k\sqrt{\tilde r_k}\,[3\cos(\theta_k/2) + \cos(3\theta_k/2)],\\
&f_2(\alpha,t) = \sum_{k=1}^{3}(-1)^k\sqrt{\tilde r_k}\,[\sin(\theta_k/2) + \sin(3\theta_k/2)],
\end{aligned} \tag{5}$$

where

$t = p/d$, $\tilde r_1 = 1$, $\tilde r_2 = \sqrt{t^2+1}$, $\tilde r_3 = t$, $\theta_1 = \alpha$,

$\theta_2 = \alpha - \pi/2 + arc\cot t + 2\pi\,\Xi(-\alpha - \pi/2 - arc\cot t)$,

$\theta_3 = \alpha - \pi/2 + arc\cot t + 2\pi\,\Xi(-\alpha - \pi/2)$, $\Xi(x)$ is the Heaviside function equal to unity at $x \ge 0$ and zero otherwise.

To account for the fracture toughness enhancement ΔK due to the crack bridging by the graphene platelets, consider the situation when all graphene platelets are oriented normally to the crack growth direction (Fig. 1). Also, assume that the UFG/NC metal-graphene matrix is a homogeneous and elastically isotropic solid and neglect the influence of the difference in the elastic moduli of the metal-graphene matrix and thin graphene platelets on the fracture toughness. In this case, according the work [17], the fracture toughness K'_{IC} of the composite, which simultaneously takes into account the crack bridging by graphene platelets and the plastic deformation due to the twin boundary migration, can be expressed from formula (4) as follows:

$$K'_{IC} = \sqrt{(K_{IC}^\sigma)^2 + \Delta K - (k_{IIC}^q)^2} - k_{IC}^q, \tag{6}$$

where $\Delta K = (1+\nu)kGLf_g/H$ [17], f_g is the graphene volume fraction, and k is the parameter describing the bridging force of a graphene platelet per its unit length.

Compare the quantities K'_{IC} and K_{IC}^σ to analyze the effect of the formation of the disclination quadrupole ABCD and the crack bridging by the graphene platelets on the crack growth. The ratio K'_{IC}/K_{IC}^σ characterizes a coefficient $q = K'_{IC}/K_{IC}^\sigma$ of increase in the fracture toughness. The disclination quadrupole formation and the crack bridging increase the fracture toughness of the composite if the coefficient $q>1$ and decrease one if $q<1$.

Results and Discussion

With the help of formulas (1)-(6), we calculated the ratio $q = K'_{IC} / K^{\sigma}_{IC}$ as a function of the distance p of the twin boundary migration and the volume fraction f_g of the graphene platelets for the case of a bimodal nanotwinned Al-graphene composite characterized by the following parameter values: $G = 27$ GPa, $\nu = 0.3$, $a = 0.405$ nm, $b = a/\sqrt{6}$ [18], $\gamma = 0.91$ J/m^2 [19]. We also put $d = 1500$ nm, $L = 300$ nm, $H = 7$ nm and $\alpha = 70°$. In the first approximation, the value of the specific bridging force $k = 6.65$ N/m was taken from the work [17] for 3C-SiC-graphene composites, since the value of k is not known for Al-graphene composites. The contour map of $q = K'_{IC} / K^{\sigma}_{IC}$ in the coordinate space (p, f_g) is presented in Fig. 2. Figure 2 clearly demonstrates that the fracture toughness of the bimodal nanotwinned Al-graphene composite increases both in the case of an increase in the distance p and in the case of an increase in the volume fraction f_g of the graphene platelets.

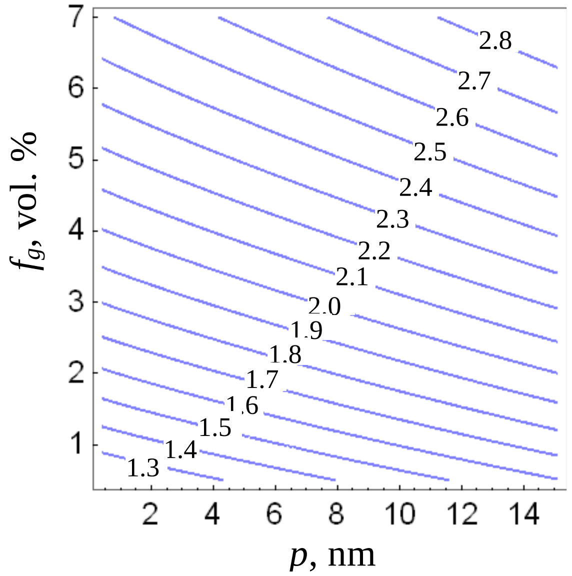

Fig. 2. Contour map of the toughening ratio $q = K'_{IC} / K^{\sigma}_{IC}$ in the space (p, f_g).

Conclusions

Thus, a theoretical model which describes the mechanism of the fracture toughness enhancement in bimodal nanotwinned metal-graphene composites with a UFG/NC matrix has been developed. The mechanism of an increase in the ductility and the fracture toughness of these composites is the interaction of microcracks with the graphene inclusions in the UFG/NC matrix and with the nanotwinned structure in the large grains. The presence of the nanotwinned structure promotes the development of the plastic deformation in the large grains near the crack tips due to the migration of the nanotwin boundaries leading to the formation of disclination configurations whose stress fields slow down the further growth of microcracks, thereby increasing the fracture toughness of such composites. At the same time, the presence of the graphene platelets in UFG/NC metal-matrix induces the crack bridging by the graphene platelets which also increases the fracture toughness of the metal-graphene composites. Within the framework of the model, it was shown that the fracture toughness of the bimodal nanotwinned metal-graphene composites can be additionally increased up to 140% (in the case of the Al-graphene composite) due to the formation of the large grains with the nanotwinned structure in the UFG/NC matrix and account for the effect of the crack bridging by the graphene platelets in comparison with UFG/NC materials without bimodal nanotwinned structure and graphene inclusions. It should be noted that the values of the toughening ratio $q = K'_{IC} / K^{\sigma}_{IC}$ calculated in the model considerably exceeds the typical experimental values, which can be attributed to an increase in porosity or the activation of other mechanisms reducing fracture toughness of the composites. Account for these mechanisms will be the subject of further investigations.

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