Reviews on Advanced Materials and Technologies, 2024, vol. 6, no. 1, pp. 29–34
DOI: 10.17586/2687-0568-2024-6-1-29-34

A Brief Review on Mechanisms of Plastic Deformation and Fracture Toughness Enhancement in Bimodal Metal-Graphene Composites with Nanotwinned Structure

N.V. Skiba*

Institute for Problems in Mechanical Engineering of the Russian Academy of Sciences, St. Petersburg 199178, Russia

Article history

Received March 18, 2024
Accepted March 22, 2024
Available online March 31, 2024

Abstract

A brief review of the theoretical models which describe mechanisms of the plastic deformation and fracture toughness enhancement in bimodal metal-graphene composites with nanotwinned structure is presented. In the framework of the models, the plastic deformation in such composites occurs due to the lattice dislocation slip and the grain boundary sliding in nanocrystalline/ultrafine-grained matrix, and the lattice dislocation slip and the migration of the twin boundaries in large grains with nanotwinned structure. Within the review, the migration of nanotwin boundaries in the large grains releases in part local stresses near crack tips and provides the fracture toughness enhancement in bimodal metal-graphene composites with nanotwinned structure. At the same time, the presence of the graphene inclusions in metal-matrix induces the crack bridging effect which also increases the fracture toughness of bimodal metal-graphene composites.

Keywords: Bimodal metal-graphene composites; Nanotwinned structure; Plastic deformation; Fracture toughness

1. INTRODUCTION

Recently, a new class of bimodal metal-graphene composites with a nanotwinned structure has been actively developed. These composites consist of large (micrometer-sized) grains with nanotwinned structure embedded into a nanocrystalline/ultrafine-grained NC/UFG matrix with graphene inclusions. Experimental studies [1,2], theoretical models [3–6] and computer simulations [7,8] demonstrate that composites with a bimodal structure simultaneously exhibit high strength and ductility. In such composites, the NC/UFG metal-matrix is responsible for high strength, while coarse grains provide good ductility. It should be noted that the formation of a nanotwinned structure in the large grains is accompanied by an additional increase in the strength and the plasticity of bimodal composite [6,9,10] while 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 [11–15]. Thus, it seems important to identify the micromechanisms responsible for the plastic deformation and fracture toughness of bimodal composites with nanotwinned structure and graphene inclusions.

The main aim of this work is a brief review on theoretical models which describe mechanisms of the plastic deformation and fracture toughness enhancement in bimodal metal-graphene composites with nanotwinned structure.

2. MECHANISMS OF PLASTIC DEFORMATION IN BIMODAL METAL-GRAPHENE COMPOSITES WITH NANOTWINNED STRUCTURE

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 a uniaxial tensile load σ (Fig. 1). According to experimental data [9,16] and theoretical models [6,17], two principal deformation mechanisms act in nanotwinned materials: twin boundary migration and dislocation motion across twins. The slip of the partial dislocations along the planes parallel to the twin boundaries serves as the primary

* Corresponding author: N.V. Skiba, e-mail: nikolay.skiba@gmail.com

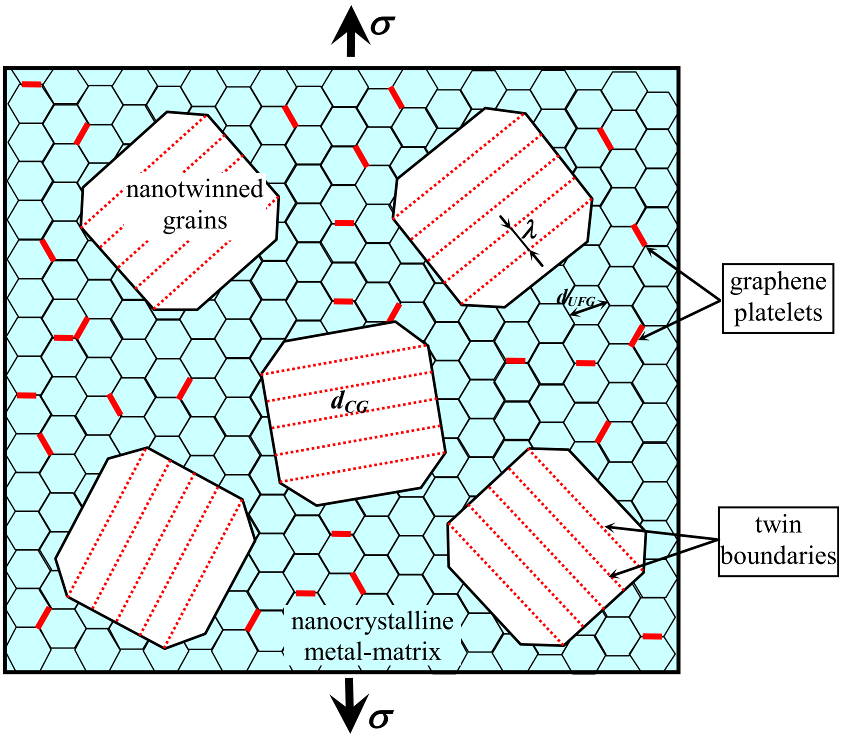

Fig. 1. Model of a bimodal metal-graphene composite consisting of large grains with nanotwinned structure embedded into NC/UFG metal matrix reinforced by graphene inclusions. Reprinted from Ref. [6]. © 2021 N.V. Skiba, published by Peter the Great St. Petersburg University. Available under the terms of the CC-BY-NC 4.0 license.

mechanism of migration of the twin boundaries in the direction normal to the twin plane.

At the same time, according to work [5], the plastic deformation of the NC/UFG metallic matrix $\sigma_{c2} = M_1\tau_{c2}$ with the graphene inclusions occurs due to the emission of the lattice dislocations from grain boundaries (GBs) and their sliding in grain interiors, and grain boundary sliding.

Taking into account the action of these deformation mechanisms, the yield stress of bimodal metal-graphene composites with nanotwinned structure was calculated [6]. Following theoretical model [17], the yield stress of nanotwinned solid is given by expression:

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

where σ_{TBM} is yield stress associated with twin boundary migration (see Ref. [17], for details), λ is a distance between adjacent twin boundaries, λ_* is the optimal distance between adjacent twin boundaries that characterizes the transition from hardening to softening, $\sigma_{HP}^{NT} = \sigma_0 + K\lambda^{-1/2}$ is the classical Hall–Petch law, σ_0 and K are the material 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 [5], the yield stress of the UFG metal-matrix 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 the GBs, $\sigma_{c0} = \sigma_0 + Kd_{UFG}^{-1/2}$, d_{UFG} is mean grain size of the UFG matrix, $\sigma_{c2} = M_1\tau_{c2}$, $\tau_{c2} = 140$ MPa [18] is the critical shear stress for slipping graphite monolayers, M_1 is the geometric factor, f_{gr} is the fraction of the GBs containing graphene and σ_{em}^{GB} is the stress necessary to free a dislocation segment pinned by obstacles (see Ref. [5], for details).

With help formulas (1) and (2) the yield stress of the bimodal metal graphene composites with nanotwinned structure can be expressed as follows [6]:

$$\sigma_y = \beta\sigma_y^{NT} + (1-\beta)\sigma_y^{UFG}, \quad (3)$$

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

In the model [6], the dependences of the yield stress σ_y on the twin thickness λ for various values of the volume fraction β (0.3, 0.5 and 0.7, the solid lines 1, 2 and 3, respectively) of large grains in the case of bimodal Cu-graphene composite were calculated (Fig. 2). 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 [17]. The horizontal dashed line 5 defines the yield stress σ_y^{UFG} of UFG metal-graphene matrix without nanotwinned grains. The dependences $\sigma_y(\lambda)$

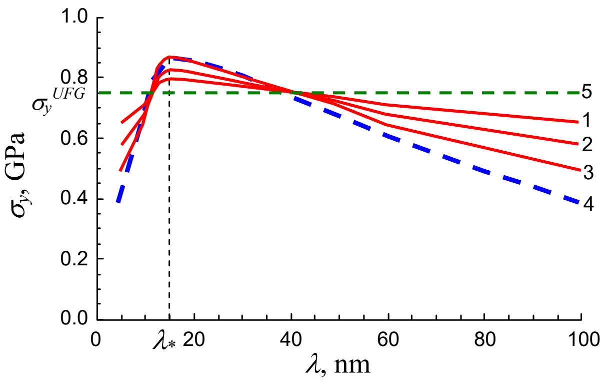

Fig. 2. The dependences of the yield stress σ_y on the twin thickness λ for bimodal nanotwinned Cu-graphene composite (curves 1–3), for UFG nanotwinned Cu (curves 4) and for NC/UFG metal-graphene composite (curve 5). Reprinted from Ref. [6].

(curves 1–3) in Fig. 2 show the transition from softening to hardening and define that optimum twin thickness λ is equal to 15 nm as well as in the case of UFG nanotwinned Cu (curve 4). Dependences in Fig. 2 also demonstrate that the yield stress σ_y of bimodal metal-graphene composite with nanotwinned structure is higher of the yield stress σ_y^{UFG} of the UFG metal-graphene composite without nanotwinned grains in the range of the twin thickness 10 nm < λ < 40 nm.

Thus, the plastic deformation mechanisms in the bimodal metal-graphene composite with nanotwinned structure that are realized due to the twin boundary migration and the dislocation motion across the twins in the large nanotwinned grains, and the lattice dislocation slip and the grain boundary sliding in the UFG metal-graphene matrix have been described. Also, it was shown that the presence of the large grains with nanotwinned structure increases the yield strength of the bimodal metal-graphene composite compared to the same composite with the large grains without nanotwinned structure.

3. MECHANISMS OF FRACTURE TOUGHNESS ENHANCEMENT IN BIMODAL METAL-GRAPHENE COMPOSITES WITH NANOTWINNED STRUCTURE

The addition of graphene inclusions to the UFG/NC matrix is often accompanied by a decrease in the plasticity and fracture toughness of metal-graphene composites. 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 the dislocation slip [11–15]. 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 the theoretical model [19], mechanism of the fracture toughness enhancement in bimodal metal-graphene composites containing the large grains with nanotwin structure and a straight semi-infinite crack of type I in the UFG/NC matrix is considered. It is assumed that under the action of the external load σ_0 the microcrack propagates

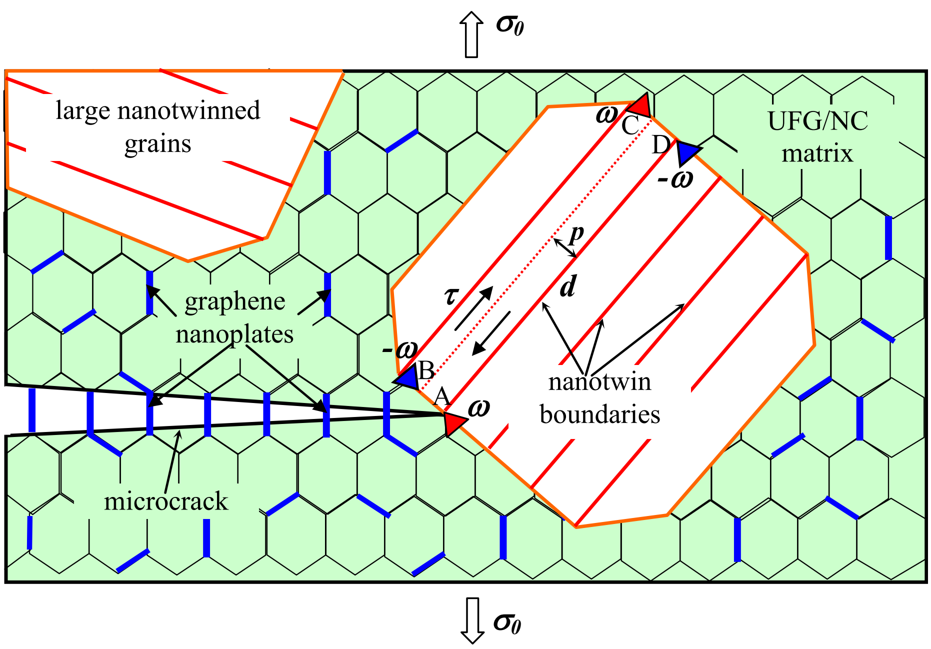

Fig. 3. Model of a bimodal metal-graphene composite containing large grains with nanotwin structure and a straight semi-infinite crack of type I in UFG/NC matrix with graphene inclusions. Reprinted from Ref. [19].

in the UFG/NC matrix crossing the configuration of identical graphene inclusions oriented perpendicular to the microcrack plane and approaching the boundary of the large grain with the nanotwinned structure (Fig. 3). Within the model, the microcrack concentrates the external stress τ near crack tip and the resulting local stress induces the migration of a nanotwin boundary to a distance p (Fig. 3). As a result of the successive migration of the twin boundary a quadrupole ABCD of the wedge ±ω-disclinations with the sizes d and p is formed (Fig. 3). Thus, stress-induced migration of the nanotwin boundary causes the plastic deformation near the crack tip accompanied by the formation of the quadrupole of ±ω-disclinations whose stress field influences the microcrack growth. At the same time, the graphene nanoplatelets create bridges between the microcrack surfaces forming a zone of so-called crack bridging and prevent crack opening.

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 [19,20]:

$$\frac{1-\nu}{2G}(K_I^2+K_{II}^2)=2\gamma, \tag{4}$$

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 [19,20]:

$$K_I=K_I^\sigma+k_I^q, \quad K_{II}=k_{II}^q, \tag{5}$$

where K_I^σ is the stress intensity factor associated with the applied load σ_0, while k_I^q and k_{II}^q are the stress intensity factors associated with the stress field of the ±ω-disclination quadrupole ABCD (Fig. 3).

The influence of the formation of the disclination quadrupole ABCD near crack tip on 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 [19,20]:

$$K_I^\sigma=K_{IC}. \tag{6}$$

Substitution of (5) to (4) and account for formula (6) allows us to obtain the expression for the fracture toughness of the composite which account for the toughness effect of the plastic deformation due to the twin boundary migration near crack tip: [19,20]

$$K_{IC}=\sqrt{(K_{IC}^\sigma)^2-(k_{IIC}^q)^2}-k_{IC}^q, \tag{7}$$

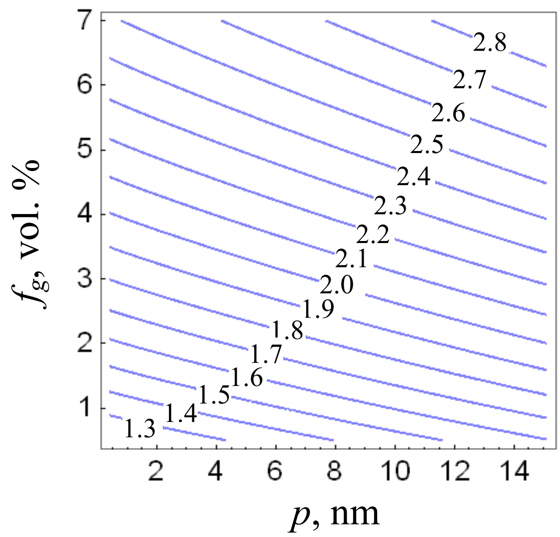

Fig. 4. Contour map of the toughening ratio $q=K'_{IC}/K_{IC}^\sigma$ in the space (p,f_g). Reprinted from Ref. [19].

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 where the disclination quadrupole and the graphene platelets is absent.

According to the work [21], the critical stress intensity factor K'_{IC} of the composite which simultaneously takes into account the crack bridging by the graphene platelets and the plastic deformation due to the twin boundary migration can be expressed from formula (7) as follows

$$K'_{IC}=\sqrt{(K_{IC}^\sigma)^2+\Delta K-(k_{IIC}^q)^2}-k_{IC}^q, \tag{8}$$

where $\Delta K=(1+\nu)kGLf_g/H$ [21] is the stress intensity factors associated with the crack bridging by the graphene platelets, L and H is length and thickness of the graphene platelets, respectively, f_g is the graphene volume fraction, and k is the parameter describing the bridging force of a graphene platelet per its unit length.

The ratio K'_{IC}/K_{IC}^σ characterizes 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 $q<1$.

Within the model [19], the ratio $q=K'_{IC}/K_{IC}^\sigma$ 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 was calculated. The contour map of $q=K'_{IC}/K_{IC}^\sigma$ in the coordinate space (p,f_g) is presented in Fig. 4. Figure 4 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.

4. CONCLUSIONS

Thus, the mechanisms of the fracture toughness enhancement in bimodal metal-graphene composites with nanotwinned structure which takes into account the crack bridging by graphene platelets and the plastic deformation due to the twin boundary migration have been described. 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.

ACKNOWLEDGEMENTS

The research is funded by the Ministry of Science and Higher Education of the Russian Federation for IPME RAS (theme no. 124041100008-5).

REFERENCES

[1] L.L. Zhu, J. Lu, Modelling the plastic deformation of nanostructured metals with bimodal grain size distribution, *Int. J. Plast*., 2012, vol. 30–31, pp. 166–184.

[2] A.G. Sheinerman, Plastic deformation of metal/graphene composites with bimodal grain size distribution: a Brief Review, *Rev. Adv. Mater. Technol.*, 2020, vol. 2, no. 4, pp. 1–8.

[3] L. Zhu, C. Wen, C. Gao, Guo X, Chen Z, Lu J, Static and dynamic mechanical behaviors of gradient-nanotwinned stainless steel with a composite structure: Experiments and modeling, *Int. J. Plast*., 2019, vol. 114, pp. 272–288.

[4] N.V. Skiba, Crossover from deformation twinning to lattice dislocation slip in metal–graphene composites with bimodal structures, *Crystals*, 2020, vol. 10, no. 1, art. no. 47.

[5] S.V. Bobylev, M.Yu. Gutkin, A.G. Sheinerman, Yield strength of metal–graphene composites with a homogeneous and bimodal grain structure, *Mech. Solids*, 2020, vol. 55, pp. 22–31.

[6] N.V. Skiba. Deformation mechanism of bimodal metal graphene composites with nanotwinned structure, *Mater. Phys. Mech*., 2021, vol. 47, no. 5, pp. 676–680.

[7] X. Guo, R. Ji, G.J. Weng, L.L. Zhu, J. Lu, Micromechanical simulation of fracture behavior of bimodal nanostructured metals, *Mater. Sci. Eng. A*, 2014, vol. 618, pp. 479–489.

[8] X. Guo, X.Y. Dai, G.J. Weng, L.L. Zhu, J. Lu, Numerical investigation of fracture behavior of nanostructured Cu with bimodal grain size distribution, *Acta Mech*., 2014, vol. 225, pp. 1093–1106.

[9] L. Lu, X. Chen, X Huang, K. Lu, Revealing the maximum strength in nanotwinned copper, *Science*, 2009, vol. 323, no. 5914, pp. 607–610.

[10] I.A. Ovid'ko, N.V. Skiba, A.G. Sheinerman, Plastic deformation modes in ultrafine-grained metals with nanotwinned structures, *Rev. Adv. Mater. Sci.*, 2015, vol. 41, no. 1, pp. 93–98.

[11] S. Zhang, P. Huang, F. Wang, Graphene-boundary strengthening mechanism in Cu/graphene nanocomposites: A molecular dynamics simulation, *Mater. Des.*, 2020, vol. 190, art. no. 108555.

[12] Y. Jiang, R. Xu, Z. Tan, G. Ji, G. Fan, Z. Li, D.-B. Xiong, Q. Guo, Z. Li, D. Zhang, Interface induced strain hardening of graphene nanosheet/aluminum composites, *Carbon*, 2019, vol. 146, pp. 17–27.

[13] M. Khoshghadam-Pireyousefan, R. Rahmanifard, L. Orovcik, P. Švec, V. Klemm, Application of a novel method for fabrication of graphene reinforced aluminum matrix nanocomposites: Synthesis, microstructure, and mechanical properties, *Mater. Sci. Eng. A*, 2020, vol. 772, art. no. 138820.

[14] O. Guler, N. Bagci, A short review on mechanical properties of graphene reinforced metal matrix composites, *J. Mater. Res. Technol.*, 2020, vol. 9, no. 3, pp. 6808–6833.

[15] L.R. Safina, J.A. Baimova, K.A. Krylova, R.T. Murzaev, R.R. Mulyukov, Simulation of metal-graphene composites by molecular dynamics: a review, *Letters on Materials*, 2020, vol. 10, no. 3, pp. 351–360.

[16] K. Lu, L. Lu, S. Suresh, Strengthening Materials by Engineering Coherent Internal Boundaries at the Nanoscale, *Science*, 2009, vol. 324, no. 5925, pp. 349–352.

[17] N.V. Morozov, I.A. Ovid'ko, N.V. Skiba, Plastic flow through widening of nanoscale twins in ultrafine-grained metallic materials with nanotwinned structures, *Rev. Adv. Mater. Sci.*, 2014, vol. 37, no. 1/2, pp. 29–36.

[18] Z. Liu, S. Zhang, J. Yang, J.Z. Liu, Y. Yang, Q. Zheng, Interlayer shear strength of single crystalline graphite, *Acta Mech. Sin.*, 2012, vol. 28, pp. 978–982.

[19] N.V. Skiba, Mechanism of fracture toughness enhancement in bimodal metal-graphene composites with nanotwinned structure, *Mater. Phys. Mech*., 2023, vol. 51, no. 2, pp. 58–64.

[20] N.F. Morozov, I.A. Ovid'ko, A.G. Sheinerman, N.V. Skiba, Formation of deformation twins through ideal nanoshear events near crack tips in deformed nanocrystalline materials, *Rev. Adv. Mater. Sci.*, 2012, vol. 32, no. 1, pp. 75–81.

[21] Y.C. Wang, Y.B. Zhu, Z.Z. He, H.A. Wu, Multiscale investigations into the fracture toughness of SiC/graphene composites: Atomistic simulations and crack-bridging model, *Ceram. Int.* 2020, vol. 46, no. 18, part A, pp. 29101–29110.

УДК 539.52+539.37

Краткий обзор механизмов пластической деформации и повышения трещиностойкости в бимодальных композитах металл-графен с нанодвойникованной структурой

Н.В. Скиба

Институт проблем машиноведения Российской академии наук, Санкт-Петербург, 199178, Россия

Аннотация. Представлен краткий обзор теоретических моделей, описывающих механизмы пластической деформации и повышения трещиностойкости в бимодальных композитах металл-графен с нанодвойникованной структурой. В рамках моделей, пластическая деформация в таких композитах происходит за счет скольжения решеточных дислокаций и зернограничного скольжения в нанокристаллической/ультрамелкозернистой матрице, и скольжения решеточных дислокаций и миграции двойниковых границ в крупных зернах с нанодвойникованной структурой. В рамках обзора, миграция границ нанодвойников в крупных зернах частично снимает локальные напряжения вблизи вершин трещин и обеспечивает повышение трещиностойкости в бимодальных композитах металл-графен с нанодвойникованной структурой. В то же время наличие графеновых включений в металлической матрице вызывает эффект бриджинга трещин, что также увеличивает трещиностойкость бимодальных композитов металл-графен.

Ключевые слова: бимодальные композиты металл-графен; нанодвойникованная структура; пластическая деформация; трещиностойкость