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Grain rotation dependent fracture toughness of nanocrystalline materials

Yingguang Liu [a], Jianqiu Zhou [a,b,*], T.D. Shen [c], David Hui [d]

[a] Department of Mechanical Engineering, Nanjing University of Technology, Nanjing 210009, Jiangsu, People's Republic of China
[b] Department of Mechanical Engineering, Wuhan Institute of Technology, Wuhan 430070, Hubei, People's Republic of China China
[c] High-Tech Research Institute and State Key Laboratory of Materials-Oriented Chemical Engineering, Nanjing University of Technology, Nanjing 210009, Jiangsu, People's Republic of China
[d] Department of Mechanical Engineering, University of New Orleans, New Orleans, LA 70148, United States

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ABSTRACT

A grain size dependent theoretical model is developed to describe the effect of special rotational deformation (SRD) on crack growth in deformed nanocrystalline (nc) materials. The SRD is driven by the stress concentration near the crack tip, and it serves as a toughening mechanism by releases part of the local stresses. The dependence of critical crack intensity factors on grain size was calculated. It was demonstrated that the SRD leads to an increase of critical crack intensity factors by 10–50%.

1. Introduction

Nc materials have been a source of great interest currently due to their unusual mechanical and physical properties [1–8]. In general, nc materials show superior strength but low tensile ductility and low fracture toughness, which limit their applications [1,3,4,6]. However, the evidence of good tensile ductility and/or enhanced toughness in nc materials has been studied and reported [9–14]. Understanding the fundamentals of toughness in the nc materials is of great importance to develop new applications. So far, many models have been developed to explain this phenomenon [15–18]. Most of them attributed the good tensile ductility and/or enhanced toughness to the alternative deformation modes such as lattice dislocation slip, intergrain sliding, Coble creep, triple junction diffusional creep, rotational deformation, and nanoscale twin deformation effectively operating in nc materials.

Many experiments [19–25] have shown that rotational deformation (plastic deformation accompanied by crystal lattice rotations) often occurs in nc materials. Besides, computer simulations [26–28] and theoretical models [29–33] have provided convincing evidence for the important role of rotational deformation in plastic flow processes in various nc materials. Morozov et al. suggested a theoretical model to study the effect of SRD on crack growth in nc materials, however, the relationship between the rotational deformation and grain size has been not well studied, and it needs to be improved. Ovid'ko et al. have pointed that the SRD effectively occurs through the formation of a quadrupole of immobile wedge disclinations whose strengths gradually increase. Their work also gives the energy change associated with the both formation of the quadrupole and the grain size. Romanov et al. indicated that at a certain grain size, there is a critical stress above which the rotation mode of the plastic deformation transfers to another mode. The remaining defects in the grain interior, such as disclination quadrupole and dislocation dipole, possess no field elastic distortions. The above three theories will be introduced briefly in Section 2. It can be seen from the above models that although the above experimental and theoretical results suggest that the rotational deformation contribute to the toughening of nc materials, the relationship between the rotational deformation and grain size has not been well quantitatively studied. In spirit of these previous works, we built a theoretical model to study the hampering effect of the SRD with grain size dependent. This mechanism is different from both standard rotational deformation, which occurs through the movement of wedge disclinations, and diffusion-accommodated grain rotations, which do not contribute to plastic flow [32,33]. The SRD can effectively operate on crack growth in nc materials, but is commonly suppressed in coarse-grained polycrystals [33]. More importantly, the dependence of critical crack intensity fac-

* Corresponding author at: Department of Mechanical Engineering, Nanjing University of Technology, Nanjing 210009, Jiangsu, People's Republic of China.
Tel.: +86 25 83588706; fax: +86 25 83374190.
E-mail addresses: zhouj@njut.edu.cn, yyzjqcc@sohu.com (J. Zhou).

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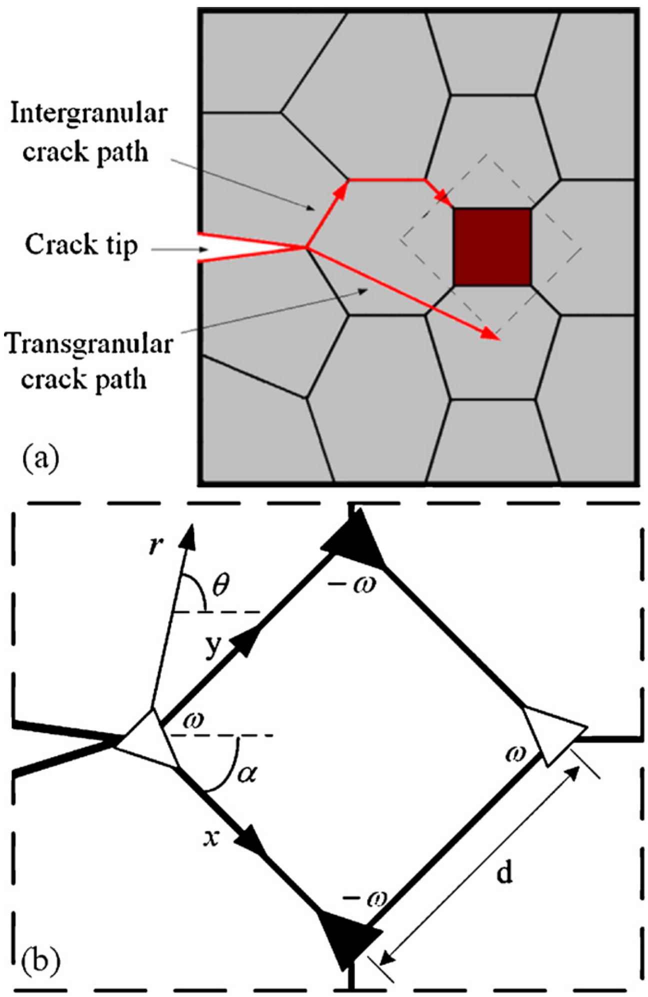

Fig. 1. (a) Special rotational deformation in a deformed nc material containing a mode I crack. (b) Magnified region in (a) highlights a disclination quadrupole near the crack tip.

tors on grain size was calculated, the results appeared to be much meaningful and inspired. So far, there are few literatures doing the similar works.

2. Model and results

In general, there are two ways for the crack propagation in polycrystals: (i) crack crosses the grain (transgranular propagation); (ii) crack travels the interface region between the grains (intergranular propagation), as schematically shown in Fig. 1a. Actually, the present model is applicable for both the transgranular and intergranular fracture mechanisms. In this paper, our aim is to study the effect of SRD. Thus, we only consider a special case that crack tip intersects GBs. and we will not study how the crack propagates. Let us consider the case where a long flat crack evolves under the action of an applied load in the deformed nc specimen under a tensile load (Fig. 1b). For simplicity, we restrict our consideration to a two-dimensional grain structure. High stress concentration near the crack tips can initiate the SRD of grains (Fig. 1b). In the present two-dimensional model, we will consider the SRD of a quadrate grain and the case when the crack tip reaches a junction of boundaries of this grain, as shown in Fig. 1b.

In terms of the theory of defects, the SRD can be described as the formation of a quadrupole of immobile wedge disclinations in such a grain. The strength of the disclinations gradually grows during the formation process [33]. The SRD is conducted by: (i) GB sliding along GBs AB and CD; (ii) diffusion-controlled climb of GB dislocations along GBs AC and BD (Fig. 2a–c). Following the concept on local shear events – shear transformations of local atomic clusters – as carriers of plastic flow in GBs in metals [34,35] and covalent solids [36], we suppose that local shear events carry sliding along GBs AB and CD. The sliding results in the formation of GB dislocations at junctions A, B, C and D [37,38], as schematically shown in Fig. 2a–c. Diffusion-controlled climb of the dislocations

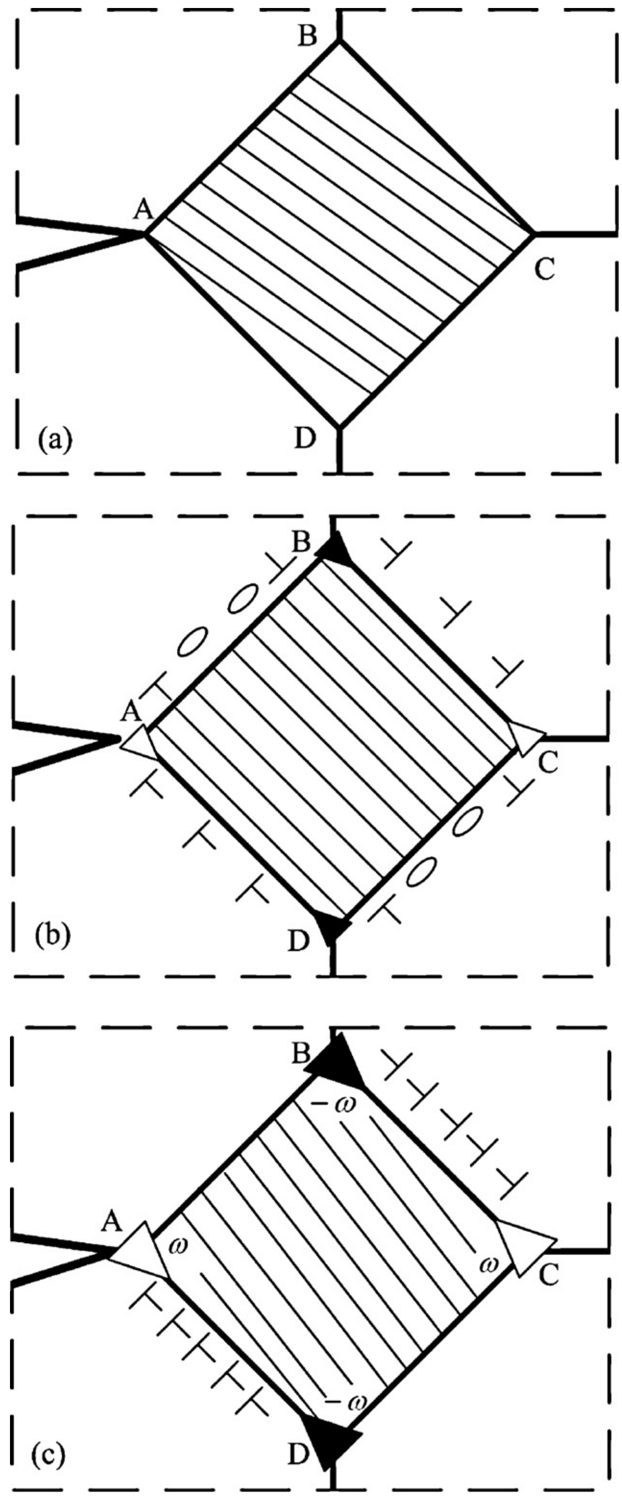

Fig. 2. Special rotational deformation occurs in a nanograin through the formation of immobile disclinations.

along GBs AC and BD provides SRD accompanied by the formation of quadrupole of wedge disclinations at GB junctions A, B, C and D (Fig. 2a–c). The disclination quadrupole creates stresses that influence crack growth.

Let us consider the effect of disclination quadrupole produced due to SRD on the fracture toughness of nc materials. Within the macroscopic mechanical description, the effect of SRD on crack growth can be accounted for through the introduction of the critical stress intensity factor K_{IC}^*. In this case, the crack growth direction is perpendicular to the tensile load direction, while the presence of the dislocations just changes the value of K_{IC}^* when compared to the case without SRD. The critical stress intensity factor K_{IC}^* can be represented as [39]:

$$K_{IC}^* = \sqrt{(K_{IC}^{\sigma})^2 - (k_{II}^q)^2} - k_I^q \tag{1}$$

where $K_{IC}^{\sigma} = \sqrt{4G\gamma_e/(1-\nu)}$ is the fracture toughness in the disclination-free case that the SRD is completely suppressed, G is the Shear modulus, ν is the Poisson's ratio and γ_e is the specific surface energy, k_I^q and k_{II}^q are the intensity factors for the stresses created by the disclinations.

Following Ref. [31], we will calculate the stress intensity factors k_{II}^q and k_I^q. In doing so, as shown in Fig. 2, $\pm\omega$ denotes the disclination strengths, α is the angle made by the crack plane and one of the quadrupole arms. We also introduce a Cartesian coordinate system (x, y) and a polar coordinate system (r, y) with the origin at the crack tip (see Fig. 2). The quadrupole arms are assumed to be equal to the grain size d and it is small compared to the crack length l. This assumption allows us to model the crack as a semi-infinite one in the calculation of the stress intensity factors k_I^q and k_{II}^q. The stress intensity factors for the disclination quadrupole shown in Fig. 2 are calculated using the way proposed by Zhang and Li [40]. This is done through the standard representation [41] of disclination dipoles as continuous distributions of edge dislocations. As a result, one can obtain the following expression for the factors k_I^q and k_{II}^q.

$$k_I^q = \frac{G\omega\sqrt{d}f_1(\theta)}{2\sqrt{2\pi}(1-\nu)}, \quad k_{II}^q = \frac{G\omega\sqrt{d}f_2(\theta)}{2\sqrt{2\pi}(1-\nu)} \tag{2}$$

$$f_1(\theta) = \sum_{k=1}^{3}(-1)^k\sqrt{\bar{r}}\left[3\cos\left(\frac{\theta_k}{2}\right) + \cos\left(\frac{3\theta_k}{2}\right)\right] \tag{3}$$

$$f_2(\theta) = \sum_{k=1}^{3}(-1)^k\sqrt{\bar{r}}\left[sin\left(\frac{\theta_k}{2}\right) + \sin\left(\frac{3\theta_k}{2}\right)\right] \tag{4}$$

where $\bar{r}_k = r_k/d$, r_k and θ_k are the coordinates of the kth disclination (k = 1, 2, 3) and $0 \le \theta_k \le \pi/2$. For the disclination quadrupole shown in Fig. 2 and α in the range $-\pi/2 \le \theta_k \le \pi/2$, we have $\bar{r}_1 = 1$, $\bar{r}_2 = \sqrt{2}$, $\bar{r}_3 = 1$; $\theta_1 = -\alpha$, $\theta_2 = \pi/4 - \alpha$, $\theta_3 = \pi/2 - \alpha$.

In our model, the disclination strength ω in Eq. (2) is arbitrary and corresponds to the minimum of the energy change ΔW associated with the formation of the disclination quadrupole. The energy change ΔW can be written as [33]

$$\Delta W = \frac{Dd^2}{2}\left(2\omega^2 \ln\ 2 - \frac{2\omega\tau}{D}\right) \tag{5}$$

where $D = G/[2\pi(1-\nu)]$. The energy ΔW has a minimum at a certain (equilibrium) value ω_0 of the absolute disclination strength. The equilibrium disclination strength ω_0 is derived from the relation $(\partial\Delta W/\partial\omega)| = 0$ as follows:

$$\omega_0 = \frac{\tau}{2D\ln\ 2} \tag{6}$$

Romanov et al. indicated that after the rotation deformation mechanism propagates trough the nc grain, a localized shear mechanism continues to occur in the initial plane or in the plane parallel to the initial one (Fig. 3d). In this case, an edge dislocation with opposite Burgers vector $-b$ forms and remains at the grain boundary. The positive dislocation (plastic shear) +b propagates further in nc materials along the easy shear grain boundary [30]. The remaining defects in the grain interior, such as disclination quadrupole and dislocation dipole, possess no field elastic distortions. The proposed transformation from the rotational deformation into plastic shear allows one to find the critical deforming stress τ_c for its realization. The critical stress τ_c, created by an applied tensile load in the vicinity of a crack tip can be written as [30]:

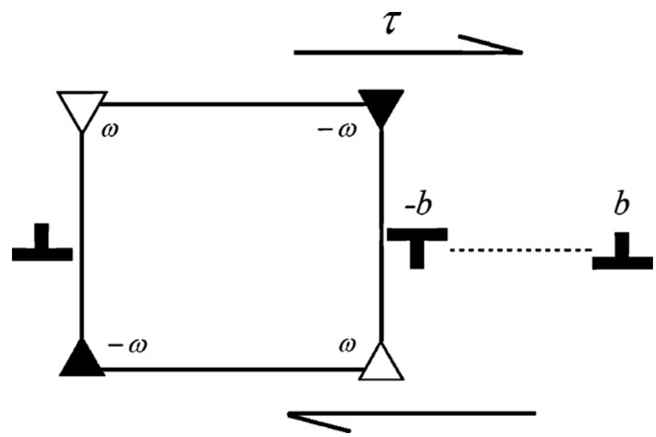

Fig. 3. The transformation from the rotational deformation into plastic shear.

$$\tau_c = \frac{Gb}{2\pi(1-\nu)d}\ln\left(\frac{0.4\varphi d}{b}\right) \tag{7}$$

where φ is the dislocation core parameter and varies from 1 to 4 for metals [42]. According to formula (7), we calculated the dependence of critical required shear stress τ_c on grain size d (Fig. 4). It can be seen that τ_c increases with decreased grain size. This is the main reason why SRD can provide more fracture toughness in nc materials than that in coarse materials.

In order to characterize the effect of SRD on crack growth, one should compare the value K_{IC}^* with the fracture toughness $K_{IC}^{\sigma} = \sqrt{4G\gamma/(1-\nu)}$ in the SRD-free case, that is, the case of brittle fracture with the SRD being completely suppressed. With the calculating results of formulas (2)–(7) substituted to formula (1) and the expression for K_{IC}^{σ} taken in to account, we obtain the depen-

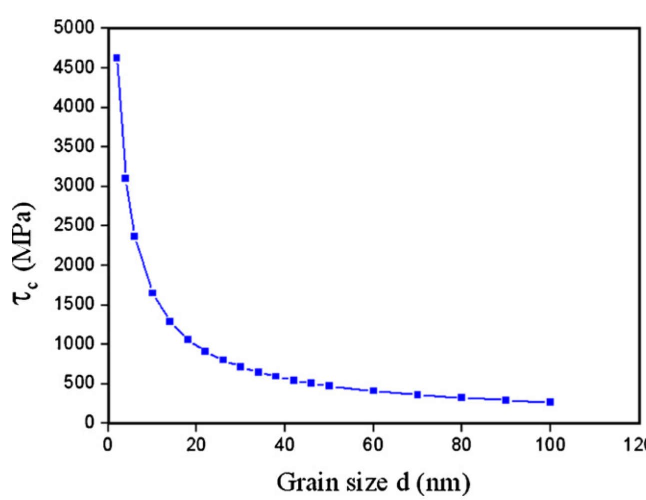

Fig. 4. Dependence of critical shear stress τ_c on grain size d in nc Ni.

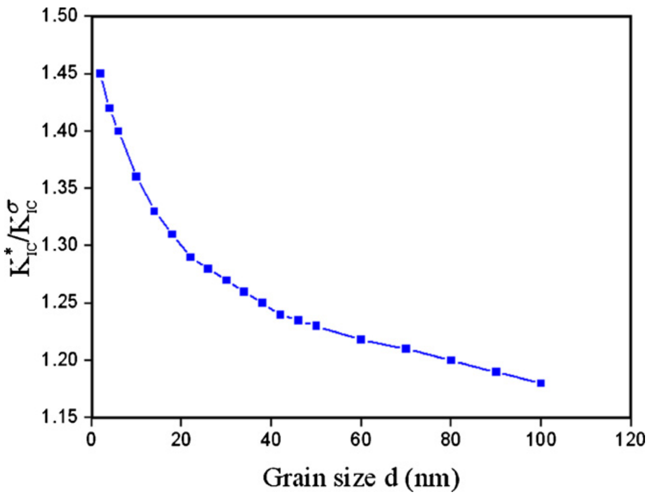

Fig. 5. K^*_{IC}/K^σ_{IC} as a function of grain size d in nc Ni.

dence of the ratio K^*_{IC}/K^σ_{IC} on the grain size of nc materials that is shown in Fig. 5. The results suggest that:

1. Owing to the SRD, fracture toughness increases by 10–50% when compared with the case without SRD. This is in agreement with the previous inference that SRD can enhance the fracture toughness of nc materials.
2. K^*_{IC}/K^σ_{IC} increases with decreased grain size in nc materials. This is because the stress concentration at the crack tip has a very strong gradient descent. When the grain size increases, the stress decreases quickly. Consequently, GB dislocation climb, driven by the stress concentration near the crack tip, becomes too slow to fully accommodate GB sliding and can no more promote fracture toughness. Thus, the suggested model is not applicable to the solids with a grain size above a hundred nanometers.

3. Conclusions

In summary, we have suggested a grain size dependent theoretical model to describe the effect of SRD on crack growth in deformed nc materials. The SRD occurs in a nanograin through the formation of immobile disclinations whose strength gradually increases during the formation process assisted by both GB sliding and diffusion. Our model suggests that (i) the SRD can significantly enhance the fracture toughness of nc materials and (ii) the reduction in the grain size of nc materials plays a dominant role in the enhancement of toughness.

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References

[1] M.A. Meyers, A. Mishra, D.J. Benson, Prog. Mater. Sci. 51 (2006) 427.
[2] S. Benkassem, L. Capolungo, M. Cherkaoui, Acta Mater. 55 (2007) 3563.
[3] K.S. Kumar, S. Suresh, H. Van Swygenhoven, Acta Mater. 51 (2003) 5743.
[4] C.C. Koch, J. Mater. Sci. 42 (2007) 1403.
[5] K.A. Padmanabhan, G.P. Dinda, H. Hahn, H. Gleiter, Mater. Sci. Eng. A 452 (2007) 462.
[6] M. Dao, L. Lu, R.J. Asaro, J.T.M. De Hosson, E. Ma, Acta Mater. 55 (2007) 4041.
[7] L. Capolungo, M. Cherkaoui, J. Qu, Int. J. Plast. 23 (2007) 561.
[8] Y.G. Liu, J.Q. Zhou, X. Ling, Mater. Sci. Eng. A 527 (2010) 1719.
[9] S. Bhaduri, S.B. Bhaduri, Nanostruct. Mater. 8 (1997) 755.
[10] R. Mirshams, S.H. Whang, C.H. Xiao, W.M. Yin, Mater. Sci. Eng. A 315 (2001) 21.
[11] J.D. Kuntz, G.D. Zhan, A.K. Mukherjee, MRS Bull. 29 (2004) 22.
[12] Y. Zhao, J. Qian, L.L. Daemen, C. Pantea, J. Zhang, G.A. Voronin, T.W. Zerda, Appl. Phys. Lett. 84 (2004) 1356.
[13] A.A. Kaminskii, M.Sh. Akchurin, R.V. Gainutdinov, K. Takaichi, A. Shirakava, H. Yagi, T. Yanagitani, K. Ueda, Crystallogr. Rep. 50 (2005) 869.
[14] Y.T. Pei, D. Galvan, J.T.M. De Hosson, Acta Mater. 53 (2005) 4505.
[15] M. Yu, I. Gutkin, A. Ovid'ko, Acta Mater. 56 (2008) 1642.
[16] F. Ashby, R.A. Verall, Acta Metall. 21 (1973) 149.
[17] W. Yang, H.T. Wang, Int. J. Sol. Struct. 45 (2008) 3897.
[18] F. Yang, W. Yang, J. Mech. Phys. Solids 57 (2009) 305.
[19] W.W. Milligan, S.A. Hackney, M. Ke, E.C. Aifantis, Nanostruct. Mater. 2 (1993) 267.
[20] M. Ke, W.W. Milligan, S.A. Hackney, J.E. Carsley, E.C. Aifantis, Nanostruct. Mater. 5 (1995) 689.
[21] S. Hackney, M. Ke, W.W. Milligan, E.C. Aifantis, in: C. Suryanarayana (Ed.), Processing and Properties of Nanocrystalline Materials, TMS, Warrendale, PA, 1996, pp. 421–426.
[22] A.K. Mukherjee, Mater. Sci. Eng. A 322 (2002) 1.
[23] M. Murayama, J.M. Howe, H. Hidaka, S. Takaki, Science 295 (2002) 2433.
[24] Zh. Shan, E.A. Stach, J.M.K. Wiezorek, J.A. Knapp, D.M. Follstaedt, S.X. Mao, Science 305 (2004) 654.
[25] I. Zizak, J.W. Gerlach, W. Assmann, Phys. Rev. Lett. 101 (2008) 065503.
[26] A. Latapie, D. Farkas, Phys. Rev. B 69 (2004) 134110.
[27] T. Shimokawa, A. Nakatani, H. Kitagawa, Phys. Rev. B 71 (2005) 224110.
[28] I. Szlufarska, A. Nakano, P. Vashista, Science 309 (2005) 911.
[29] S.P. Joshi, K.T. Ramesh, Phys. Rev. Lett. 101 (2008) 025501.
[30] A.E. Romanov, A.L. Kolesnikova, I.A. Ovid'ko, E.C. Aifantis, Mater. Sci. Eng. A 503 (2009) 62.
[31] N.F. Morozov, I.A. Ovid'ko, A.G. Sheinerman, E.C. Aifantis, J. Mech. Phys. Solids 58 (2010) 1088.
[32] P. Cavaliere, Int. J. Fatigue 31 (2009) 1476.
[33] I.A. Ovid'ko, A.G. Sheinerman, Scripta Mater. 59 (2008) 119.
[34] H. Conrad, J. Narayan, Scripta Mater. 42 (2000) 1025.
[35] K.A. Padmanabhan, H. Gleiter, Mater. Sci. Eng. A 381 (2004) 28.
[36] M.J. Demkowicz, A.S. Argon, D. Farkas, M. Frary, Philos. Magn. 87 (2007) 4253.
[37] S.V. Bobylev, M.Y. Gutkin, I.A. Ovid'ko, Phys. Rev. B 73 (2006) 064102.
[38] S.V. Bobylev, A.K. Mukherjee, I.A. Ovid'ko, Scripta Mater. 60 (2009) 36.
[39] S.V. Bobylev, A.K. Mukherjee, I.A. Ovid'ko, A.G. Sheinerman, Int. J. Plast. 26 (2010) 1629.
[40] T.Y. Zhang, J.C.M. Li, Acta Metall. Mater. 39 (1991) 2739.
[41] A.E. Romanov, V.I. Vladimirov, in: F.R.N. Nabarro (Ed.), Dislocations in Solids, vol. 9, North-Holland Publ. Co., Amsterdam, 1992, pp. 191–302.
[42] J.P. Hirth, J. Lothe, Theory of Dislocations, McGraw-Hill, New York, 1982.