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Generation of Nanocracks at Deformation Twins in Nanomaterials

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The formation of cracks at nanoscale deformation twins stopped by grain boundaries (GBs) is theoretically described as a new fracture mode in nanocrystalline and ultrafine-grained materials. It is noted that dipoles of partial wedge disclinations are formed at GBs, where they stop deformation twins and create high local stresses capable of initiating crack generation. Within this scenario, the critical parameters for crack generation at deformation twins stopped by GBs are revealed. The results of the theoretical analysis explain the corresponding data of experiments and computer simulations and predict novel specific features of the crack formation in deformed nanomaterials.

Keywords: Nanocrystalline Materials, Fracture, Cracks, Twins

Nanocrystalline and ultrafine-grained materials (hereinafter called nanomaterials) are typically characterized by superior strength and show deformation behaviors controlled by specific mechanisms of plastic flow; see, e.g. reviews [1–8] and book.[9] Therefore, in parallel with conventional lattice slip (dominating in coarse-grained polycrystals), specific deformation mechanisms – nanoscale twin deformation and grain boundary (GB) deformation modes – effectively operate in nanomaterials and strongly affect their mechanical properties.[1–9] In particular, following numerous experimental data, computer simulations, and theoretical models, twin deformation highly contributes to plastic flow in various nanomaterials at certain conditions; see, e.g. original research papers [10–25] and review.[8]

In most cases, nanocrystalline materials exhibit superior strength, but disappointingly low tensile ductility at ambient temperatures. The low ductility is the key problem that prevents wide structural applications of nanomaterials.[1–9] Despite the recent progress in solving this problem in several partial cases (see reviews [26–28]), its general solution (opening an opportunity to systematically fabricate nanomaterials with simultaneously high strength and good ductility) is still not found and represents the subject of intense debates. The crucial

role in the optimization of strength and ductility of nanomaterials is played by competition/interaction between plastic deformation and fracture processes having their specific features in nanomaterials due to the nanoscale and GB effects. In particular, crack generation and growth processes often occur at GBs and their triple junctions in nanomaterials characterized by large amounts of GBs and deformed by GB deformation mechanisms; for a review, see [29]. A typical example of such processes is represented by the generation of nanocracks in the stress field of GB disclination defects arising due to GB sliding; see theoretical model.[30] Besides, in nanomaterials, twin deformation and fracture can occur cooperatively. For instance, nanoscale twins can be generated at GBs near large preexistent cracks in nanocrystalline materials.[31]

In general, with large contribution of nanoscale twin deformation to plastic flow in nanomaterials, of utmost interest is the search for the specific fracture modes initiated by nanoscale twins in such materials. Recently, computer simulations [32] have demonstrated that a new fracture mode can operate in nanocrystalline Mo deformed by nanoscale twinning. This mode represents crack generation at nanoscale deformation twins stopped by GBs. The computer simulations [32] are well

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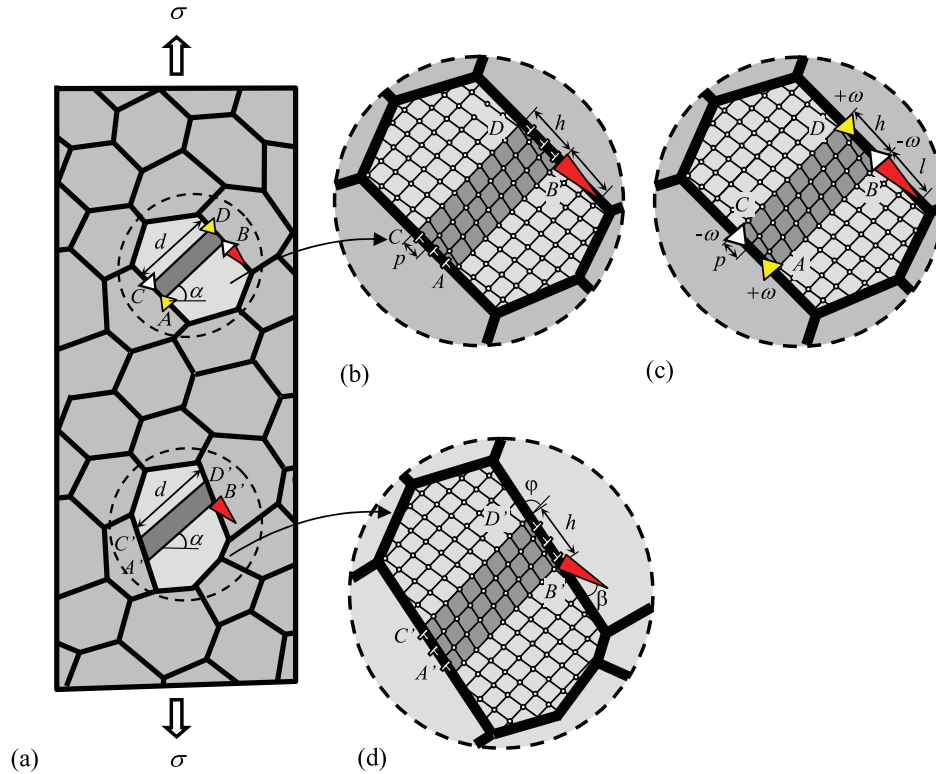


Figure 1. Nanocracks at nanoscale deformation twins in deformed nanocrystalline solids. (a) General view. (b)–(d) Magnified insets highlighting nanoscale twins and nanocracks. (b) Magnified inset highlights nanoscale twin $ABCD$ restricted by opposite parallel GBs within a nanograin. Here, dipoles of partial Shockley dislocations are generated in the neighboring planes under the action of the applied stress. This results in the formation of the deformation nanotwin $ABCD$ with boundaries AB and CD being perpendicular to the GB planes restricting the twin lamella. (c) The stress field created by the two walls of edge Shockley dislocations having opposite Burgers vectors is equivalent to that created by a quadrupole of wedge disclinations. This stress field induces the generation of a nanocrack at a GB. (d) Magnified inset highlights nanoscale twin $A'B'C'D'$ and an intragrain nanocrack generated in its stress field. The twin boundaries $A'B'$ and $C'D'$ are not perpendicular to the GB planes restricting the twin lamella.

consistent with the experimental observations [33,34] of cracks formed at intersection sites for deformation twins and GBs in coarse-grained γ -TiAl. The papers [32–34] reported on computer simulations and experimental observations of crack generation in nano- and polycrystalline materials, but did not analyze the conditions for the realization of this new fracture mode. At the same time, in order to understand if the new fracture mode is typical in nanomaterials with various crystal lattices and other materials deformed by twinning, it is crucially important to reveal the conditions of crack generation at deformation twins stopped by GBs. The main aims of this Letter are to theoretically describe the conditions of crack generation at deformation twins and identify the critical parameters that control this new fracture mode in nanomaterials.

Let us discuss the geometric characteristics of deformation twins stopped by GBs in a nanocrystalline solid consisting of nanoscale grains divided by GBs. A two-dimensional section of the solid is schematically shown in Figure 1(a). The solid is under a remote one-axis tensile load σ . Within our model, during plastic flow in the nanocrystalline solid, deformation twin lamellas,

$ABCD$ and $A'B'C'D'$, in nanoscale grains are generated (Figure 1(a)). Each of these lamellas is restricted by opposite parallel GBs (Figure 1(a) and 1(b)). Following, [30, 35–37] we assume that the twin lamellas are composed of overlapping stacking faults that join opposite twinning partial dislocations whose dipoles form in adjacent slip planes (Figure 1(a) and 1(b)). In the case of fcc crystals, the dipoles of Shockley partials form in adjacent slip planes $\{111\}$.

Let us consider the nanoscale deformation twin $ABCD$. The twin lamella is perpendicular to the GBs that stop its growth, as it is schematically shown in Figure 1(b). We denote the twin lamella thickness (equal to the length of the GB segments AB and CD) as h , the twin lamella length (Figure 1(b)) as d , and the distance between the neighboring dislocations in the dislocation walls at the GB segments AB and CD as p . In doing so, the distance p between identical Shockley dislocations producing the deformation twin lamella equals to the distance between the $\{111\}$ crystallographic planes and is related to the crystal lattice parameter a as $p = a/\sqrt{3}$. Within our model, the Shockley partials are of edge character, and their Burgers vectors $\pm \mathbf{b}$ are of the

$(a/6) < 112 >$ type. The magnitude b of such Burgers vectors is equal to $a/\sqrt{6}$.

The nanoscale twin $ABCD$ (Figure 1(a) and 1(b)) stopped by GBs creates internal stresses in the specimen. Following,[36] the two walls, AC and BD, of edge Shockley partials can be represented as a quadrupole of wedge disclinations with the strengths $\pm\omega$ (Figure 1(c)). Within this representation, according to the theory of disclinations,[36] the disclination strength magnitude ω is in the following relationship with the Burgers vector magnitude b of the Shockley partials and the distance p between neighboring dislocation dipoles: $\omega = 2 \arctan(b/(2p))$.

The stress fields of the disclination quadrupole and the applied load σ are capable of inducing the generation of a nanocrack. For definiteness, let us consider the generation of a GB nanocrack located as shown in Figure 1(a)–(c). In order to estimate the conditions for the nanocrack generation and growth, in the following we assume that the twin length d is large compared with both the twin thickness h and the nanocrack length l . Then, we can neglect the effects of disclinations located at points A and C on the nanocrack generation and growth. In other words, we consider the generation and growth of the nanocrack in superposition of the stress field created by the disclination dipole BD and the applied load.

In order to analyze the conditions for the nanocrack generation and growth, we employ the energetic criterion of nanocrack growth [38]

$$F > 2\gamma - \gamma_b, \quad (1)$$

where F is the energy release rate, γ is the specific surface energy, and γ_b is the specific (per unit area) GB energy. The expression on the left-hand side of formula (1) designates the strain energy released due to nanocrack advance by unit length, while the expression on the right-hand side of formula (1) describes the energy associated with the formation of two new free surfaces and elimination of a GB fragment in the course of nanocrack propagation. The energy release rate is calculated in the standard way [31] using the expressions for the stress field of a disclination dipole in an isotropic infinite solid with the shear modulus G and the Poisson's ratio ν . As a result, we obtain the following condition for nanocrack growth: $q > q_c$, where q and q_c are the parameters defined as follows:

$$q = \frac{2Gl}{2\gamma - \gamma_b} \left[g^2 \left(\frac{l}{h} \right) + \left(\frac{\pi(1-\nu)\sigma \sin(2\alpha)}{G\omega} \right)^2 \right], \quad (2)$$

$$g(\tilde{l}) = \ln \frac{\sqrt{\tilde{l}+1}+1}{\sqrt{\tilde{l}+1}-1} - \frac{2(\sqrt{\tilde{l}+1}-1)}{\tilde{l}}, \quad (3)$$

$$q_c = \frac{32\pi(1-\nu)}{\omega^2}, \quad (4)$$

ω is the disclination strength (for details, see our previous discussion), and $\tilde{l}$ is the argument of the function $g(\tilde{l})$.

Let us plot the dependences $q(l)$ in the case of nanocrystalline Ni characterized by the following values of parameters: $G = 79$ GPa, $\nu = 0.31$, $\gamma = 1.725$ J/m², $\gamma_b = 0.69$ J/m², $a = 0.352$ nm. The above values of γ and γ_b are the characteristic mean values of specific surface energy and specific tilt GB energy, respectively.[39] We also put $\sigma = 1$ GPa and $\alpha = \pi/4$. (The value of $\sigma = 1$ GPa is typical for the flow stress in nanocrystalline Ni,[40] while $\alpha = \pi/4$ corresponds to the direction of the maximum shear stress (induced by the external tensile load) at which the nanotwin generation is most favorable.) The dependences $q(l)$ are presented in Figure 2(a), for various values of the twin width h . The horizontal line in Figure 2(a) shows the value of q_c . The nanocrack growth is energetically favored, if the curve $q(l)$ lies higher than the horizontal line q_c . As it follows from Figure 2(a), two situations can take place. In particular, if the twin width h is small (see the lowest curve in Figure 2(a)), the nanocrack generation is not favored. If the twin width h exceeds a critical value, the nanocrack generation is favored. In this case, nanocrack growth is energetically favorable until the nanocrack length reaches its equilibrium value l_e . The equilibrium length l_e is determined by the intersection of the curve $q(l)$ with the horizontal line q_c . It is seen in Figure 2(a) that the equilibrium nanocrack length l_e increases with h . In particular, for $h = 3$ nm, we have $l_e \approx 4.3$ nm, whereas for $h = 4$ nm, we have $l_e \approx 13.3$ nm. The analysis demonstrates that the critical value of h (the minimum value at which the nanocrack generation is favored) is approximately equal to 2.6 nm.

In calculation of the dependences $q(l)$ presented in Figure 2(a), we have chosen a value of 0.69 J/m² for the specific GB energy. In general, however, real values of tilt GB energies in nanocrystalline Ni can vary in a wide range from 0.3 to 1.5 J/m²; see, e.g. [41,42].

Therefore, in Figure 2(b), we plot the dependence $q(l)$ at $h = 3$ nm and three different values of γ_b (0.4, 0.8 and 1.2 J/m²). It is seen in Figure 2(b) that an increase in the specific GB energy γ_b leads to an increase in the equilibrium nanocrack length l_e . For example, for $\gamma_b = 0.4$ J/m², we have $l_e \approx 3.9$ nm, while at $\gamma_b = 1.2$ J/m², we have $l_e \approx 9.4$ nm.

Now let us consider a nanoscale deformation twin $A'B'C'D'$ whose boundaries, A' and $C'D'$, make an arbitrary angle φ with the GBs (Figure 1(a) and 1(d)). In this case, the Burgers vectors of Shockley partial dislocations are not normal to the GBs, and the dislocation ensemble cannot be represented as a pure quadrupole of wedge disclinations. As a corollary, the stress field of the dislocation ensemble at segments $A'B'$ and $C'D'$ is different from that created in the case shown in Figure 1(b). In doing so, in the case illustrated in Figure 1(d), the nanocrack formed in the stress field of the Shockley partial dislocations can

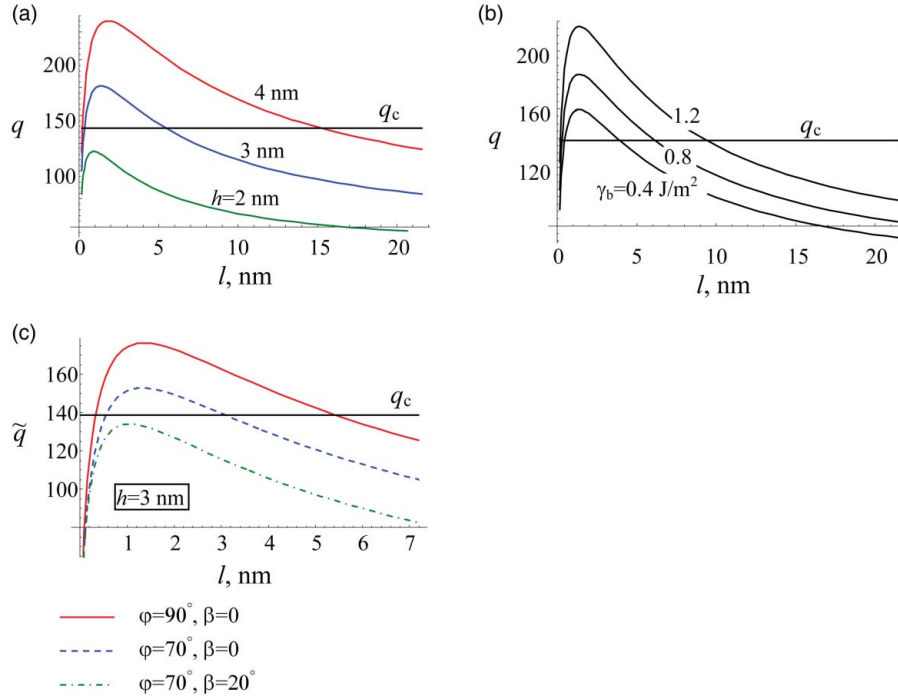


Figure 2. Dependences of the parameter q (a, b) and $\tilde{q}$ (c) on the nanocrack length l . The horizontal lines show the value of the parameter q_c .

either grow along a GB or inside the grain, making an angle β with the GB. The latter case is illustrated in Figure 1(d).

Let us calculate the conditions for the nanocrack generation and growth in the stress field of the Shockley partials producing the nanotwin (Figure 1(d)). To do so, as with our previous consideration, we assume that the twin length d is large compared with both the twin thickness h and the nanocrack length l . In these circumstances, we can neglect the effects of Shockley partials located at the twin boundary AC on the nanocrack generation and growth. In other words, we consider the generation and growth of the nanocrack in superposition of the applied load σ and the stress field created by an array of Shockley partials located only at the twin boundary BD .

In order to calculate the conditions for nanocrack growth, we use the energetic criterion.[38] The calculation is very similar to that given in the first part of this Letter. Here we omit the details of the calculation and present only its final results. Therefore, the condition for energetically favorable nanocrack growth is as follows: $\tilde{q}(l) > q_c$, where $\tilde{q}(l)$ is a function of the nanocrack length l , depending on the angles α , β and ϕ , elastic constants of the solid, applied load σ , the nanotwin width h , the Burgers vector magnitudes b of the Shockley partials, their interspacing p , and the specific surface energy γ (as well as the specific GB energy γ_b , if the nanocrack grows along the GB).

The dependences $\tilde{q}(l)$ in the exemplary situation with nanocrystalline Ni are presented in Figure 2(c), for

$h = 3$ nm, $\sigma = 1$ GPa, $\alpha = \pi/4$, $\gamma_b = 0.69$ J/m² and different values of the angles β and ϕ . The horizontal line in Figure 2(c) shows the value of q_c . The three curves in Figure 2(c) correspond to three different cases. The upper curve illustrates the case where the twin boundaries AB and CD are normal to GBs and the nanocrack grows along the GB. The intermediate curve corresponds to the case where the twin boundaries AB and CD make the angle $\phi = 70^\circ$ with the GBs, and the nanocrack also grows along the GB. The lower curve illustrates the case where the twin boundaries AB and CD make the angle $\phi = 70^\circ$ with the GBs, and the nanocrack grows inside a grain. As it follows from Figure 2(c), for the parameter values used, the nanocrack generation and growth inside the grain are not energetically favored (in this situation, $\tilde{q} < q_c$, for any nanocrack length l ; see the lowest curve in Figure 2(c)). In the case of the GB nanocrack, its growth is the easiest when the twin boundaries AB and CD are normal to GBs. In doing so, the interval of nanocrack lengths where nanocrack growth is energetically favorable (that is, the curve $\tilde{q}(l)$ lies higher than the horizontal line q_c) is wider than that in the case of $\phi = 70^\circ$; see the two upper curves in Figure 2(c)). Thus, the case where the twin lamella is normal to GBs is most favorable for the generation and growth of nanocracks.

To summarize, crack generation at nanoscale deformation twins stopped by GBs serves as a special fracture mode (alternative to crack generation driven by GB deformation and/or conventional activities of lattice dislocations) effectively operating in nanocrystalline and

ultrafine-grained materials. This theoretically revealed statement is well consistent with the corresponding experimental data [33,34] and computer simulations.[32] Within our theoretical approach, the key critical parameters influencing the crack generation process at deformation twins stopped by GBs are revealed to be the twin width, the angle of intersection of deformation twin and GB plane, and the external stress. Also, GB misorientation (which specifies geometric opportunity for a twin to penetrate through a GB to a neighboring grain) is expected to play a prominent role in crack generation at deformation twins in nanomaterials.

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References

- [1] Wolf D, Yamakov V, Phillpot SR, Mukherjee AK, Gleiter H. Deformation of nanocrystalline materials by molecular-dynamics simulation: relationship to experiments? *Acta Mater.* 2005;53:1–40.
- [2] Meyers MA, Misra A, Benson DJ. Mechanical properties of nanostructured materials. *Progr Mater Sci.* 2006;51:427–556.
- [3] Dao M, Lu L, Asaro RJ, De Hosson JTM, Ma E. Toward a quantitative understanding of mechanical behavior of nanocrystalline metals. *Acta Mater.* 2007;55:4041–4065.
- [4] Koch CC. Structural nanocrystalline materials: an overview. *J Mater Sci.* 2007;42:1403–1414.
- [5] Kawasaki M, Langdon TG. Principles of superplasticity in ultrafine-grained materials. *J Mater Sci.* 2007;42:1782–1796.
- [6] Pande CS, Cooper KP. Nanomechanics of Hall–Petch relationship in nanocrystalline materials. *Progr Mater Sci.* 2009;54:689–706.
- [7] Ovid'ko IA, Sheinerman AG. Micromechanisms for improved fracture toughness in nanoceramics. *Rev Adv Mater Sci.* 2011;29:105–125.
- [8] Zhu YT, Liao XZ, Wu XL. Deformation twinning in nanocrystalline materials. *Progr Mater Sci.* 2012;57:1–62.
- [9] Koch CC, Ovid'ko IA, Seal S, Veprek S. Structural nanocrystalline materials: fundamentals and applications. Cambridge: Cambridge University Press; 2007.
- [10] Liao XZ, Zhou F, Lavernia EJ, He DW, Zhu YT. Deformation twins in nanocrystalline Al. *Appl Phys Lett.* 2003;83:5062–5064.
- [11] Chen M, Ma E, Hemker KJ, Sheng H, Wang Y, Cheng X. Deformation twinning in nanocrystalline aluminum. *Science.* 2003;300:1275–1277.
- [12] Liao XZ, Zhao YH, Srinivasan SG, Zhu YT, Valiev RZ, Gunderov DV. Deformation twinning in nanocrystalline copper at room temperature and low strain rate. *Appl Phys Lett.* 2004;84:592–594.
- [13] Wang YM, Hodge AM, Biener J, Hamza AV, Barnes DE, Liu K, Nieh TG. Deformation twinning during nanoindentation of nanocrystalline Ta. *Appl Phys Lett.* 2005;86:101915.
- [14] Wu XL, Zhu YT. Partial-dislocation-mediated processes in nanocrystalline Ni with nonequilibrium grain boundaries. *Appl Phys Lett.* 2006;89:031922.
- [15] Gutkin MY, Ovid'ko IA, Skiba NV. Generation of deformation twins in nanocrystalline metals: theoretical model. *Phys Rev B.* 2006;74:172107.
- [16] Zhang J-Y, Liu G, Wang RH, Li J, Sun J, Ma E. Double-inverse grain size dependence of deformation twinning in nanocrystalline Cu. *Phys Rev B.* 2008;81:172104.
- [17] Wu X-L, Liao XZ, Srinivasan SG, Zhou F, Lavernia EJ, Valiev RZ, Zhu YT. New deformation twinning mechanism generates zero macroscopic strain in nanocrystalline metals. *Phys Rev Lett.* 2008;100:095701.
- [18] Wu X-L, Zhu YT. Inverse grain-size effect on twinning in nanocrystalline Ni. *Phys Rev Lett.* 2008;101:025503.
- [19] Zhang XY, Wu XL, Zhu AW. Growth of deformation twins in room-temperature rolled nanocrystalline nickel. *Appl. Phys. Lett.* 2009;94:121907.
- [20] Zhu YT, Wu XL, Liao XZ, Narayan J, Mathaudhu SN, Kecskes LJ. Twinning partial multiplication at grain boundary in nanocrystalline fcc metals. *Appl Phys Lett.* 2009;95:031909.
- [21] Li Q, Sui ML, Mao SX. Pseudoelastic stacking fault and deformation twinning in nanocrystalline Ni. *Appl Phys Lett.* 2010;97:241912.
- [22] Wang YM, Ott RT, Hamza AV, Besser MF, Almer J, Kramer MJ. Achieving large uniform tensile ductility in nanocrystalline metals. *Phys Rev Lett.* 2010;105:215502.
- [23] Ovid'ko IA, Sheinerman AG. Deformation twinning through nanoscale ideal shears in nano- and polycrystalline materials at ultra high stresses. *Rev Adv Mater Sci.* 2011;27:189–194.
- [24] Ovid'ko IA. Nanoscale multiplane shear and twin deformation in nanowires and nanocrystalline solids. *Appl Phys Lett.* 2011;99:061907.
- [25] Beyerlein IJ, Wang J, Kang K, Zheng SJ, Mara NA. Twinnability of bimetal interfaces in nanostructured composites. *Mater Res Lett.* 2013;1:89–95 (doi: 10.1080/21663831.2013.78207).
- [26] Ma E. Eight routes to improve the tensile ductility of bulk nanostructured materials and alloys. *JOM.* 2006;54:49–53.
- [27] Zhao Y, Zhu YT, Lavernia EJ. Strategies for improving tensile ductility of bulk nanostructured materials. *Adv Eng Mater.* 2010;12:769–778.
- [28] Ovid'ko IA, Langdon TG. Enhanced ductility of nanocrystalline and ultrafine-grained metals. *Rev Adv Mater Sci.* 2012;30:103–111.
- [29] Ovid'ko IA. Review on the fracture processes in nanocrystalline materials. *J Mater Sci.* 2007;45:1694–1708.
- [30] Gutkin MY, Ovid'ko IA, Skiba NV. Crack-stimulated generation of deformation twins in nanocrystalline metals and ceramics. *Philos Mag.* 2006;88:1137–1151.
- [31] Ovid'ko IA, Sheinerman AG. Special strain hardening mechanism and nanocrack generation in nanocrystalline materials. *Appl Phys Lett.* 2007;90:171927.
- [32] Zhang Y, Millett PC, Tonks M, Biner B. Deformation-twin-induced grain boundary failure. *Sci Mater.* 2012;66:117–120.
- [33] Ng BC, Simkin BA, Crimp MA, Bieler TR. The role of mechanical twinning on microcrack nucleation and crack propagation in a near- γ TiAl alloy. *Intermetallics.* 2004;12:1317–1323.
- [34] Simkin BA, Ng BC, Crimp MA, Bieler TR. Crack opening due to deformation twin shear at grain boundaries in near- γ TiAl. *Intermetallics.* 2007;15:55–60.

- [35] Sutton AP, Balluffi RW. Interfaces in crystalline materials. Oxford: Oxford Science Publications; 1996.
- [36] Romanov AE, Vladimirov VI. Disclinations in crystalline solids. In: Nabarro FRN, editor. Dislocations in solids. Amsterdam: North-Holland; 1992. vol. 9, p. 402.
- [37] Gutkin MY, Ovid'ko IA, Skiba NV. Generation of deformation twins in nanocrystalline metals: theoretical model. *Phys Rev B*. 2006;74:172107.
- [38] Irwin RG. Analysis of stresses and strains near the end of a crack traversing a plate. *J Appl Mech*. 1957;24:361–364.
- [39] Hirth JP, Lothe J. Theory of dislocations. New York: Wiley; 1982.
- [40] Li H, Ebrahimi F. Transition of deformation and fracture behaviors in nanostructured face-centered-cubic metals. *Appl Phys Lett*. 2004;84:4307.
- [41] Rohrer GS, Holm EA, Rollett AD, Foiles SM, Li J, Olmsted DL. Comparing calculated and measured grain boundary energies in nickel. *Acta Mater*. 2010;58:5063.
- [42] Udler D, Seidman DN. Grain boundary and surface energies of fcc metals. *Phys Rev B*. 1996;54:R11133.