Rev. Adv. Mater. Sci. 39 (2014) 9-14

NANOCRACK GENERATION DUE TO STRESS-DRIVEN WIDENING OF TWINS IN NANOTWINNED METALS

I.A. Ovid'ko[1,2] and A.G. Sheinerman[1,2]

[1]St. Petersburg State Polytechnical University, St. Petersburg 195251, Russia
[2]Department of Mathematics and Mechanics, St. Petersburg State University, St. Petersburg 198504, Russia

Received: September 17, 2014

Abstract. A theoretical model is suggested which describes generation of nanocracks in nanotwinned metals during their plastic deformation occurring through stress-driven widening of nanoscale twins in nanotwinned metals. In the framework of the suggested model, widening of pre-existent growth twins under mechanical load carries plastic deformation and leads to formation of wedge disclination structures at junctions of twin and grain boundaries. These disclinations create high local stresses capable of inducing nanocrack generation. The conditions for such a crack generation in nanotwinned metals are calculated.

1. INTRODUCTION

Nanotwinned metals represent ultrafine-grained metallic materials containing high-density ensembles of nanoscale twins within ultrafine grains [1-3]. Such nanotwinned metals often show both high strength and good ductility at room temperature; see, e.g., [1-10]. This remarkable combination of high strength and good ductility is very important for structural applications of nanotwinned metals, and its nature is of utmost interest from a fundamental viewpoint [1-10]. In terms of mechanics of materials, strength and ductility of nanotwinned metals are strongly influenced or even controlled by competition between plastic deformation and fracture processes in such metals. These plastic deformation and fracture processes as well as their competition have their specific features due to the specific structural features of nanotwinned solids. For instance, in nanotwinned metals, plastic deformation can effectively occur through a rather specific mode, the namely widening of nanoscale growth twins bounded by grain boundaries [2]. In the context discussed, it is highly interesting to understand and describe competition of the specific deformation mode with fracture processes. The main aim of this paper is to suggest a theoretical model that describes nanocrack generation in high local stresses created due to previous plastic deformation through widening of nanoscale growth twins bounded by grain boundaries in nanotwinned metals.

2. STRESS-DRIVEN MIGRATION OF TWIN BOUNDARIES IN A NANOTWINNED SOLID. MODEL

Let us consider a nanotwinned metallic solid under the action of a uniaxial tensile load σ_0 (Fig. 1a). For simplicity, we examine a two-dimensional model of the nanotwinned metal (Fig. 1a). Within the model, the grains of the nanotwinned solid contain rectangular twins of nanoscopic thickness (nanotwins) bounded by both coherent twin boundaries and fragments of grain boundaries (Figs. 1a and 1b). Consider a typical grain containing N+2 nanotwins di-

Corresponding author: I.A. Ovidko, e-mail: ovidko@nano.ipme.ru

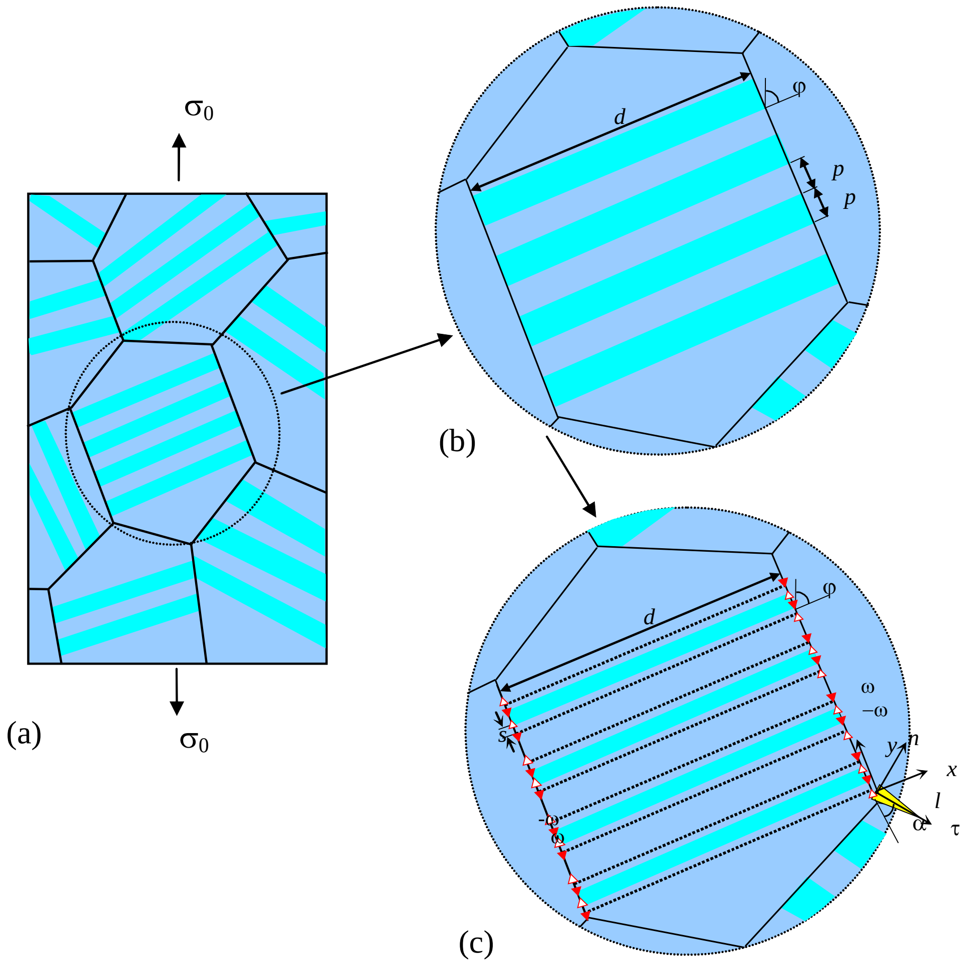

Fig. 1. (Color online) Formation of a nanocrack in a deformed nanotwinned metallic solid. (a) Deformed nanotwinned metallic solid (general view). The insets (b) and (c) show twin boundary migration and formation of a nanocrack in a typical grain. (b) The model grain contains N+1 twin boundaries. (c) Twin boundary migration – stress-driven widening of twins – in the grain is accompanied by the formation of an array of disclination quadrupoles and induces the generation of a nanocrack.

vided by N+1 coherent twin boundaries. We assume that the distances between the twin boundaries are the same and equal to p, and the lengths of these boundaries are equal to d (Fig. 1b).

Also, we assume that the applied tensile load induces twin boundary migration leading to widening of twins (and playing the role of a plastic deformation mode in nanotwinned solids [2]). In nanotwinned metals with face-centered cubic (fcc) lattices twin boundary migration occurs through the glide of Shockley partials over twin boundaries [11–16]. In turn, the glide of Shockley partials over twin boundaries can occur either through emission of preexistent Shockley partials from one grain boundary to another or via the homogeneous generation of the dipoles of Shockley partials at opposite grain boundaries. Let us denote the twin boundaries by index n, where n runs from 0 to N. We suppose that the lengths of twin boundary migration are the same and equal to s. Also, we designate the angle between twin boundaries and the direction of the applied load as φ (Figs. 1b and 1c).

It should be noted that here we consider the situation where in the initial state (before twin boundary migration) the junctions of twin and grain boundaries do not contain defects. This is in contrast to model [17] that considered nanotwinned solids containing junction disclinations even in the non-deformed state. At the same time, in our case of the initially defect-free solid, twin boundary migration results in the formation of wedge disclination quadrupoles. Indeed, according to the theory of defects in solids [18], migration of each twin boundary results in the formation of a quadrupole of wedge disclinations whose strengths ω and -ω are equal (in terms of their absolute value) to the misorientation angle of the migrating twin boundary [17]. As a consequence, migration of twin boundaries leads to the formation of an array of disclination quadrupoles (Fig. 1c). If the stresses created by these quadrupoles are high enough, the quadrupole can induce the generation of nanocrack at a junction disclination (Fig. 1c).

3. CALCULATION OF THE CONDITIONS FOR NANOCRACK GENERATION IN THE STRESS FIELD OF DISCLINATION QUADRUPOLES AND THE APPLIED LOAD IN A NANOTWINNED SOLID

Let us calculate the conditions for nanocrack generation in a deformed nanotwinned solid containing a regular array of disclination quadrupoles (Fig. 1c). To do so, we will model the nanotwinned solid as an isotropic medium with the shear modulus G and Poisson's ratio ν. We assume that the nanocrack nucleates at the lowest right disclination of the array, that is, in the region where the tensile stresses are highest (see Fig. 1c). We denote the nanocrack length as l and the angle between the nanocrack and grain boundary planes as α (Fig. 1c). Also, we introduce two Cartesian coordinate systems (x,y) and (τ,n) with the same origin, as shown in Fig. 1c. To calculate the condition for nanocrack generation and growth, we use the energetic criterion of nanocrack growth, suggesting that the strain energy release rate associated with crack growth exceeds the specific energy of the newly formed crack free surfaces. This criterion has the following quantitative form [19]:

$$F > 2\gamma, \tag{1}$$

where F is the energy release rate, and γ is the specific surface energy.

The energy release rate associated with nanocrack growth is given [19] by

$$F = \frac{\pi(1-\nu)l}{4G}\left(\bar{\sigma}_{nn}^2 + \bar{\sigma}_{\tau n}^2\right), \tag{2}$$

where $\bar{\sigma}_{nn}$ and $\bar{\sigma}_{\tau n}$ are the mean weighted stresses calculated [19] as

$$\bar{\sigma}_{\left\{ nn \atop \tau n \right\}} = \frac{2}{\pi l}\int_0^l \sigma_{\left\{ nn \atop \tau n \right\}}(\tau, n=0)\sqrt{\frac{\tau}{l-\tau}}\,d\tau \tag{3}$$

and σ_{nn} and $\sigma_{\tau n}$ are the components of the tensor of the total stress created by the array of disclination quadrupoles and the applied load in the absence of the nanocrack.

For convenience, we introduce the normalized stresses $g_{ij} = \sigma_{ij}/(D\omega)$, where $i,j = x,y$ and $D = G/[2\pi(1-\nu)]$. The normalized stress tensor components g_{nn} and $g_{\tau n}$ can be expressed in terms of the normalized components g_{xx}, g_{yy}, and g_{xy} of the total stress tensor in the coordinate system (x,y) as follows:

$$g_{nn} = g_{xx}\cos^2\alpha + g_{yy}\sin^2\alpha + g_{xy}\sin(2\alpha), \tag{4}$$

$$g_{\tau n} = (1/2)\left(g_{xx} - g_{yy}\right)\sin(2\alpha) - g_{xy}\cos(2\alpha). \tag{5}$$

In turn, the normalized stresses g_{xx}, g_{yy}, and g_{xy} can be calculated using the expressions [18] for the stress fields of wedge disclinations in an infinite solid as

$$\begin{aligned} g_{ij} = \sum_{n=0}^{N}(-1)^n\Big[g_{ij}^{\Delta}(x, y-np-s) - \\ g_{ij}^{\Delta}(x, y-np-s+s(-1)^n) - g_{ij}^{\Delta}(x+d, y-np-s) + \\ g_{ij}^{\Delta}(x+d, y-np-s+s(-1)^n)\Big] + \sigma_{ij}^{e}/(D\omega), \end{aligned} \tag{6}$$

where $\sigma_{xx}^e = \sigma_0\cos^2\varphi$, $\sigma_{yy}^e = \sigma_0\sin^2\varphi$, $\sigma_{xy}^e = \sigma_0\sin(2\varphi)$,

$$\begin{aligned} g_{xx}^{\Delta}(x,y) &= \frac{\ln\left(x^2+y^2\right)}{2} + \frac{y^2}{x^2+y^2}, \\ g_{yy}^{\Delta}(x,y) &= \frac{\ln\left(x^2+y^2\right)}{2} + \frac{x^2}{x^2+y^2}, \\ g_{xy}^{\Delta}(x,y) &= -\frac{xy}{x^2+y^2}. \end{aligned} \tag{7}$$

Now substitution of formulae (2) and (3) to criterion (1) and the relation $g_{ij} = \sigma_{ij}/(D\omega)$ yields the following condition of nanocrack growth: $q > q_c$, where $q_c = 8p^3(1-\nu)\gamma/(G\omega^2)$,

$$\begin{aligned} q = (1/l)\Bigg[\left(\int_0^l g_{nn}(\tau, n=0)\sqrt{\frac{\tau}{l-\tau}}\,d\tau\right)^2 + \\ \left(\int_0^l g_{\tau n}(\tau, n=0)\sqrt{\frac{\tau}{l-\tau}}\,d\tau\right)^2\Bigg], \end{aligned} \tag{8}$$

and the coordinate τ at the nanocrack plane $n = 0$ is related to the coordinates x and y as follows: $x = \tau\sin\alpha$ and $y = \tau\cos\alpha$.

Let us plot the dependences $q(l)$ in the case of nanotwinned Cu characterized by the following values of parameters: $G = 48$ GPa, $\nu = 0.34$, $\gamma = 1.725$ J/m^2, $\omega = 2\arctan(\sqrt{2}/4) \approx 39°$, and $d = 400$ nm.

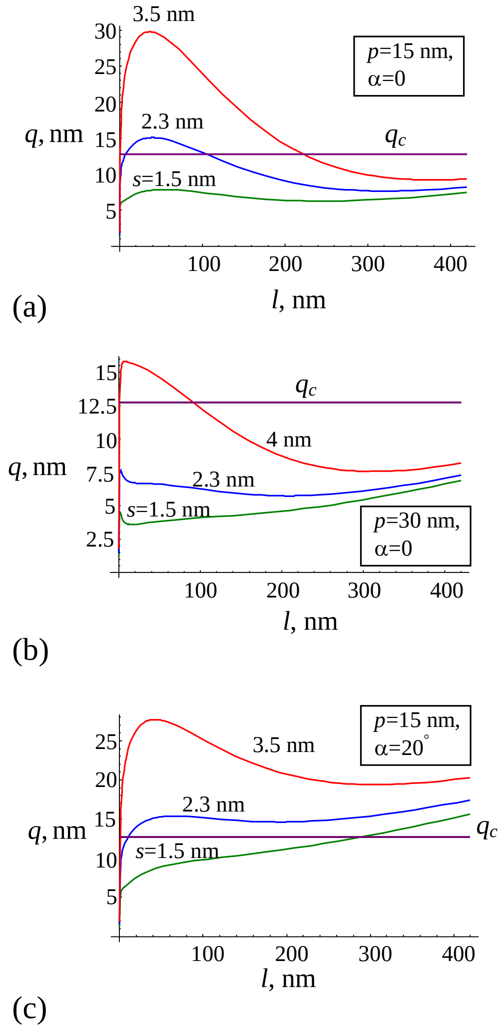

Fig. 2. (Color online) Dependences of the parameter q on the nanocrack length l, for various values of the parameters s,p, and α. The horizontal lines show the values of the parameter q_c.

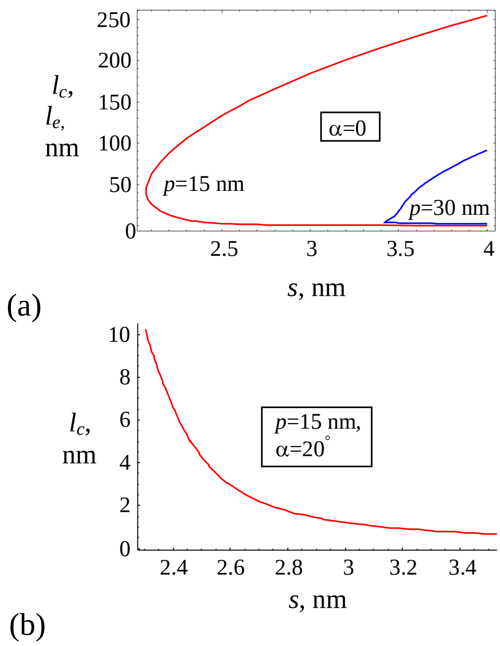

Fig. 3. (Color online) Critical nanocrack length l_c (a,b) and equilibrium nanocrack length l_e (a) vs. twin boundary migration length s, for various values of the twin thickness p and angle α.

We also put σ_0 = 1 GPa and $\varphi = \pi/4$. Besides, we consider the case of approximately equiaxed grains and choose N from the relation $(N + 2)p \approx d$. The dependences $q(l)$ for nanotwinned Cu are presented in Fig. 2, for various values of the nanotwin boundary migration length s, twin thickness p and the angle α characterizing nanocrack orientation with respect to the nearest grain boundary plane. The horizontal lines in Fig. 2 show the values of q_c. Nanocrack growth is energetically favored, if the curve $q(l)$ lies higher than the horizontal line q_c. As it follows from Fig. 2, two situations can take place. If the twin boundary migration length s is small (see the lowest curve in Figs. 2a, 2b, and 2c), nanocrack generation is not favored. If the twin boundary migration length s exceeds a critical value, nanocrack generation is favored. In the latter case, nanocrack can grow in two different modes. In the situation shown in Figs. 2a and 2b, nanocrack growth is energetically favorable in some crack length interval $l_c<l<l_e$. The critical nanocrack length l_c and equilibrium nanocrack length l_e correspond to the left and right points of intersection of the curve $q(l)$ with the horizontal line q_c, respectively. A stable nanocrack is generated when the crack length reaches its critical value of l_c through thermal fluctuations. Then the crack growth is energetically favorable until the crack length reaches its equilibrium value of l_e. In contrast, in the situation depicted in Fig. 2c, nanocrack growth is favored in crack length interval $l>l_c$. In the latter situation, the crack has to reach its critical length l_c through thermal fluctuations as well. However, at $l>l_c$, the crack can grow catastrophically under the action of the applied load unless its growth is stopped by disclinations or other stress sources in neighboring grains.

Figs. 2a and 2b demonstrate that the critical nanocrack length l_c decreases, and the equilibrium nanocrack length l_e increases with increasing s and/or decreasing p (the latter is accompanied by increasing the number N+1 of disclination quadrupoles). This tendency is also illustrated in Fig. 3a showing the dependences of l_c (lower branches of the curves) and l_e (upper branches of the curves) on twin boundary migration length s, for two different values of twin thickness p. In particular, for s = 2.5 nm and p = 15 nm, we have: $l_c \approx 2.7$ nm and $l_e \approx 132$

nm, for s = 3.6 nm and p = 15 nm, we have: $l_c \approx 0.55$ nm and $l_e \approx 229$ nm, whereas, for s = 3.6 nm and p = 30 nm, we have: $l_c \approx 2$ nm and $l_e \approx 42$ nm. The observed decrease in l_c and increase in l_e with decreasing p (accompanied by increasing N) is associated with higher stresses that a larger and denser array of disclination quadrupoles creates near the crack tip.

We now consider the case shown in Fig. 2c, where the equilibrium crack l_e does not exist, and the crack, if its length reaches the critical length l_c, can grow catastrophically. In this case, the dependences of the critical length l_c on the twin boundary migration length s are shown in Fig. 3b, for p = 15 nm and α = 20. Fig. 3b demonstrates that l_c decreases with increasing s, as above. For example, the value l_c =1 nm is reached at $s \approx 3.1$ nm, while the value l_c =2 nm is reached at $s \approx 2.7$ nm.

Let us suppose that the nanocrack can grow through thermal fluctuations until the length of around 1 to 2 nm. In this case, Figs. 2 and 3 demonstrate that the formation of a nanocrack in deformed nanotwinned Cu with ultrafine grains is possible, if the twin boundary migration length s is high enough, that is, $s \approx 2$–3 nm. At the same time, Fig. 2c shows that if the collective twin boundary migration does occur over such a length, it can lead to the formation of a catastrophic crack resulting in the fracture of the nanotwinned solid.

Now let us consider the case where twin boundary migration length s is equilibrium, that is, corresponds to a minimum of the energy of the nanotwinned solid in the absence of cracks. To do so, we calculate the energy variation associated with the collective migration of twin boundaries in a specified grain (see Fig. 1). For definiteness, we consider the most favorable situation for twin boundary migration, where twin boundaries make the angle $\varphi = \pi/4$ with the direction of the tensile load and the shear strain $\tau = \sigma_0 \sin(2\varphi)$ acting on the twinning partials is maximum. For definiteness, we also focus on the case where the number N-1 of twin boundaries is odd, that is, $N = 2M$, where M is an integer.

The energy variation ΔW due the formation of $2M$-1 disclination quadrupole (per unit disclination length) can be presented as

$$\Delta W = W^q + W^{q-\sigma}, \qquad (9)$$

where W^q is the proper energy of the array of disclination quadrupoles and $W^{q-\sigma}$ is the energy of their interaction with the applied load.

The energy W^q can be calculated using expressions [18] for the self-energies of wedge disclination dipoles and the energies of the interaction between wedge disclinations in an isotropic infinite solid as

$$W^q = \frac{D\omega^2 d^2}{2}\Bigg[\sum_{k=1}^{M-1}(M-k)\times \big(f((2k-1)p/d, s/d) + f((2k-1)p/d, -s/d)\big) + (2M-1)h(s/d)\Bigg], \qquad (10)$$

where $f(u,t) = h(2t + u) + h(u) - 2h(t + u)$ and $h(x) = (x^2 + 1)\ln(x^2 + 1) - x^2\ln(x^2)$.

The energy $W^{q-\sigma}$ is calculated [18] as

$$W^{q-\sigma} = -(2M-1)\tau\omega s d. \qquad (11)$$

The minimum (critical) shear stress for the collective migration of twin boundaries by the distance s follows from $\partial \Delta W / \partial s|_{\tau=\tau_c} = 0$. Substitution of formulas (9) to (11) to the latter relation yields

$$\tau_c = D\omega\Bigg(h_1(t) + \frac{2}{2M-1}\sum_{k=1}^{M-1}(M-k)f_1\big((2k-1)p/d, t\big)\Bigg), \qquad (12)$$

where $t = s/d$, $h_1(t) = t\ln(1 + 1/t^2)$ and

$$f_1(u,t) = (1/4)\partial\big(f(u,t) + f(u,-t)\big)/\partial t = h_1(u+2t) - h_1(u-2t) + h_1(u-t) - h_1(u+t). \qquad (13)$$

In the examined case of $\varphi = \pi/4$, the critical applied load σ_c for the collective twin boundary migration is related to the critical shear stress τ_c as $\sigma_c = 2\tau_c$.

The dependences of the critical stress σ_c on the normalized migration length s/d for the equiaxed grain, characterized by $d = N/p$, in nanotwinned Cu are presented in Fig. 4, for N = 12, 24, and 50. The critical stress σ_c = 1 GPa corresponds to the nor-

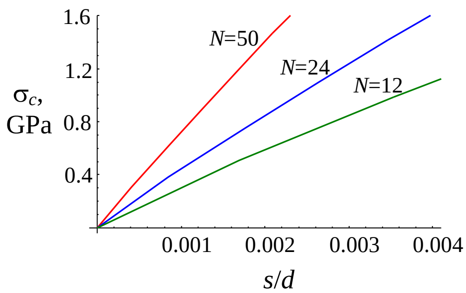

Fig. 4. (Color online) Dependences of the critical applied load σ_c for collective twin boundary migration in a specified grain of nanotwinned Cu on the normalized twin boundary migration length s/d, for various numbers of twin boundaries.

malized migration lengths *s*/*d* equal to 0.0036, 0.0024, and 0.0014, for N = 12, 24, and 50, respectively. In the exemplary case of p = 15 nm, this corresponds to the equilibrium migration lengths of 0.65, 0.86, and 1.05 nm, respectively. These values are much smaller than the characteristic values of migration length (around 3 nm) at which the nanocrack is expected to nucleate in the case of p = 15 nm. This explains observations [2,3] of good strength of nanotwinned metals.

At the same time, one should note that with increasing the number N+1 of twin boundaries, the equilibrium twin boundary migration length increases, while the value of the twin boundary migration length, at which nanocrack nucleation is expected, decreases. Therefore, nanocracks can nucleate, if the number of twin boundaries within the grains of nanotwinned solids is very high (e.g., several hundreds or more). In particular, nanocracks are expected to nucleate in nanotwinned solids with large enough grains containing dense or ultradense ensembles of twin boundaries.

4. CONCLUDING REMARKS

Thus, as it has been demonstrated in this paper, nanocracks in nanotwinned metals can be generated in high local stresses created due to previous plastic deformation through widening of nanoscale growth twins bounded by grain boundaries. At the same time, according to our estimates, stress-driven widening of twins induces generation of nanocracks only in the situation where very high external stresses operate. This theoretical conclusion is well consistent with the observations [2,3] of good strength exhibited by nanotwinned metals.

ACKNOWLEDGEMENTS

This work was supported, in part, (for IAO) by the St. Petersburg State University research grant 6.37.671.2013 and (for AGS) by the Russian Ministry of Education and Science (Zadanie 9.1964. 2014/K).

REFERENCES

[1] L. Lu, Y. Shen, X. Chen, L. Qian and K. Lu // *Science* **304** (2004) 422.

[2] L. Lu, X. Chen, X. Huang and K. Lu // *Science* **323** (2009) 607.

[3] K. Lu, L. Lu and S. Suresh // *Science* **324** (2009) 349.

[4] I.-C. Choi, Y.-J. Kim, Y.M. Wang, U. Ramamurty and J.-I. Jang // *Acta Mater.* **61** (2013) 7313.

[5] J.R. Greer // *Nature Mater*. **12** (2013) 689.

[6] Y.M. Wang, F. Sansoz, T. LaGrange, R.T. Ott, J. Marian, T.W. Barbee and Jr & Alex V. Hamza // *Nature Mater*. **12** (2013) 697.

[7] Z. Zhang, Y. Huo, F. Huo, X. Zhang, L. Zhang and D. Guo // *Scr. Mater*. **68** (2013) 747.

[8] Z. Zhang, F. Li, G. Ma, R. Kang and X. Guo // *Scr. Mater*. **69** (2013) 231.

[9] Z. You, X. Li, L. Gui, Q. Lu, T. Zhu, H. Gao and L. Lu // *Acta Mater*. **61** (2013) 217.

[10] Y. Tian, B. Xu, D. Yu, Y. Ma, Y. Wang, Y. Jiang, W. Hu, C. Tang, Y. Gao, K. Luo, Z. Zhao, L.-M. Wang, B. Wen, J. He and Z. Liu // *Nature* **493** (2013) 385.

[11] J.W. Yan and G.P. Zhang // *Appl. Phys. Lett.* **102** (2013) 211905.

[12] R. Niu and K. Han // *Scr. Mater.* **68** (2013) 960.

[13] J. Wang, N. Li, O. Anderoglu, X. Zhang, A. Misra, J.Y. Huang and J.P. Hirth // *Acta Mater.* **58** (2010) 2262.

[14] H. Mirkhani and S.P. Joshi // *J. Mech. Phys. Sol.* **68** (2014) 107.

[15] Z.J. Jie, X. FangDa, Y. YongDa and S. Tao // *Chin. Sci. Bull.* **58** (2013) 684.

[16] Y. Wei // *Mater. Sci. Eng.* A **528** (2011) 1558.

[17] N.F. Morozov, I.A. Ovid'ko and N.V. Skiba // *Rev. Adv. Mater. Sci.* **37** (2014) 29.

[18] A.E. Romanov and V.I. Vladimirov, In: *Dislocations in Solids*, vol. 9, ed. by F.R.N. Nabarro (North-Holland, Amsterdam, 1992).

[19] *Mechanics of Fracture and Strength of Materials*, *Vol. 2*, ed. by V.V. Panasyuk (Naukova Dumka, Kiev, 1988).