Twin Boundary Migration and Nanocrack Generation in Ultrafine-Grained Materials with Nanotwinned Structure

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Abstract: A theoretical model is suggested which describes plastic flow and crack generation through twin boundary migration in nanotwinned metals (ultrafine-grained metallic materials containing high-density ensembles of nanoscale twins within grains). Within the suggested model, migration of twin boundaries under a mechanical load carries plastic deformation and leads to formation of wedge disclinations at the junctions of twin and grain boundaries. These disclinations create high local stresses that produce strengthening of nanotwinned metals and can induce nanocrack generation. Within the model, we calculate the flow stress as a function of twin thickness in nanotwinned metals in the situation where twin boundary migration significantly contributes to plastic flow. We also consider generation of nanocracks in nanotwinned metals during migration of twin boundaries and calculate the conditions for crack formation. Besides, our theoretical results and their comparison with corresponding experimental data are briefly discussed.

Key Words: Nanotwinned materials, plastic deformation, yield strength, fracture, cracks, defects, modeling

1 Introduction

Nanotwinned metals (ultrafine-grained metallic materials containing high-density ensembles of nanoscale twins within grains) represent new materials with simultaneously high strength and good ductility at room temperature (see, e.g., [1–4]). This combination of high strength and good ductility is very promising for a wide range of technologies exploiting the mechanical properties of materials. In terms of mechanics of materials, strength and ductility of nanotwinned metals are strongly influenced or even controlled by the competition between plastic deformation and fracture processes in such metals.

However, its fundamental nature is not fully understood and represents the subject of intensive debates; see, e.g., [1–4]. In particular, the specific deformation modes operating in nanotwinned metals are of crucial interest for understanding the role of the nanotwinned structure in optimization of strength and ductility. One specific deformation mechanism in nanotwinned metals is viewed to be plastic deformation occurring through migration of twin boundaries [2]. Previous research on this topic focused mainly on dislocation reactions resulting in formation of the twinning partial dislocations that move along twin boundaries and provide twin boundary migration [2, 5–10]. At the same time, in parallel with dislocations, grain boundaries (whose amounts are rather large in nanotwinned metals with ultrafine grains) can significantly influence plastic deformation carried by twins. When twin boundaries migrate, special defects – wedge disclinations – are typically formed at the junctions of grain and twin boundaries [11,12]. Such disclinations create stress fields, and their ensemble is often characterized by a high strain energy which can strongly influence the flow stresses of a nanotwinned metal. This factor should be taken into account in analysis of plastic flow and fracture of nanotwinned metals. The main aims of this paper are to suggest a theoretical model which describes plastic deformation through migration of twin boundaries in nanotwinned metals and to reveal the effect of defects formed at the junctions of twin and grain boundaries on the yield stress of nanotwinned metals and generation of nanocracks in these solids.

2 Geometry of Twin Boundary Migration in Nanotwinned Metals

Let us consider a mechanically loaded metallic specimen with the ultrafine grained structure, whose grains contain high-density ensembles of nanoscale twins (Fig. 1a). For simplicity, we will examine an idealized two-dimensional model of a nanotwinned metallic specimen under a uniaxial tensile load σ (Fig. 1). In the framework of our model, each grain of a nanotwinned metallic specimen contains periodically arranged rectangular twins whose short segments terminate at opposite grain boundaries (Fig. 1a and b). We consider a typical model grain containing N identical nanoscale twins periodically arranged with a period l (Fig. 1b). Each nanoscale twin in its initial state is specified by the thickness h_0 and the length d (Fig. 1b). In the framework of our model, the external stress σ induces the maximum shear stress $\tau = \sigma / 2$ that operates along twin boundaries and drives slip of partial Shockley dislocations along these boundaries. When such a dislocation slips along a twin boundary from one grain boundary to its opposite counterpart across a grain interior, the twin thickness h_0 increases by the distance δ between neighbouring crystallographic slip planes. Following Ref. [2], this deformation mode associated with twin boundary migration can significantly contribute to plastic flow in nanotwinned copper.

Since many studies of the nanotwinned metals are concerned with copper, we will focus on twin boundary migration in fcc metals, that is, metals with the face-centered cubic crystal lattice. In the framework of our model, we consider edge partial dislocations of $(a/6) < 11\overline{2} >$ type as carriers of the dislocation slip in slip planes {111} along twin boundaries in the typical model grain. Such Shockley dislocations are characterized by the Burgers vector magnitude $b = a / \sqrt{6}$, and their slip along twin boundaries leads to twin boundary migration. In the framework of our model, dislocation slip in the typical grain occurs simultaneously along N twin boundaries (including one twin boundary per each twin) within the grain and leads to simultaneous increase of the nanotwin thickness h_0 by the value of δ for all the N twins located within the grain (Fig. 1c).

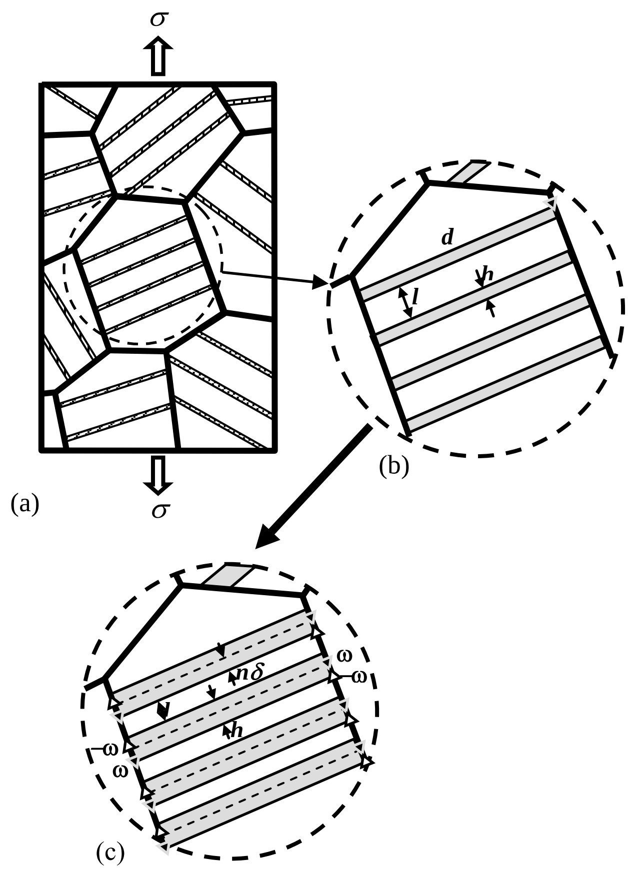

Fig. 1. Twin boundary migration in a nanotwinned metal specimen. (a) A nanotwinned metal specimen is under a tensile load (general view). Subfigures (b) and (c) illustrate a manified region of subfigure (a) and show evolution of twins and disclinations (formed at the junctions of twin and grain boundaries) in a typical model grain during plastic deformation occurring through twin boundary migration. (b) A typical model grain contains N periodically arranged identical nanotwins whose short segments are located on opposite grain boundaries. (c) The system of N nanotwins after n elementary acts of widening of nanotwins in the typical grain.

As a result of such elementary events of the dislocation slip, all the twins within the typical grain are widened, in which case the thickness of each twin becomes equal to $h_1 = h_0 + \delta$, and the distance between neighbouring twins decreases by value of δ and becomes equal to $l_1 = l - \delta$. The distance δ between neighbouring crystallographic slip planes {111} in fcc metals is in the following relationship with the crystal lattice parameter a: $\delta = a/\sqrt{3}$.

Within our model, the dislocation slip in the typical model grain occurs simultaneously along N twin boundaries of N twins (along one twin boundary per each twin) within the grain and leads to simultaneous increase of the nanotwin thickness h_0 by the value of δ for all the twins located within the grain. The process of nanotwin thickness widening by δ can occur many times and thus carry plastic deformation in a nanotwinned metal. After n events of nanotwin widening, the typical grain contains N twins, each having the thickness of $h = h_0 + n\delta$ (Fig. 1c). In doing so, the characteristic distance between neighbouring twins decreases down to the value of $l_n = l - n\delta$ (Fig. 1c).

It is important to note that twin boundary migration results in the formation of wedge disclination quadrupoles. Indeed, according to the theory of defects in solids [13], migration of each twin boundary results in the formation of a quadrupole of wedge disclinations whose strengths ω and $-\omega$ are equal (in terms of their absolute value) to the misorientation angle of the migrating twin boundary [11,12]. As a consequence, migration of twin boundaries leads to the formation of an array of disclination quadrupoles (Fig. 1c).

Each event of nanotwin widening is characterized by the critical shear stress τ_n^{crit} defined as the minimum external stress at which the twin widening process is energetically favourable. In next section, we will calculate the energy associated with twin boundary migration and the critical applied load needed to initiate this process.

3 Energy and Critical Stress for Twin Boundary Migration in Nanotwinned Metals

Let us consider the energy characteristics of N identical nanoscale twins (each having the thickness h_0 and the length d) periodically arranged with a period l in the typical grain (Fig. 1b). We assume that all the twin boundaries have migrated to their new positions by the distance $n\delta$. The strain energy of the twin system under examination can be approximated by the energy W_n associated with the formation of the disclination configuration consisting of N quadrupoles of $\pm\omega$- disclinations (Fig. 1c). The latter energy is given as:

$$W_n = E_N^q + E_N^{q-q} + E_N^{\tau}, \qquad (1)$$

where E_N^q is the total proper energy of N quadrupoles of $\pm\omega$- disclinations, E_N^{q-q} is total energy that characterizes the pair interactions between all the disclination quadrupoles, and E_N^{τ} is the work done by the external shear stress τ on widening of N nanotwins by the value of $n\delta$. In the approximation of an elastically isotropic solid, the total proper energy E_N^q is given by the following standard expression [14]:

$$E_N^q = \frac{ND\omega^2}{2}\left((\Delta h)^2 \ln\frac{(\Delta h)^2 + d^2}{(\Delta h)^2} + d^2 \ln\frac{(\Delta h)^2 + d^2}{d^2} \right), \qquad (2)$$

where $D = G/2\pi(1-\nu)$, G is the shear modulus, and ν is the Poisson ratio.

The energy that characterizes the pair interaction between the ith and jth quadrupoles of $\pm\omega$- disclinations is calculated in the standard way as the work spent to the generation of the jth quadrupole in the shear stress field created by the ith quadrupole. The energy E_N^{q-q} represents the sum of the above energies that characterize the pair interactions and is calculated using the expressions [13] for the stress fields of wedge disclinations in an infinite isotropic solid. For brevity, we do not present the expressions for E_N^{q-q} here.

The energy E_N^{τ} is given by the following formula:

$$E_N^{\tau} = -N\omega(\tau - \tau_y)n\delta d, \qquad (3)$$

where τ_y is an effective friction stress associated with the energetic barrier that each Shockley dislocation has to overcome to be emitted from a grain boundary in the absence of disclinations. In the most favorable case for twin boundary migration, where twin boundaries make an angle of 45° with the direction of the applied stress, we have: $\tau_y \approx \sigma_y/2$, where σ_y is the tensile yield stress of the nanotwinned solid. Formulae (1)–(3) allow us to calculate the total energy W_n of the system as a function of the initial twin thickness h_0 and twin boundary migration length $n\delta$.

In order to quantitatively describe the strain hardening (that is, an increase of the flow stress with rising plastic strain), let us calculate the energy change $\Delta W_n = W_n - W_{n-1}$ related to an elementary widening of N twins by δ within the typical grain. Here W_{n-1} is the energy of the system in its (n-1)th state with N twins each having the thickness $h_{n-1} = h_0 + (n-1)\delta$ (after $n-1$ previous events of widening of twins), and W_n is the energy of the system in its nth state with N twins each having the thickness $h_n = h_0 + n\delta$ (after n previous events of widening of twins) (Fig. 1c).

The nth widening process is energetically favourable if $\Delta W_n < 0$. In terms of stresses, the nth widening process is energetically favourable, if the external shear stress τ reaches its critical value τ_n^{crit}. The critical stress τ_n^{crit} is defined as the minimum stress at which the following condition is valid: $\Delta W_n = 0$.

The nth widening process is also characterized by the plastic strain ε associated with twin boundary migration. The plastic strain ε within the typical grain is approximately as follows:

$$\varepsilon \approx \frac{nN\delta}{d}. \quad (4)$$

Formula (4) for the plastic strain ε and the expression $\sigma = 2\tau_n^{crit}$ allow us to calculate the dependence of the flow stress on the plastic strain in the case of nanotwinned Cu. With the previously used values of parameters characterizing copper and its nanotwinned structure within the typical model grain, we calculated the dependences $\sigma(\varepsilon)$. This dependences are presented in Fig. 2, for the case $h_0 = l$ and various values of the nanotwin thickness h_0. In plotting Fig. 2, the number N of nanotwins in the typical grain was taken as $N = \lfloor d/(h_0 + l) \rfloor$, where $\lfloor X \rfloor$ means an integer part of a rational number X. The experimental values of the yield stress for nanotwinned Cu have been taken from Ref. [2]. As it follows from Fig. 2, the flow stress increases when the twin thickness h_0 increases.

Note that the experimentally measured [2,3] ultimate stresses for nanotwinned copper are lower than typical values of the flow stress (Fig. 2) obtained in our theoretical estimates. This discrepancy can be logically explained by the fact the ultrafine-grained structure of a nanotwinned metallic specimen and configurations of nanotwins in its grains are not identical. We have considered plastic deformation of a typical model grain. Plastic deformation through twin boundary migration is favoured in this grain, because of "stress-favoured" orientation of its twin boundaries. More precisely, the twin boundaries in the typical grain are oriented along the direction of the maximum shear stress action which drives the partial dislocation slip along these boundaries and leads to twin boundary migration. At the same time, in parallel with grains containing "stress-favoured" twin boundaries in a nanotwinned metal specimen, there are grains containing twins that cannot be deformed by twin boundary migration due to their unfavourable orientation relative to the applied shear stress. The grains of the second sort are deformed by plastic flow modes different from twin boundary migration. In these circumstances, the flow stresses of a nanotwinned metal specimen are controlled by contributions from two or more plastic flow modes (including plastic deformation through twin boundary migration), and, in particular, the values of the flow stress can be lower than those (Fig. 2) that characterize migration of twin boundaries.

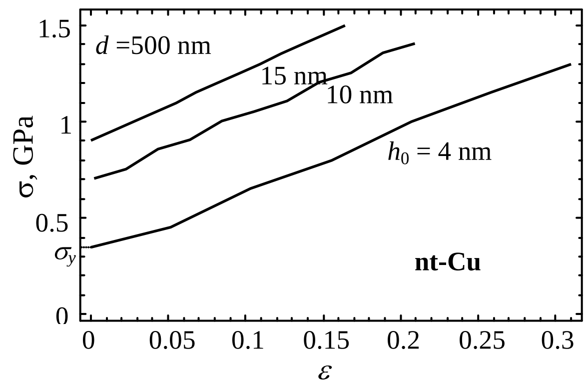

Fig. 2. Dependences of the flow stress σ on the plastic strain ε at various values of the initial (before plastic deformation) nanotwin thickness h_0 = 4 nm, 10 nm and 15 nm.

4 Nanocrack Generation in the Stress Field of Disclination Quadrupoles and Applied Load in a Nanotwinned Solid

In the previous section, we have calculated the flow stress associated with the migration of twin boundaries in nanotwinned solids. At the same time, besides producing plastic flow, twin boundary migration in nanotwinned solids can result in the formation of nanocracks.

To examine the formation of nanocracks, let us consider a nanotwinned metallic solid under the action of a uniaxial tensile load σ_0 (Fig. 3a). For simplicity, we examine a two-dimensional model of the nanotwinned metal (Fig. 3a). 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 (Fig. 3a). Consider a typical grain containing $N+2$ nanotwins divided 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.

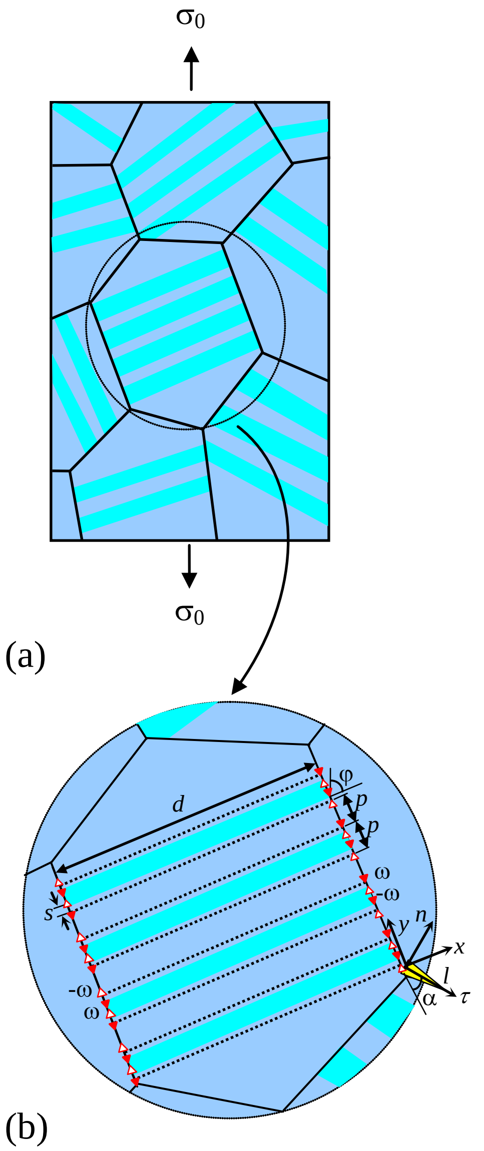

Fig. 3. Formation of a nanocrack in a deformed nanotwinned metallic solid. (a) Deformed nanotwinned metallic solid (general view). (b) Twin boundary migration in the grain is accompanied by the formation of an array of disclination quadrupoles and induces the generation of a nanocrack.

As above, we assume that the applied tensile load induces twin boundary migration. 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 (Fig. 3b). As above, within our model, migration of each twin boundary results in the formation of a quadrupole of wedge disclinations whose strengths ω and $-\omega$ are equal (in terms of their absolute value) to the misorientation angle of the migrating twin boundary. As a consequence, migration of twin boundaries leads to the formation of an array of disclination quadrupoles (Fig. 3b). If the stresses created by these quadrupoles are high enough, the quadrupole can induce the generation of nanocrack at a junction disclination (Fig. 3b).

Let us calculate the conditions for nanocrack generation in a deformed nanotwinned solid containing a regular array of disclination quadrupoles (Fig. 3b). As above, we 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. 3b). We denote the nanocrack length as l and the angle between the nanocrack and grain boundary planes as α (Fig. 3b). Also, we introduce two Cartesian coordinate systems (x, y) and (τ, n) with the same origin, as shown in Fig. 3b. 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 [17]:

$$F > 2\gamma, \tag{5}$$

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

The energy release rate associated with nanocrack growth is given [17] by

$$F = \frac{\pi(1-\nu)l}{4G}\left(\bar{\sigma}_{nn}^2 + \bar{\sigma}_{\tau n}^2\right), \tag{6}$$

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

$$\bar{\sigma}_{\left\{ {nn \atop \tau n} \right\}} = \frac{2}{\pi l}\int_0^l \sigma_{\left\{ {nn \atop \tau n} \right\}}(\tau, n=0)\sqrt{\frac{\tau}{l-\tau}}\,d\tau \tag{7}$$

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

$D = G/[2\pi(1-\nu)]$, as above. 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:

$$g_{nn} = g_{xx}\cos^2\alpha + g_{yy}\sin^2\alpha + g_{xy}\sin(2\alpha), \qquad (8)$$

$$g_{\tau n} = (1/2)(g_{xx} - g_{yy})\sin(2\alpha) - g_{xy}\cos(2\alpha). \qquad (9)$$

In turn, the normalized stresses g_{xx}, g_{yy} and g_{xy} can be calculated using the expressions [13] for the stress fields of wedge disclinations in an infinite solid as

$$\begin{aligned} g_{ij} = \sum_{n=0}^{N}(-1)^n \Big[& g_{ij}^{\Delta}(x, y-np-s) \\ & - g_{ij}^{\Delta}(x, y-np-s+s(-1)^n) \\ & - g_{ij}^{\Delta}(x+d, y-np-s) \\ & + g_{ij}^{\Delta}(x+d, y-np-s+s(-1)^n)\Big] + \sigma_{ij}^{e}/(D\omega), \end{aligned} \qquad (10)$$

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

$$g_{xx}^{\Delta}(x,y) = \frac{\ln(x^2+y^2)}{2} + \frac{y^2}{x^2+y^2},$$

$$g_{yy}^{\Delta}(x,y) = \frac{\ln(x^2+y^2)}{2} + \frac{x^2}{x^2+y^2},$$

$$g_{xy}^{\Delta}(x,y) = -\frac{xy}{x^2+y^2}. \qquad (11)$$

Now substitution of formulae (6) and (7) to criterion (5) and the relation $g_{ij} = \sigma_{ij}/(D\omega)$ yields the following condition of nanocrack growth: $q > q_c$, where $q_c = 8\pi^3(1-\nu)\gamma/(G\omega^2)$,

$$q = (1/l)\left[\left(\int_0^l g_{nn}(\tau, n=0)\sqrt{\frac{\tau}{l-\tau}}\,d\tau\right)^2 + \left(\int_0^l g_{\tau n}(\tau, n=0)\sqrt{\frac{\tau}{l-\tau}}\,d\tau\right)^2\right], \qquad (13)$$

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, $\omega = 2\arctan(\sqrt{2}/4) \approx 39^{\circ}$, and $d = 400$ nm. We also put $\sigma_0 = 1$ 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. 4, 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.

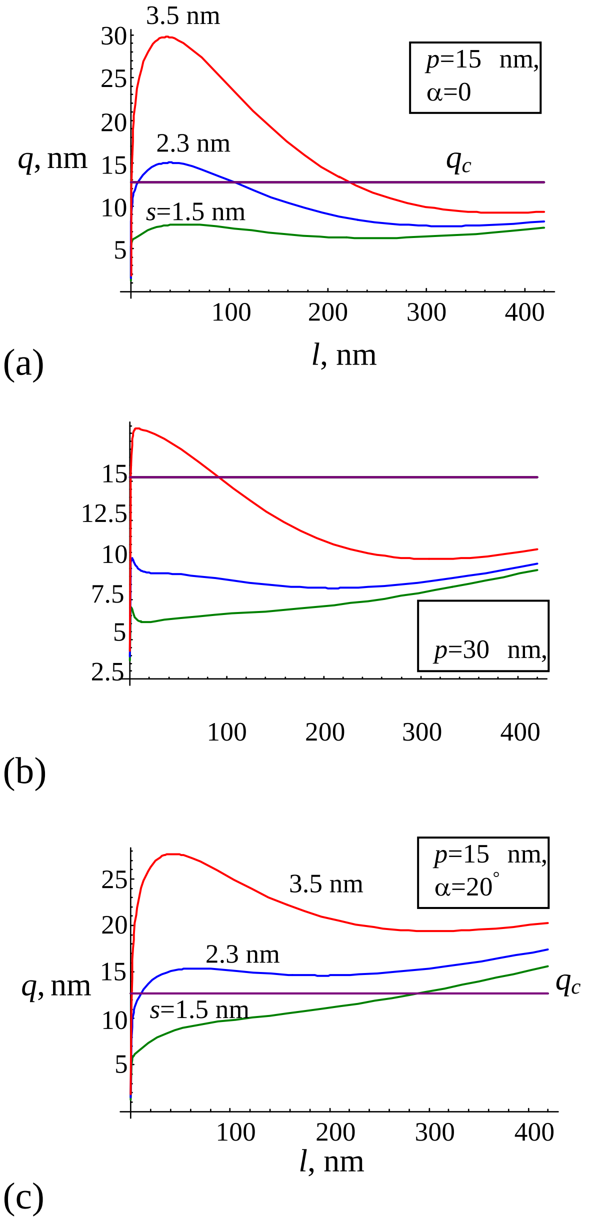

Fig. 4. Dependences of the parameter q on the nanocrack length l, for various values of the parameters s, p and α. The horizontal lines show the values of the parameter q_c.

The horizontal lines in Fig. 4 show the values of q_c. Nanocrack growth is energetically favoured if the curve $q(l)$ lies higher than the horizontal line q_c. As it follows from Fig. 4, two situations can take place. If the twin boundary migration length width s is small (see the lowest curve in Figs. 4a, 4b and 4c), nanocrack generation is not favoured. If the twin boundary migration length s exceeds a critical value, nanocrack generation is favoured. In the latter case, nanocrack can grow in two different modes. In the situation shown in Figs. 4a and 4b, nanocrack growth is energetically favourable 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 crack growth is energetically favourable until the crack length reaches its equilibrium value of l_e. In contrast, in the situation depicted in Fig. 4c, nanocrack growth is favoured 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 neighbouring grains.

Figures 4a and 4b 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. 5a 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. 4c, 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. 5b, for $p = 15$ nm and $\alpha = 20^\circ$. Figure 5b 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.

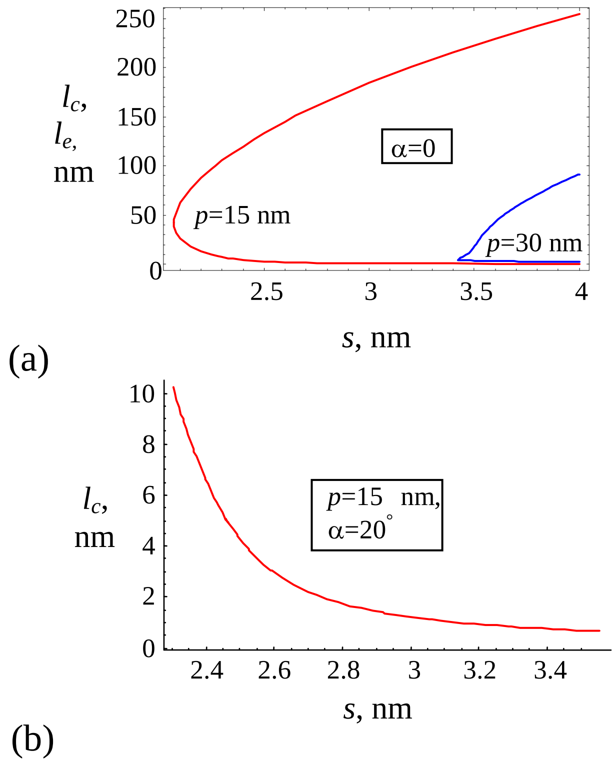

Fig. 5. Critical nanocrack length l_c (a,b) and equilibrium nanocrack length l_e (a) vs. twin boundary migration length s, for various values of the twin thickness p and angle α.

Let us suppose that the nanocrack can grow through thermal fluctuations until the length of around 1 to 2 nm. In this case, Figs. 4 and 5 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. 4c 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. 3). For definiteness, we consider the most favourable 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.

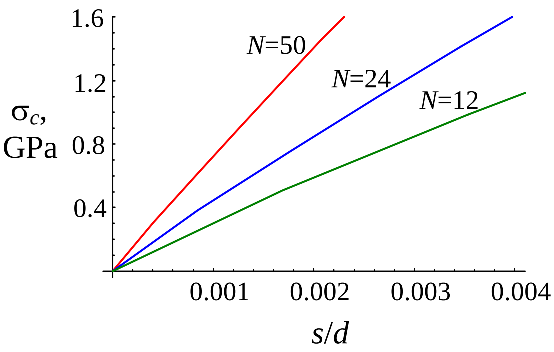

Fig. 6. Dependences of the critical applied load σ_c for collective twin boundary migration in a specified grain of nanotwinned Cu on the normalized twin boundary migration length s/d, for various numbers of twin boundaries.

The dependences of the critical stress σ_c on the normalized migration length s/d (obtained using formulae (1) to (3)) for the equiaxed grain, characterized by $d = Np$, in nanotwinned Cu are presented in Fig. 6, for $N = 12$, 24 and 50. The critical stress $\sigma_c = 1$ GPa corresponds to the normalized 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.

5 Conclusions

To summarize, we have suggested a model describing plastic flow and nanocrack generation in nanotwinned solids where migration of twin boundaries occurs in the course of plastic deformation. Within the model, twin boundary migration leads to the formation of wedge disclinations at the junctions of twin and grain boundaries (Figs. 1 and 3). We have calculated the flow stress of nanotwinned solids as a function of twin thickness in nanotwinned copper in the situation where twin boundary migration significantly contributes to plastic flow. In addition, we have calculated the conditions for nanocrack generation in the stress field of disclinations formed during twin boundary migration and the applied load. The calculations demonstrated that nanocracks are expected to nucleate in nanotwinned solids with large enough grains containing dense or ultradense ensembles of twin boundaries.

Acknowledgements

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References:

[1] L. Lu, Y. Shen, X. Chen, L. Qian, K. Lu, Ultrahigh Strength and High Electrical Conductivity in Copper, *Science*, vol. 304, No. 5669, 2004, pp. 422–426.

[2] L. Lu, X. Chen, X. Huang, K. Lu, Revealing the Maximum Strength in Nanotwinned Copper, *Science*, vol. 323, No. 5914, 2009, pp. 607–610.

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

[4] Z. You, X. Li, L. Gui, Q. Lu, T. Zhu, H. Gao, L. Lu, Plastic Anisotropy and Associated Deformation Mechanisms in Nanotwinned Metals, *Acta Materialia*, vol. 61, No. 1, 2013, pp. 217–227.

[5] J.W. Yan, G.P. Zhang, Revealing the Tunable Twinning/Detwinning Behavior in 25nm Cu/Au Multilayers, *Applied Physics Letters*, vol. 102, 2013, art. 211905.

[6] R. Niu, K. Han, Strain Hardening and Softening in Nanotwinned Cu, *Scripta Materialia*, vol. 68, 2013, pp. 960–963.

[7] J. Wang, N. Li, O. Anderoglu, X. Zhang, A. Misra, J.Y. Huang, J.P. Hirth, Detwinning Mechanisms for Growth Twins in Face-Centered Cubic Metals, *Acta Materialia*, vol. 58, 2010, pp. 2262–2270.

[8] H. Mirkhani, S.P. Joshi, Mechanism-Based Crystal Plasticity Modeling of Twin Boundary Migration in Nanotwinned Face-Centered-Cubic Metals, *Journal of the Mechanics and Physics of Solids*, vol. 68, 2014, pp. 107–133.

[9] Z.J. Jie, X. FangDa, Y. YongDa, S. Tao, Detwinning-Induced Reduction in Ductility of Twinned Copper Nanowires, *Chinese Science Bulletin*, vol. 58, No. 6, 2013, pp. 684–688.

[10] Y. Wei, The Kinetics and Energetics of Dislocation Mediated De-Twinning in Nano-Twinned Face-Centered Cubic Metals, *Materials Science and Engineering* A, vol. 528, No. 3, 2011, pp. 1558–1566.

[11] I.A. Ovid'ko, A.G. Sheinerman, Nanoscale Cracks at Deformation Twins Stopped by Grain Boundaries in Bulk and Thin-Film Materials with Nanocrystalline and Ultrafine-Grained Structures, *Journal of Physics* D, vol. 47, No. 1, 2014, art. 015307.

[12] I.A. Ovid'ko, N.V. Skiba, Nanotwins Induced by Grain Boundary Deformation Processes in Nanomaterials, *Scripta Materialia*, vol. 71, 2014, pp. 33–36.

[13] A.E. Romanov, V.I. Vladimirov, Disclinations in Crystalline Solids, In: *Dislocations in Solids*, vol. 9, ed. by F.R.N. Nabarro, North-Holland, 1992.

[14] A.E. Romanov, A.L. Kolesnikova, Application of Disclination Concept to Solid Structures, *Progress in Materials Science*, vol. 54, No. 6, 2009, pp. 740–769.

[15] R.A. Masumura, P.M. Hazzledine, C.S. Pande, Yield Stress of Fine Grained Materials, *Acta Materialia*, vol. 46, No. 13, 1998, pp. 4527–4534.

[16] M.Yu. Gutkin, I.A. Ovid'ko, Disclinations and Yield Stress of Metallic Glass-Nanocrystal Composites, *Nanostructured Materials*, vol. 2, No. 6, 1993, pp. 631–636.

[17] *Mechanics of Fracture and Strength of Materials,* vol. 2, ed. by V.V. Panasyuk, Naukova Dumka, 1988.