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PLASTIC FLOW THROUGH WIDENING OF NANOSCALE TWINS IN ULTRAFINE-GRAINED METALLIC MATERIALS WITH NANOTWINNED STRUCTURES

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Abstract. A theoretical model is suggested which describes plastic flow through widening of nanoscale twins in nanotwinned metals (ultrafine-grained metallic materials containing high-density ensembles of nanoscale twins within grains). In the framework of the suggested model, widening of pre-existent growth twins under mechanical load carries plastic deformation and leads to rearrangements of defect structures at junctions of twin and grain boundaries. With these factors (changes in twin widths, and rearrangements of defect structures), we calculated the yield stress as a function of twin thickness in nanotwinned metals in the situation where widening of nanoscale twins significantly contributes to plastic flow. Our theoretical results and their comparison with corresponding experimental data (reported in the literature) are discussed.

1. INTRODUCTION

Nanotwinned metals (ultrafine-grained metallic materials containing high-density ensembles of nanoscale twins within grains) are novel materials exhibiting simultaneously high strength and good ductility at room temperature; see, e.g., [1-11]. This combination of high strength and good ductility is very promising for a wide range of technologies exploiting the mechanical properties of materials. However, its fundamental nature is not fully understood and represents the subject of intensive debates; see, e.g., [1-11]. 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 of the specific modes in nanotwinned metals is viewed to be plastic deformation occurring through widening of nanoscale twins [2]. In previous description of this deformation mode, focuses were placed on dislocation reactions resulting in formation of the twinning partial dislocations that move along twin boundaries and provide widening of twins [2]. At the same time, in parallel with dislocations, grain boundaries (whose amounts are rather large in nanotwinned metals having ultrafine grains) can significantly influence plastic deformation carried by twins. For instance, grain boundaries can serve as plane defects where deformation twins are generated and/or stopped; see, e.g., [12-16]. When twins are generated and stopped by grain boundaries, special defects – wedge disclinations – are typically formed at junctions of grain and twin boundaries [17,18]. Such disclinations create stress fields, and their ensemble is often characterized by a rather high elastic energy which can crucially influence the yield and flow stresses of a nanotwinned

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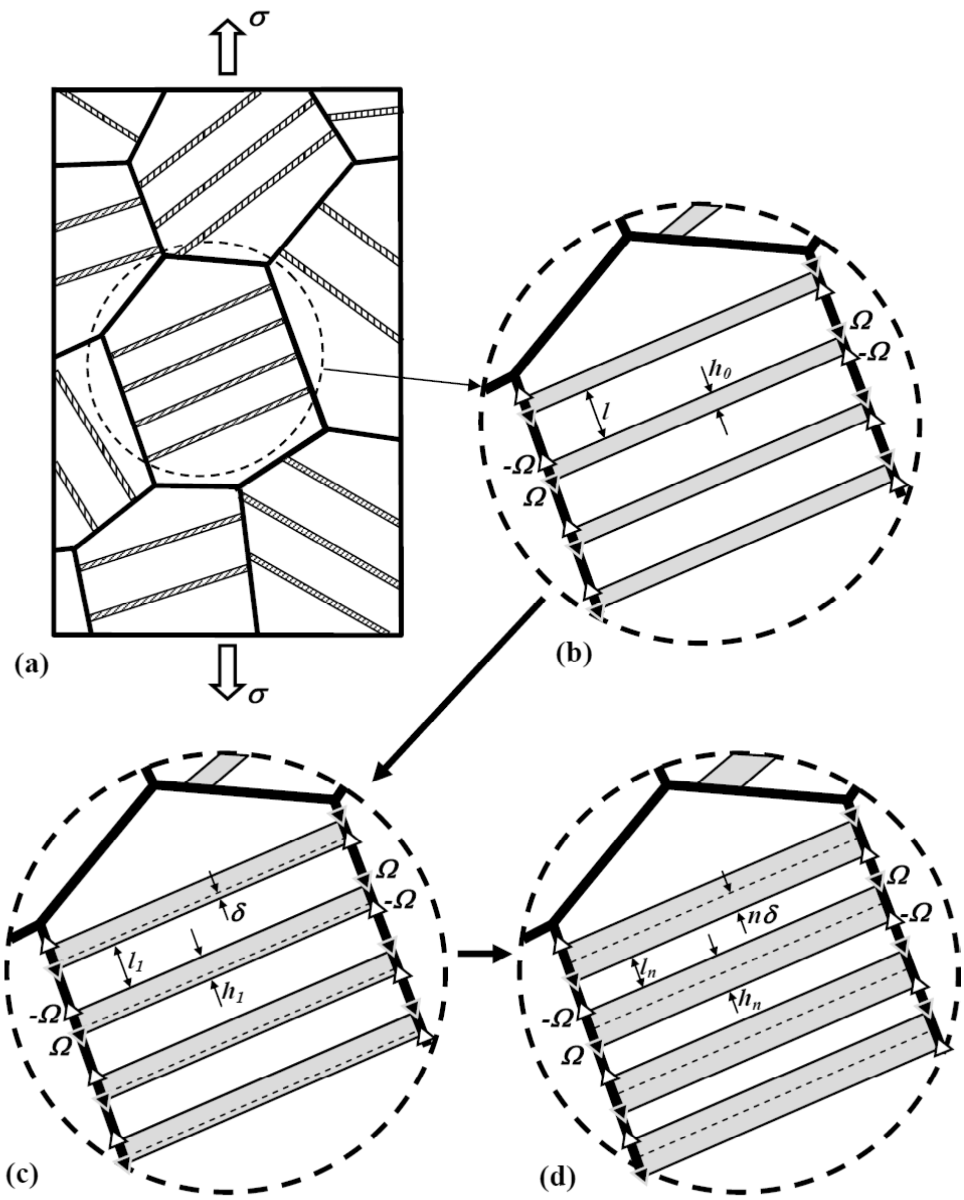

Fig. 1. Plastic flow in a nanotwinned metal specimen (having the ultrafine-grained structure with grains containing high-density ensembles of nanoscale twins) occurs through widening of twins and is accompanied by evolution of disclinations. (a) A nanotwinned metal specimen is under tensile load (a general view). Magnified insets (b)-(d) show evolution of twins and disclinations (formed at junctions of twin and grain boundaries) in a typical model grain during plastic deformation occurring through widening of twins. (b) The typical model grain contains N periodically arranged identical nanotwins whose short segments are located on opposite grain boundaries. (c) An elementary act of widening of nanotwins in the typical grain. (d) The system of N nanotwins after n elementary acts of widening of nanotwins in the typical grain.

metal. This factor should be definitely taken into account in analysis of plastic flow in nanotwinned metals. The main aim of this paper is to suggest a theoretical model which describes plastic deformation through widening of nanoscale twins in nanotwinned metals, with a special attention being paid to the effects of the disclinations (formed at junctions of twin and grain boundaries) on the yield stress characterizing these metals.

2. GEOMETRIC FEATURES OF PLASTIC FLOW OCCURRING THROUGH WIDENING OF NANOSCALE TWINS IN NANOTWINNED METALS

Let us consider a mechanically loaded metallic specimen having the ultrafine grained structure with grains containing high-density ensembles of nanoscale twins (Fig. 1a). For simplicity of our description focused on the geometric features of plastic flow mode occurring through evolution of nanoscale twins, we will examine an idealized two-dimensional model of a nanotwinned metallic specimen under uniaxial tensile load σ (Fig. 1). Despite of its simplicity, the model catches the essential physics of both the plastic flow mode and its sensitivity to the effects of the disclinations formed at junctions of twin and grain boundaries. In the framework of our model, each grain of a nanotwinned metallic specimen contains periodically arranged rectangular twins having short segments terminated at opposite grain boundaries (Figs. 1a and 1b). We consider a typical model grain containing N identical nanoscale twins periodically arranged with 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 dislocations (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 value of δ, the distance between neighboring crystallographic slip planes (Fig. 1c). Following Ref. [2], this deformation mode associated with widening of twins can crucially contribute to plastic flow in nanotwinned copper.

Since many studies of the nanotwinned metals are concerned with copper [1-6,10], we will focus our further theoretical analysis on widening of twins in fcc metals, that is, metals with face-centered cubic crystal lattice. In the framework of our model, we consider edge partial dislocations of $(a/6)\langle 11\bar{2}\rangle$ 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 widening of nanotwins [6]. In the framework of our model, the 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 value of d for all the N twins located within the grain (Fig. 1c). 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 neighboring twins decreases by value of δ and becomes equal to $l_1 = l - \delta$ (Fig. 1c). The distance d between neighboring crystallographic slip planes {111} in fcc metals is in the following relationship with the crystal lattice parameter a: $\delta = a/\sqrt{3}$.

For geometric reasons, wedge disclinations are typically formed at junctions of grain and twin boundaries [17,18]. More precisely, since crystal lattice orientation changes at twin boundaries, tilt misorientation of a grain boundary (that is, tilt misorientation of crystal lattices of two grains adjacent to the grain boundary) changes at its junction with a twin boundary. As a corollary, a wedge disclination exists at such a junction and is characterized by the strength related to the change in the grain boundary misorientation; for details, see [17,18]. In spirit of the approach [17,18], when a twin has its short segments terminated at opposite grain boundaries (Figs. 1a and b), four wedge disclinations exist at its junctions with the grain boundaries, and these disclinations form a quadrupole configuration (Fig. 1b). The disclinations are characterized by strengths $\pm\Omega$ which, according to the theory of disclinations in solids [19,20], is in the following relationship with the Burgers vector magnitude b characterizing the Shockley dislocations: $\Omega = 2\arctan(b/2\delta) \approx 39°$. (Hereinafter, for shortness, the disclinations characterized by strengths $\pm\Omega$ will be called the $\pm\Omega$ -disclinations). In the initial state of the system under examination (Fig. 1b), the distances between neighboring disclinations of a quadrupole associated with a twin are h_0 and d (Fig. 1b).

In the framework of 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 value of δ for all the twins located within the grain (Fig. 1c). The process/event 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. 1d). In doing so, the characteristic distance between neighboring twins decreases down to value of $l_n = l - n\delta$ (Fig. 1d). 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 favorable. In next section, we will examine in detail the energy and stress characteristics of the twin widening process.

3. ENERGY AND STRESS CHARACTERISTICS OF WIDENING OF NANOSCALE TWINS 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 period l in the typical grain (Fig. 1b). The elastic energy of the twin system under examination is well approximated by the energy of disclination configuration consisting of N quadrupoles of $\pm\Omega$-disclinations (Fig. 1b). The latter energy is given as:

$$W_0 = E_N^q + E_N^{q-q} + E_N^{\gamma}, \tag{1}$$

where E_N^q is the sum proper energy of N quadrupoles of $\pm\Omega$- disclinations; E_N^{q-q} is the sum energy that characterizes the pair interactions between all the disclination quadrupoles; and E_N^{γ} is the sum specific energy (per unit area) of all the stacking faults.

The sum proper energy E_N^q is given by the following standard expression [20]:

$$E_N^q = \frac{ND\Omega^2}{2}\left(h_0^2 \ln\frac{h_0^2 + d^2}{h_0^2} + d^2 \ln\frac{d^2 + h_0^2}{d^2} \right), \tag{2}$$

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 i-th and j-th quadrupoles of $\pm\Omega$-disclinations is calculated in the standard way as the work spent to the generation of the j-th quadrupole in the shear stress field created by the i-th quadrupole. The energy E_N^{q-q} represents the sum of the above energies that characterize the pair interactions and can be written as the following double sum over indexes i and j:

$$E_N^{q-q} = \frac{D\Omega^2}{2} \times \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\left((h_0 + y_{ij})\ln\frac{d^2 + (h_0 + y_{ij})}{(h_0 + y_{ij})} + (h_0 + y_{ij})\ln\frac{d^2 + (h_0 + y_{ij})^2}{(h_0 + y_{ij})^2} + d^2\left(\ln\frac{d^2 + (h_0 + y_{ij})^2}{d^2 + y_{ij}^2} + \ln\frac{d^2 + (h_0 + y_{ij})^2}{d^2 + y_{ij}^2} \right) - 2y_{ij}^2 \ln\frac{d^2 + y_{ij}^2}{y_{ij}^2} \right), \tag{3}$$

where $y_{ij} = (j - i)(h_0 + l)$.

The sum specific energy E_N^{γ} of all the stacking faults is evidently given by the following formula:

$$E_N^{\gamma} = 2Nd\gamma, \tag{4}$$

with γ being the specific (per unit area) energy of a stacking fault.

Formulas (1)-(4) allow us to calculate the total energy W_0 of the system as a function of both the twin thickness h_0 and the distance l between the neighboring twins. Let us perform such calculations in the exemplary case of a nanotwinned copper (Cu) characterized the following values of parameters: G = 44 GPa, ν = 0.38, a = 0.352 nm [21], γ = 45 mJ m^{-2} [22], and d = 500 nm. With these parameters, we calculated maps $W_0(h_0,l)$, for various values of N. A typical example of the map $W_0(h_0,l)$ is presented in Fig. 2, for N = 5. As it follows from Fig. 2, the total energy $W_0(h_0,l)$ of the nanotwin system under examination (Fig. 2b) monotonously increases when the nanotwin thickness h_0 increases and/or the distance l between the nanotwins decreases. Thus, the energy of the nanotwin system monotonously grows with widening of twins. This trend is indicative of strain hardening of nanotwinned metals during their plastic deformation occurring through widening of twins.

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 n-th state with N twins each having the thickness $h_n = h_0 + n\delta$ (after n previous events of widening of twins) (Fig. 1d). The energy change $\Delta W_n = W_n - W_{n-1}$ can be written as follows:

$$\Delta W_n = E_N^{q(n)} - E_N^{q(n-1)} + E_N^{q-q(n)} - E_N^{q-q(n-1)} + E_N^{\tau}, \tag{5}$$

where $E_N^{q(n)}$ and $E_N^{q(n-1)}$ are the proper energies of N quadrupoles of $\pm\Omega$-disclinations in the n-th and (n-1)-th states, respectively; $E_N^{q-q(n)}$ and $E_N^{q-q(n-1)}$ are the energies that specify the pair interactions between all the quadrupoles of $\pm\Omega$-disclinations in the n-th and (n-1)-th states, respectively; and E_N^{τ} is the work spent by the external shear stress τ on widening of N nanotwins by value of δ.

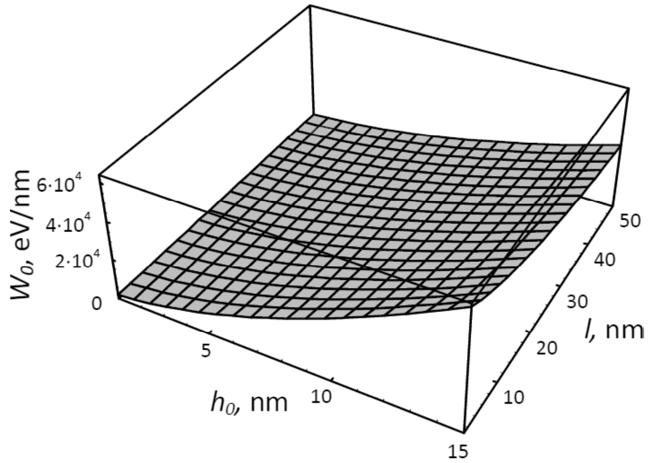

Fig. 2. Dependence of the energy W_0 of the system containing N nanotwins on the nanotwin thickness h_0 and the distance l between neighboring nanotwins.

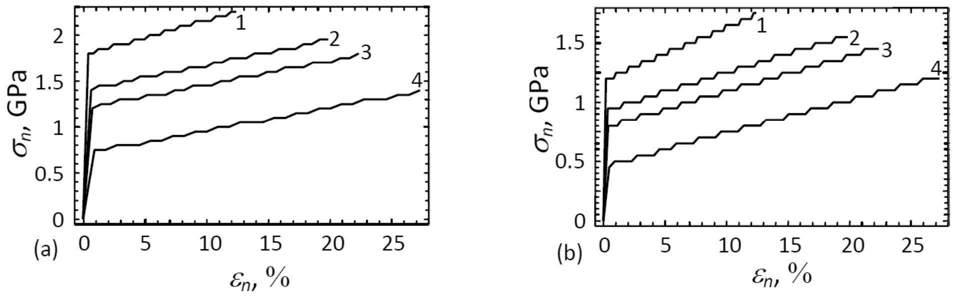

Fig. 3. Dependence of the flow stress σ_n on the plastic strain degree ε_n at various values of the initial (before plastic deformation) nanotwin thickness h_0 = 15 nm, 10 nm, 8 nm, and 4 nm (curves 1, 2, 3, and 4, respectively), for (a) l = 50 nm and (b) l = 25 nm.

The energies $E_N^{q(n)}$ and $E_N^{q(n-1)}$ are given by formula (2) with the replacements $h_0 \to h_n$, $l \to l_n$ and $h_0 \to h_{n-1}$, $l \to l_{n-1}$ taken into account, respectively. The energies $E_N^{q-q(n)}$ and $E_N^{q-q(n-1)}$ are given by formula (3) where the same replacements $h_0 \to h_n$, $l \to l_n$ and $h_0 \to h_{n-1}$, $l \to l_{n-1}$ are taken into consideration, respectively.

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

$$E_N^{\tau} = -N\tau\sigma d. \tag{6}$$

Formulas (2), (3), (5), and (6) allow us to calculate the energy change ΔW_n characterizing the n-th elementary act of plastic deformation occurring through widening of twins in the typical grain. The n-th widening process is energetically favorable, if ΔW_n<0. In terms of stresses, the n-th widening process is energetically favorable, 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 n-th widening process is also characterized by plastic strain ε_n carried by this process. The plastic strain ε_n within the typical grain is approximately as follows:

$$\varepsilon \approx \frac{nN\delta}{d}. \tag{7}$$

Both the approximate formula (7) for the plastic strain ε_n and the expression $\sigma_n = 2\tau_n^{crit}$ 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 dependence $\sigma_n(\varepsilon_n)$. It is presented in Fig. 3, for various values of the nanotwin thickness h_0 in the cases of l = 50 nm (Fig. 3a) and l = 25 nm (Fig. 3b). In these cases, the number N of nanotwins in the typical grain was taken as $N = [d/(h_0+l)]$, where [X] means an integer part of a rational number X. As it follows from Fig. 3, the flow stress increases when the twin thickness h_0 increases and/or the distance l between the neighboring twins diminishes.

Note that the experimentally measured [2,3] ultimate stresses for nanotwinned copper are 1.5÷2 times lower than typical values of the flow stress (Fig. 3) 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 widening of twins is favored in this grain, because of "stress-favored" 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 widening of twins. At the same time, in parallel with grains containing "stress-favored" twin boundaries in a nanotwinned metal specimen, there are grains containing twins that cannot be deformed by widening due to their unfavorable orientation relative to the applied shear stress. Grains of the second sort are deformed by plastic flow modes different from widening of twins. In these circumstances, the flow and yield stresses of a nanotwinned metal specimen are controlled by contributions from two or more plastic flow modes (including plastic deformation through widening of twins), and, in particular, values of the flow stress can be lower than those (Fig. 3) that characterize widening of twins.

Let us estimate the yield stress of a nanotwinned metal specimen, using the above representations on various sorts of grains. In doing so, we divide grains in a nanotwinned metal specimen in the two categories: grains I (with "stress-favored" twin boundaries) deformed by widening of twins and grains II deformed by conventional lattice slip (Fig. 4). That is, the nanotwinned metal specimen is viewed as a "structural composite" with grains I and II playing the roles of its constituent structural phases (Fig. 4). Plastic deformation through widening of twins in grains I is characterized by the yield stress $\sigma_1 = 2\tau_1$, where τ_1 denotes the critical shear stress for the 1st event of plastic flow realized though widening of twins. Plastic deformation in grains II is assumed to occur by conventional slip of perfect lattice dislocations, and twin boundaries (by analogy with grain boundaries in polycrystals) serve as stoppers for such lattice dislocations. In this case, plastic deformation in grains II is characterized by the yield stress σ_{HP} obeying the Hall-Petch relationship $\sigma_{HP} = \sigma_0 + K_{HP} d_m^{-1/2}$, with $d_m = l$ being the distance between twin boundaries, σ_0 and K_{HP} are the material constants. In the case of copper, one has: $\sigma_0 = 200$ MPa and K_{HP} =1750 MPa [23].

In the framework of our model, in a first approximation, the yield stress σ_y^{th} of the nanotwinned metal is estimated by the mixture rule (conventionally exploited in the theory of nanomaterials and composites; see, e.g., [24]) as follows:

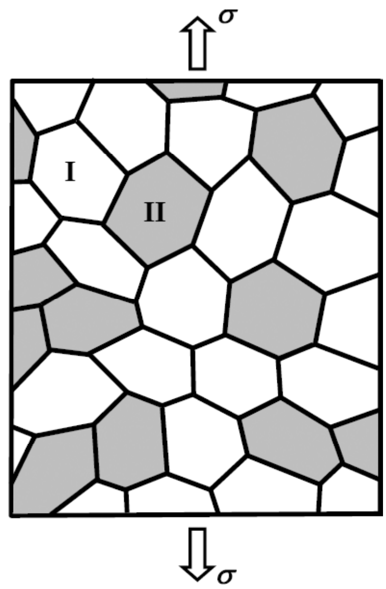

Fig. 4. A nanotwinned metal specimen is schematically shown as a structural composite consisting of grains I and II (white and grey hexagons, respectively) where plastic flow occurs through widening of twins and conventional slip of lattice dislocations, respectively (for details, see text).

$$\sigma_y^{th} = \alpha\sigma_1 + \beta\sigma_{HP}, \tag{8}$$

where α and β are the volume fractions occupied by grains I and II, respectively.

With formula (8), we estimated the yield stress σ_y^{th} that characterizes nanotwinned copper, for α = 0.6, β = 0.4, l = 50 nm and various values of the nanotwin thickness h_0. In doing so, in particular, we found σ_y^{th} = 450 MPa at h_0 = 4 nm, σ_y^{th} = 650 MPa at h_0 = 8 nm, σ_y^{th} = 750 MPa at h_0 = 10 nm, and σ_y^{th} = 900 MPa at h_0=15 nm. These theoretical values are rather well consistent with the experimentally measured [2,3] values of the yield stress σ_y^{exp} = 300, 550, 750, and 900 MPa in nanotwinned copper specimens characterized by the following mean values of the nanotwin thickness: h_0 = 4,8,10, and 15 nm, respectively. This agreement between our theoretical predictions and corresponding experimental data [2] is indicative in favor of the suggested theoretical representations on the effects caused by disclinations (formed at junctions of twin and grain boundaries; see Fig. 1b) on plastic flow occurring through widening of twins in nanotwinned metals.

Note that our theoretical estimates are not consistent with the experimental data [2] concerning the yield stress of nanotwinned copper specimens characterized by the mean nanotwin thickness exceeding 15 nm. More precisely, in the discussed case, the experimental values of the yield stress are lower than those obtained in our theoretical examinations. This disagreement can be logically explained by the statement that widening of twins stops significantly contributing to plastic flow of grains containing nanotwins with thicknesses > 15 nm, in which case our model does not operate for such grains with comparatively wide twins.

4. DISCUSSION. CONCLUDING REMARKS

To summarize, plastic flow through widening of nanoscale twins can effectively occur in nanotwinned metals where this specific deformation mode leads to formation of disclinations at junctions of twin and grain boundaries (Fig. 1). The disclinations create stresses and typically are characterized by a rather high elastic energy which crucially influences the yield and flow stresses in nanotwinned metals. The discussed effect is of critical significance in namely nanotwinned metals, since they contain both high-density ensembles of nanoscale twins and very large amounts of grain boundaries.

We have elaborated a theoretical model describing the role of the disclinations in plastic flow through widening of twins in nanotwinned metals. In particular, we calculated in a first approximation the yield stress of as a function of twin thickness in nanotwinned copper in the situation where widening of nanoscale twins significantly contributes to plastic flow. Our theoretical estimates are rather well consistent with the experimentally measured [2] values of the yield stress in nanotwinned copper specimens characterized by low mean values ($h_0 \leq$ 15 nm) of the nanotwin thickness. This agreement between our theoretical results and corresponding experimental data [2] is indicative in favor of the suggested theoretical representations on the important role of the disclinations in plastic flow through widening of twins in nanotwinned metals containing ultranarrow twins.

Plastic flow in conventional nanocrystalline and ultrafine-grained metallic materials (that is, nanomaterials which do not contain high-density ensembles of growth twins) often occurs through specific deformation modes; see, e.g., [12-16,25-35]. These modes are crucially influenced by very large amounts of grain boundaries that exist in nanocrystalline and ultrafine-grained metallic materials [12-16,25-35]. In particular, deformation carried by nanoscale twins generated and stopped at grain boundaries essentially contributes to plastic flow in such materials; for a review, see [16]. In these circumstances, results of our theoretical model presented in this paper are also important for understanding the unusual mechanical behaviors of nanocrystalline and ultrafine-grained metallic materials whose plastic flow involves nanoscale deformation twinning.

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