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DEFORMATION TWINNING THROUGH NANOSCALE IDEAL SHEARS IN NANO- AND POLYCRYSTALLINE MATERIALS AT ULTRA HIGH STRESSES

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

[1]Institute of Problems of Mechanical Engineering, Russian Academy of Sciences, Bolshoj 61, Vasilievskii Ostrov, St. Petersburg 199178, Russia
[2]St. Petersburg State University, St. Petersburg 198504, Russia

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Abstract. A special micromechanism of deformation twinning in nano- and polycrystalline materials is suggested and theoretically described. The micromechanism represents the formation of nanoscale deformation twins through consequent events of nanoscale ideal shear. It is theoretically demonstrated that the special micromechanism of deformation twinning can occur in the non-barrier way in nano- and polycrystalline materials deformed at ultra high stresses.

1. INTRODUCTION

Deformation behavior of materials is strongly influenced by their structural features, specimen sizes and the conditions of mechanical loading. For instance, materials with the nanocrystalline or ultrafine-grained structure are characterized by the flow stress and strength values which are 2–10 times larger than those of coarse-grained polycrystalline materials with the same chemical composition; see, e.g., [1-9]. Single crystalline metallic nanopillars ranging in diameter between 100 nm and several micrometers are deformed in uniaxial compression at stresses exceeding 10–50 times those for their bulk counterparts [10-17]. Also, very high values of the flow stress are typical for conventional bulk polycrystals under dynamic deformation (see, e.g., [18-20]), in contrast to quasistatic deformation regimes characterized by comparatively low stresses.

High applied stresses often initiate operation of specific modes of plastic deformation in mechanically loaded materials. For instance, plastic flow modes conducted by grain boundaries effectively come into play in nanocrystalline and ultrafine-grained materials [1-6,21-25], in contrast to coarse-grained polycrystals where lattice dislocation slip dominates. Also, deformation twinning significantly contributes to plastic flow in nanocrystalline materials (like Al) with high stacking fault energies [1-3,26-28], in contrast to their coarse-grained counterparts. In recent years, particular attention has been paid to the nanodisturbance deformation mode occurring through nanoscale ideal shear events in various solids at high stresses [29-35]. It was theoretically demonstrated that the nanodisturbance deformation mode can effectively contribute to plastic flow in Gum metals (special Ti-based alloys) [29], nanocrystalline materials [31,32], nanocomposites [30] and nanowires [33,35]. These theoretical representations were confirmed by "in situ" observation (by high resolution electron microscopy) of nanodisturbances – carriers of nanoscale ideal shear – in Gum metals during their plastic deformation [34]. Also, nanoscale stacking faults resulting from nanoscale ideal shear events were experimentally observed in deformed Au nanowires with lateral sizes $\approx$ 1-2 nm [36].

Corresponding author: I.A. Ovid'ko, e-mail: ovidko@nano.ipme.ru

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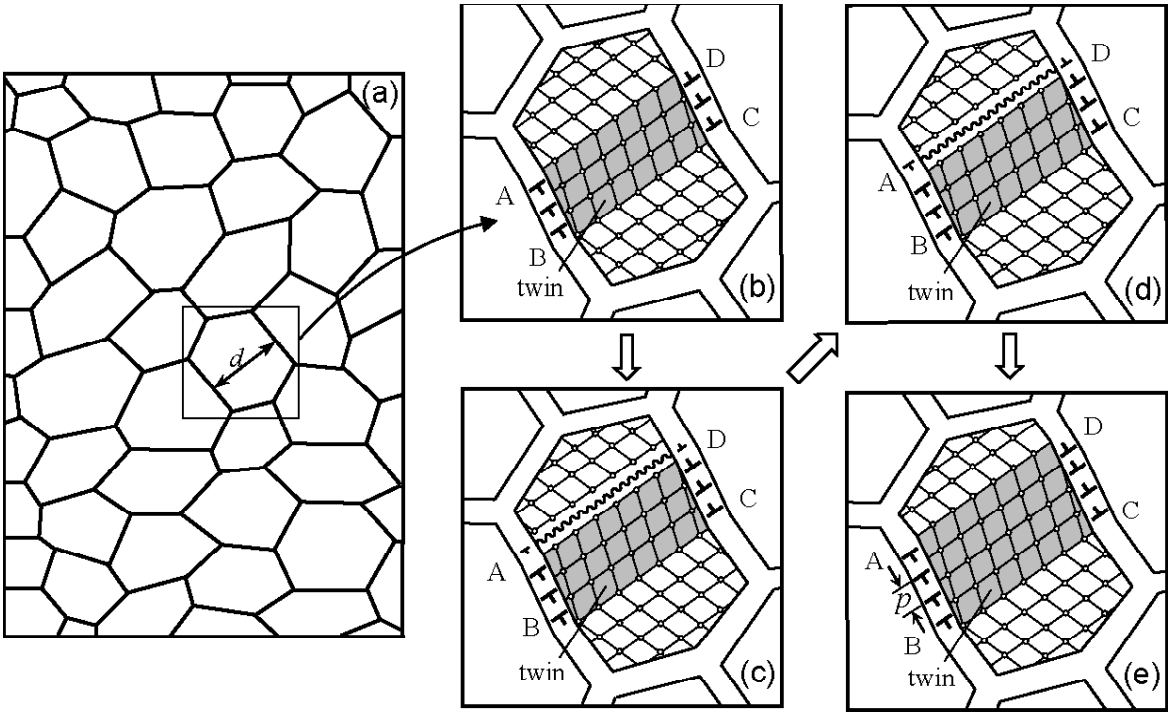

Fig. 1. Nanoscale deformation twin grows through a nanoscale ideal shear (a schematic two-dimensional illustration). (a) Deformation twinning in a nanoscale grain of a mechanically loaded nanocrystalline specimen (general view). (b) Magnified inset of the initial state of a nanoscale twin consisting of *n*-1 layers. (c) Nanoscale ideal shear occurs in plane AD adjacent to the nanoscale twin boundary. The shear is specified by a tiny shear magnitude *s* and results in formation of a dipole of non-crystallographic dislocations (located at points A and D) with the Burgers vector magnitude *s*. A generalized stacking fault (wavy line) is formed between the non-crystallographic dislocations. (d) The magnitude *s* of nanoscale ideal shear (also playing the role of the Burgers vector magnitude of the non-crystallographic dislocations A and D) increases. (e) The dislocations A and D transform into Shockley partials, in which case the new twin boundary AD is formed, and the twin thickness increases by one layer.

In paper [35], it was theoretically shown that deformation-induced formation of nanoscale twin nuclei (two-layer twins of nanoscopic length) in nanowires can occur through consequent ideal shear events. It was found that this deformation twinning is energetically favorable in Au and Cu nanowires with lateral sizes ranging from 1 to 100 nm, when they are deformed at ultra high stresses. That is, deformation twinning and nanodisturbance deformation mode can occur cooperatively in mechanically loaded nanowires. Following [35], the cooperative action of these deformation modes is strongly affected by the free surfaces and nanoscopic sizes of nanowires, which determine the ultra high level of the flow stress. In the context discussed, it is very interesting to find out if deformation twinning and the nanodisturbance deformation mode can occur cooperatively in solids with structures and sizes different from those of nanowires. The main aim of this paper is to suggest and theoretically describe a new micromechanism for deformation twinning – formation of nanoscale deformation twins through the consequent events of nanoscale ideal shear (that is, the nanodisturbance deformation mode) – in nano- and polycrystalline materials.

2. GEOMETRY OF DEFORMATION TWINNING THROUGH CONSEQUENT IDEAL SHEAR EVENTS IN NANOCRYSTALLINE MATERIALS

Let us consider the generation of deformation twins in a nanocrystalline solid. Following [37-40], we assume that twin lamellas are composed of overlapping stacking faults that join opposite twinning partial dislocations whose dipoles form in adjacent slip planes (Figs. 1a and 1b). In the case of fcc

crystals, the dipoles of Shockley partials form in adjacent slip planes {111} (Figs. 1a and 1b). Growth of a nanoscale deformation twin is supposed to occur through consequent nanoscale ideal shears in the neighboring crystallographic planes under the action of a shear stress τ (Figs. 1b-e). More precisely, within our model, growth of a nanoscale deformation twin can be divided into several stages, each occurring through a nanoscale ideal shear. In general, the *n*th stage of nanotwin growth is realized as follows. In the initial state (resulted from the (*n*-1)-th growth stage), the nanotwin consists of (*n*-1) nanoscale stacking faults bounded by (*n*-1) dipoles of Shockley partials (Fig. 1b). Then, a nanoscale ideal shear occurs in the crystallographic plane AD adjacent to one of the nanoscale twin boundaries (Fig. 1c). The shear is specified by a tiny shear magnitude *s* (*s* << *b*, where *b* is the Burgers vector magnitude of a Shockley partial dislocation). The nanoscale ideal shear results in formation of a dipole of non-crystallographic dislocations A and D (that is, dislocations located at points A and D) with the Burgers vectors $\pm\mathbf{s}$. A generalized stacking fault (GSF) is formed between the non-crystallographic dislocations (Fig. 1c). Then, the magnitude *s* of the nanoscale ideal shear increases (Fig. 1d), and so does the Burgers vector magnitude *s* of the non-crystallographic dislocations A and D (Fig. 1d). Finally, the magnitude *s* reaches the value of *b*, and the dislocations A and D transform into twinning partials (Fig. 1e). As a result, the new twin boundary AD is formed, and the nanotwin thickness increases by one layer (Fig. 1e).

The situation with $n = 1$ corresponds to the formation of one stable nanoscale stacking fault bounded by two Shockley partials that form a dipole configuration. In terms of Refs. [29-32], the formation of one stable nanoscale stacking fault occurs through the nanodisturbance deformation mode. The formation of the first stable stacking fault and associated dipole of Shockley partial dislocations is possible when the external shear stress τ reaches a critical value of τ_{c1}. The formation of subsequent Shockley dislocation dipoles occurs at stresses whose values, in general, are different from τ_{c1}. If the external shear stress τ is large enough, many Shockley partials and thereby a rather thick twin lamella can form in the nanograin.

Let us consider the situation where a periodic array of n - 1 dipoles of Shockley partials has already been formed in a solid with the fcc crystal lattice structure (Figs. 1a and 1b). We denote the distance between the dislocations composing a dipole configuration (Fig. 1a) as *d*, and the distance between the neighboring dislocations in the walls 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 $p = a\sqrt{3}$. The Burgers vectors $\pm\mathbf{b}$ of the Shockley partials are of the kind (*a*/6)<112>. For the typical case where the lines of Shockley partials are directed along one of the <110> planes, these dislocations are of 60° character. In this case, their edge and screw components, $\pm b_1$ and $\pm b_2$, follow from $b_1 = b\sqrt{3}/2$ and $b_2 = b/2$, where $b = a/\sqrt{6}$ is the magnitude of the Shockley dislocation Burgers vector.

3. ENERGY AND STRESS CHARACTERISTICS OF DEFORMATION TWINNING THROUGH CONSEQUENT IDEAL SHEAR EVENTS

Let us examine the energy and stress characteristics of deformation twinning through consequent ideal shear events in nano- and polycrystalline materials. In doing so, we consider the situation where the *n*th dipole of Shockley partials nucleates through a nanoscale ideal shear at a crystallographic plane neighboring to a twin consisting of *n*-1 stable stacking faults, as shown in Figs. 1b-1e. That is, we consider the *n*th stage of deformation twin growth through consequent ideal shear events. Within our approach, the nucleation occurs through a gradual increase of the dislocation Burgers vector magnitudes from zero to *b* (Figs. 1b-e). We examine the defect configuration at the time moment at which the Burgers vectors of the nucleating *n*th dislocation dipole are $\pm\mathbf{s}$. At this moment, the edge and screw components, $\pm s_1$ and $\pm s_2$, of the Burgers vectors follow from $s_1 = s\sqrt{3}/2$ and $s_2 = s/2$.

Let us calculate the change ΔW in the total energy of the system due to the formation of the dipole of dislocations with the Burgers vectors $\pm\mathbf{s}$ in the stress field created by n - 1 dipoles of Shockley partials and the external shear stress τ. The energy change ΔW (per unit dislocation length) is given as follows:

$$\Delta W = W_{dip} + \sum_{k=1}^{n-1} W_{\text{int}}^{n-k} + W_{\gamma} - A, \qquad (1)$$

where W_{dip} is the self-energy of the *n*th dipole of dislocations with the Burgers vectors $\pm\mathbf{s}$, W_{int}^{n-k} is the energy of the elastic interaction between the *n*th and *k*th dipoles of Shockley partials (k =

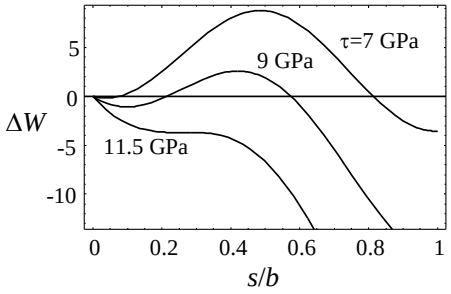

Fig. 2. Dependences of the energy change ΔW (characterizing the nucleation of the nth Shockley dislocation dipole through a nanoscale ideal shear) on the normalized dislocation Burgers vector magnitude s/b, for d = 20 nm, n = 10 and various values of the applied shear stress τ. The energy ΔW is given in units of $Gb^2/[2\pi(1-\nu)]$.

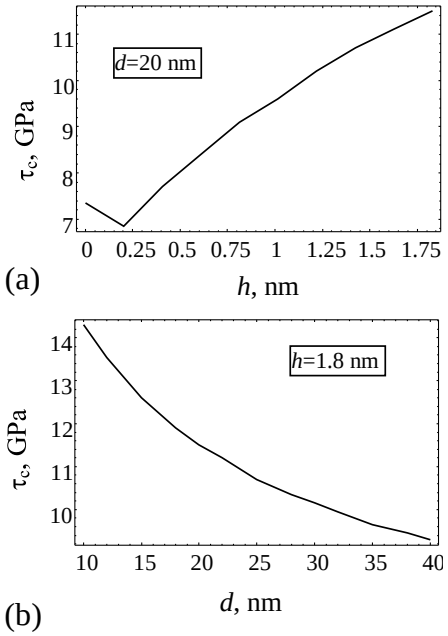

Fig. 3. Critical stress τ_c for the consequent formation of the dipoles of twinning dislocations through nanoscale ideal shear events in nanocrystalline Ni vs (a) twin lamella thickness h and (b) twin lamella width d.

1,2,…,n-1), W_γ is the energy of the GSF that joins the dislocations of the nth dipole, and A is the work done to generate the nth dislocation dipole under the stress τ. The standard calculations for the case of an elastically isotropic solid yield the following final expression for the energy change ΔW:

$$\Delta W = D\left\{s_1^2\left(\ln\frac{d}{s_1}+1\right)+(1-\nu)s_2^2\left(\ln\frac{d}{s_2}+1\right)\right\}+ D\sum_{k=1}^{n-1}\left[\left(s_1b_1+(1-\nu)s_2b_2\right)\ln\frac{p^2k^2+d^2}{p^2k^2}- 2s_1b_1\frac{d^2}{p^2k^2+d^2}\right]+\left(\gamma_n(s)-\tau s_1\right)d, \quad (2)$$

where $D = G/[2\pi(1-\nu)]$, G denotes the shear modulus, ν the Poisson's ratio, and $\gamma_n(s)$ the specific energy of the GSF that joins the dislocations of the nth dipole.

The energy $\gamma_n(s)$ can be calculated as the difference between the total specific stacking fault energy in the state with the GSF and the corresponding specific energy before its formation. The energy $\gamma_n(s)$ can be written [35,41] using the following relations:

$$\gamma_n(s) = \left(\gamma_{ut} - 2\gamma_{tsf}\right)\sin^2\left(\pi s/b\right),\ n \geq 3, \quad (3)$$

$$\gamma_1(s) = \begin{cases}\gamma_{us}\sin^2\left(\pi s/b\right), & 0 \leq s/b < 1/2,\\ \gamma_{isf} + \left(\gamma_{us} - \gamma_{isf}\right)\sin^2\left(\pi s/b\right), & \\ 1/2 \leq s/b \leq 1,\end{cases} \quad (4)$$

$$\gamma_2(s) = \begin{cases}\left(\gamma_{ut} - \gamma_{isf}\right)\sin^2\left(\pi s/b\right), & \\ 0 \leq s/b < 1/2,\\ \left(\gamma_{ut} - 2\gamma_{tsf}\right)\sin^2\left(\pi s/b\right), & \\ 1/2 \leq s/b \leq 1,\end{cases} \quad (5)$$

where γ_{ut}, γ_{tsf}, γ_{us}, and γ_{isf} are material parameters. In the case of Ni, one has [41]: γ_{ut} = 0.324 J/m^2, γ_{tsf} = 0.055 J/m^2, γ_{us} = 0.273 J/m^2, and γ_{isf} = 0.110 J/m^2. In formulae (3)–(5), the case of n = 1 corresponds to the formation of an isolated GSF, the case of n = 2 corresponds to the formation of a GSF adjacent to a pre-existent stable stacking fault, and the case of $n \geq 3$ corresponds to the formation of a GSF adjacent to a pre-existent nanotwin consisting of n - 1 layers.

Fig. 2 presents the dependences $\Delta W(s/b)$, for Ni (characterized by the following parameter values: G = 73 GPa, ν = 0.34, a = 0.352 nm) at d = 20 nm, n = 10 and various values of τ. As it follows from Fig. 2, for τ = 7 and 9 GPa, the generation of the nth dislocation dipole requires overcoming energy barriers (see the two upper curve in Fig. 2). For higher values of τ, the energy ΔW always decreases with increasing s/b, in which case the formation of the nth dipole of Shockley partials occurs in the non-

barrier way (see the lowest curve in Fig. 2). As it is seen, the applied stresses are very high which are needed for the non-barrier formation of the *n*th dislocation dipole and associated growth of the twin lamella.

Let us calculate the critical stress τ_c defined as the minimum stress at which the formation of the *n*th dipole of Shockley partials occurs in the non-barrier way. The critical stress τ_c is calculated numerically using formulae (2)–(5). Let us denote the thickness of the deformation twin lamella as *h*. The quantity *h* can be related to the number *n* of dislocation dipoles using the relation $h = (n - 1)p$. The dependences of τ_c on *h* and *d* are depicted in Figs. 3a and 3b, respectively, for the case of nanocrystalline Ni with the parameter values used in plotting the curves in Fig. 2. As it follows from Fig. 3a, with increasing the twin lamella thickness *h*, τ_c first decreases and then increases. Also, Fig. 3a shows that, for $d = 20$ nm, the critical stress τ_c increases from 6.9 to 11.5 GPa, when the twin lamella thickness increases from 0 nm to 1.8 nm. For $h = 1.8$ nm, with increasing the twin lamella width *d* from 10 to 40 nm, τ_c decreases from 14.3 down to 9.3 GPa (Fig. 3b). Therefore, wide and thin twin lamellas are the easiest to form. The values of τ_c are ultra high. However, they can be reached in the course of shock loading in some deformation regimes.

4. CONCLUDING REMARKS

Thus, in this paper a special micromechanism of deformation twinning – formation of nanoscale deformation twins through the consequent events of nanoscale ideal shear (Fig. 1) – in nano- and polycrystalline materials has been suggested. According to our analysis of its energy and stress characteristics, the special micromechanism can effectively occur in the non-barrier way in nano- and polycrystalline materials deformed at ultra high stresses. Such conditions are realized, for instance, in solids under high-strain-rate deformation. At the same time, operation of the special micromechanism of deformation twinning (Fig. 1) is hardly possible in solids at conventional applied stresses typical for quasistatic deformation regimes.

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