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FORMATION OF PAIRED TWINS AT GRAIN BOUNDARIES IN NANOSTRUCTURED AND COARSE-GRAINED MATERIALS UNDER PLASTIC DEFORMATION

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Abstract. A theoretical model is suggested which describes plastic flow through formation of paired deformation twins at grain boundaries in nanostructured and coarse-grained polycrystalline metallic materials. In the framework of the suggested model, formation and evolution of paired twins at a grain boundary are mediated by successive emission of partial dislocation pairs from this boundary to adjacent grains. It is found that formation of paired deformation twins at grain boundaries can be significantly enhanced due to stress fields created by triple junction disclinations produced by preceding plastic deformation. Energy and stress characteristics of formation of paired twins in nanostructured and coarse-grained polycrystalline metallic materials (Ti, Mg) with hcp lattices are calculated. Results of the suggested theoretical model are consistent with experimental data reported in literature.

1. INTRODUCTION

Plastic deformation in coarse-grained polycrystalline and especially nanostructured materials is crucially affected by grain boundaries (GBs); see, e.g., [1-14]. For instance, the role of GBs as obstacles for lattice dislocation slip is responsible for Hall-Petch dependences of the yield stress and hardness on grain size [15,16]. In nanostructured materials where amounts of GBs are extremely large, GBs can effectively mediate plastic deformation and serve as sources of lattice dislocations and twins [3,5,18-25]. In particular, following numerous experimental data, computer simulations and theoretical models [3,5,17,19,21,24,25], twin deformation carried by nanoscale twins generated at GBs effectively contributes to plastic flow of nanostructured metals specified by low values of stacking fault energy. Also, recently, generation of paired deformation twins at GBs has been experimentally observed in coarse-grained polycrystalline titanium [26]. Such a paired twin consists of two twins generated at one GB segment and emitted to opposite grains adjacent to the GB segment [26] (Fig. 1). Twins that compose paired twins are inclined by comparatively large angles (~ 60-80°) relative to parent GB plane and have an edge-like shape (Fig. 1) [26]. Following Refs. [24,25], individual edge-shaped twins are generated at GBs through successive emission of partial dislocations (resulted from transformations of extrinsic sessile GB dislocations) to adjacent grains. In Ref. [9], a theoretical model was suggested describing generation of deformation twin pairs at gliding GB dislocation pile-ups. However, this model predicts formation of only twins inclined by low angles relative to GB plane [9]. Besides, the

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critical stress level needed to initiate formation of paired twins at gliding GB dislocation pile-ups is estimated to be very high [9], in which case this stress level hardly can be achieved in conventional quasistatic deformation tests. Both these predictions of the model [9] are not consistent with the experimental observations [26] of paired twins inclined by comparatively large angles relative to GB plane in quasistatically deformed titanium. In the context discussed, it is interesting to describe the experimental data [26] in order to understand the nature of plastic deformation processes mediated by paired twins in metallic materials under conventional quasistatic load. The main aim of this paper is to theoretically describe plastic flow through formation of paired deformation twins at GBs in nanostructured and coarse-grained polycrystalline metallic materials.

2. FORMATION OF PAIRED DEFORMATION TWINS AT GRAIN BOUNDARIES. GEOMETRIC ASPECTS

We now consider a two-dimensional model of a polycrystalline metallic specimen specified by an average grain size *d* (Fig. 2a). The specimen is under tensile stress σ that initiates plastic flow (Fig. 2a). In the framework of our model, the twin pair formation occurs through successive generation of pairs of partial dislocations at the GB AA' and their emission to adjacent grains (Fig. 2). An elemental act of the twin pair formation at the GB AA' represents generation of a pair of partial dislocations at this GB; see, e.g., Fig. 2c. In doing so, we assume that the partial dislocations (that move to grains adjacent to the GB AA') are resulted from homogeneous generation of one immobile GB dislocation and the two partial dislocations, as shown in Fig. 2c. The sum Burgers vector of the dislocations involved in the homogeneous generation process (Fig. 2c) is the zero-vector.

In terms of the theory of dislocations in solids, the homogeneous generation of one GB dislocation and two partial lattice dislocations (Fig. 2c) can be described as formation of two dipoles, AD and AF, of partial dislocations with Burgers vectors $\pm\mathbf{b}_1$ and $\pm\mathbf{b}_2$ all having magnitude *b* (Fig. 2d). In doing so, the partial dislocations D and F move in adjacent grain interiors, whereas two immobile dislocations are located at a GB point A (Fig. 2d), and their superposition is equivalent to the GB dislocation with Burgers vector $\mathbf{b}_s$ (Figs. 2c and 2d).

Following experimental data [26], in hcp titanium, paired twins are formed in crystal slip of $\{10\bar{1}2\}$

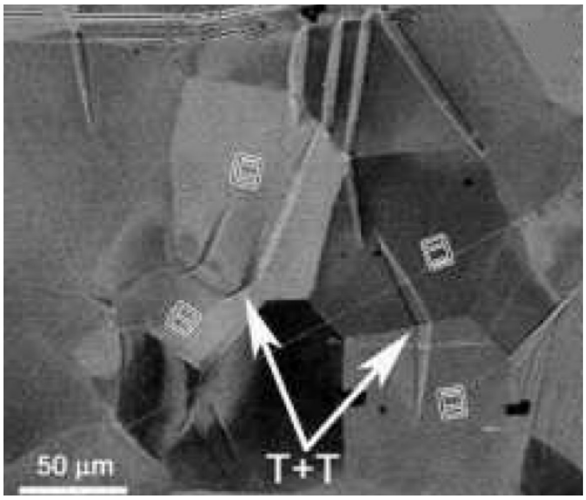

Fig. 1. Backscattered electron images showing matching pairs of twins (T + T) at grain boundaries. Two T + T pairs where it appears that both twins nucleated from the same location on the grain boundary and grew into the parent grains in opposite directions. Reprinted from Scripta Materialia, Vol. 63, L. Wang, P. Eisenlohr, Y. Yang, T.R. Bieler, M.A. Crimp, Nucleation of paired twins at grain boundaries in titanium, P.827-830, Copyright (2010), with permission from Elsevier.

$<\bar{1}011>$ type. Twinning partial dislocations that mediate formation of such twins are specified by Burgers vector magnitude $b = a/\sqrt{3}$, with *a* being the lattice parameter. Their slip planes $\{10\bar{1}2\}$ make the angle a with a normal to GB AA' (Fig. 2). Partial dislocation pairs are successively emitted from the GB AA' and thus form a twin pair (Fig. 2). More precisely, behind the partial dislocations, F and D, that compose the first pair of emitted dislocations, stacking faults are formed which have lengths $p_{1(1)}^{(1)}$ and $p_{1(1)}^{(2)}$, respectively (Fig. 2e). The stacking faults are characterized by the specific (per unit area) surface energy γ. Then the emission of the second pair of partial dislocations occurs which move along slip planes neighbouring to those for the dislocations D and F (Fig. 2f). As a result, two nuclei ABCD and ABEF of deformation twins are generated (Fig. 2f). Further events of dislocation pair emission from GB AA' give rise to thickening of the nuclei and formation of a pair of deformation twins ABCD and ABEF (Figs. 2e-2h). With a simplifying assumption that GB AA' is a symmetric tilt boundary, one finds the twins to be inclined by the same angle to the GB AA' plane (Fig. 2).

In the framework of our model, we examine the situation where triple junctions, O and O′, of GBs contain wedge disclinations with strengths $\pm\omega$ (hereinafter called $\pm\omega$-disclinations) due to previous

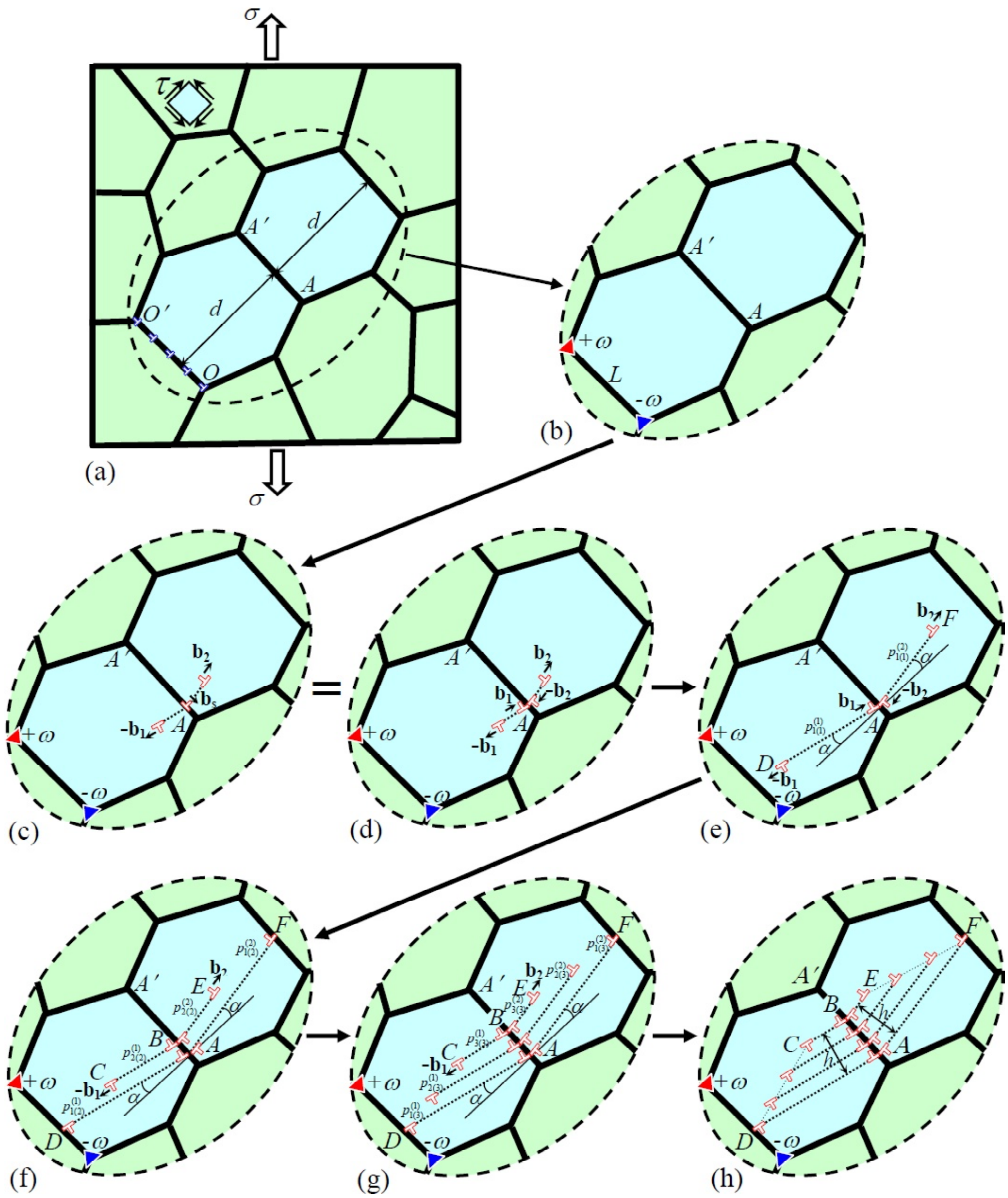

Fig. 2. Generation of a deformation twin pair at a grain boundary through successive emission of partial dislocation pairs to adjacent grain interiors. (a) Metallic specimen under tensile mechanical load. (b) Grain boundary OO′ containing a dipole of ±ω-disclinations. (c) Homogeneous generation of one GB dislocation with Burgers vector $\mathbf{b}_s$ and two partial lattice dislocations (that move to adjacent grains) occurs at the GB AA′. (d) Generation of two dislocation dipoles AD and AF at grain boundary AA′. They are equivalent to the dislocation configuration shown in (c). (e) Movement of partial dislocations D and F in grain interiors is followed by formation of stacking faults behind them. (f)-(h) Successive generation of dislocation dipoles leads to formation of deformation twins ABCD and ABEF.

plastic deformation processes (Fig. 2b). Such wedge disclinations at triple junctions of GBs are often present in coarse-grained and nanostructured metals processed by severe plastic deformation; see, e.g., reviews [27,28]. These defects are typically formed due to inhomogeneous plastic deformation which produces various plastic strains in various grains of a mechanically loaded metal [28]. In the situation under examination, for definiteness, we assume that triple junction disclinations, O and O′, are formed as defects – stress sources – terminating a wall of extrinsic GB dislocations located at the GB OO′ of length *L* (Fig. 2b).

Note that the effect exerted by the triple junction disclinations O and O′ on the emission of partial dislocations towards the GB OO′ is more pronounced, as compared to that on emission of partial dislocations in opposite direction. As a corollary, the twin ABCD in the grain adjacent to the GB OO’ has larger area, as compared to its counterpart ABEF (Fig. 2h).

3. ENERGY AND STRESS CHARACTERISTICS OF TWIN PAIR FORMATION

We now examine energy characteristics of the twin pair formation through successive emission of partial dislocation pairs from the GB AA′ (Fig. 2). Let W_{n-1} and W_n denote the energies of the (*n*-1)th state of the system containing 2(*n*-1) dislocation pairs and the *n*th state with *n* dislocation pairs, respectively. The transformation from the (*n*-1)th state to the *n*th state is energetically favourable, if $\Delta W_n = W_n - W_{n-1} < 0$. In this case, the expression $\Delta W_n = 0$ allows one to find the critical shear stress $\tau_{c(n)}$ for the transformation, that is, the minimum critical stress at which the (*n*-1)-to-*n* transformation is energetically favourable.

The energy change ΔW_n in its general form is given as:

$$\Delta W_n = E^{b}_{n} - E^{b}_{n-1} + E^{b-b}_{n} - E^{b-b}_{n-1} + E^{\Delta-b}_{n} - E^{\Delta-b}_{n-1} + E^{\gamma}_{n} - E^{\gamma}_{n-1} + E^{\tau}_{n} - E^{\tau}_{n-1}, \tag{1}$$

where E^{b}_{n-1} and E^{b}_{n} are the sums of the proper energies of 2(*n*-1) and 2*n* dislocation dipoles, respectively; E^{b}_{n-1} and E^{b-b}_{n} are the sums of the energies that specify pair interactions between 2(*n*-1) and 2*n* dislocation dipoles, respectively; E^{γ}_{n-1} and E^{γ}_{n} are the energies of twin boundaries and adjacent stacking faults in the sates with 2(*n*-1) and 2*n* dislocation dipoles, respectively; $E^{\Delta-b}_{n-1}$ and $E^{\Delta-b}_{n}$ are the sums of the energies that specify the interactions of the ±ω-disclination dipole with 2(*n*-1) and 2*n* dislocation dipoles, respectively; E^{τ}_{n-1} and E^{τ}_{n} are the sums of the energies that specify the interaction of the external shear stress τ with 2(*n*-1) and 2*n* dislocation dipoles, respectively.

The sum of the proper energies of 2(*n*-1) dislocation dipoles is given as follows [29]:

$$E^{b}_{n-1} = Db^2 \sum_{k=1}^{2}\sum_{i=1}^{n-1}\left(\ln\frac{p^{(k)}_{i(n-1)} - r_c}{r_c} + 1\right), \tag{2}$$

where $D = G/[2\pi(1-\nu)]$, *G* is the shear modulus, ν is the Poisson ratio, $p^{(k)}_{i(n-1)}$ is the distance moved by the *i*th partial dislocation, $r_c \approx b$ denotes the dislocation core radius.

The energy of elastic interaction between the *i*th and *j*th dislocation dipoles is calculated as the work spent to generation of the *i*th dislocation dipole in the stress field created by the *j*th dislocation dipole; see, e.g., Ref. [30]. The energy E^{b-b}_{n-1} represents the sum of such energies that specify all pair interactions between 2(*n*-1) dislocation dipoles and can be written as the following double sum over indexes *i* and *j*:

$$\begin{aligned}
E^{b-b}_{n-1} = {} & \frac{Db^2}{2}\sum_{k=1}^{2}\Bigg\{\sum_{i=1}^{n-2}\sum_{j=i+1}^{n-1}\Big\{2y_{ij}^2 \times \\
& \times\Bigg(\frac{p^{(k)2}_{i(n-1)} - 2p^{(k)}_{i(n-1)}x_{ij} - 2p^{(k)}_{i(n-1)}p^{(k)}_{j(n-1)}}{(p^{(k)2}_{j(n-1)} + x_{ij}^2 + y_{ij}^2 + 2p^{(k)}_{j(n-1)}x_{ij})(p^{(k)2}_{j(n-1)} + p^{(k)2}_{i(n-1)} + x_{ij}^2 + y_{ij}^2 + 2p^{(k)}_{j(n-1)}x_{ij} - 2p^{(k)}_{i(n-1)}x_{ij} - 2p^{(k)}_{i(n-1)}p^{(k)}_{j(n-1)})} \\
& - \frac{p^{(k)2}_{i(n-1)} - 2p^{(k)}_{i(n-1)}x_{ij}}{(x_{ij}^2 + y_{ij}^2)(p^{(k)2}_{j(n-1)} + x_{ij}^2 + y_{ij}^2 - 2p^{(k)}_{i(n-1)}x_{ij})}\Bigg) + \ln\Bigg[1 + \frac{p^{(k)2}_{i(n-1)} - 2p^{(k)}_{i(n-1)}x_{ij}}{x_{ij}^2 + y_{ij}^2}\Bigg] - \\
& \ln\Bigg[1 + \frac{p^{(k)2}_{i(n-1)} - 2p^{(k)}_{i(n-1)}x_{ij} - 2p^{(k)}_{i(n-1)}p^{(k)}_{j(n-1)}}{p^{(k)2}_{j(n-1)} + x_{ij}^2 + y_{ij}^2 + 2p^{(k)}_{j(n-1)}x_{ij}}\Bigg]\Big\} + \sum_{i=1}^{n-1}\sum_{j=1}^{n-1}\cos 2\alpha \ln\Bigg[1 + \frac{p^{(k)2}_{j(n-1)} - 2p^{(k)}_{j(n-1)}x_{ij}}{x_{ij}^2 + y_{ij}^2}\Bigg] - \\
& \cos 2\alpha \ln\Bigg[1 + \frac{p^{(k)}_{j(n-1)}(p^{(k)}_{j(n-1)} + 2x_{ij} + 2p^{(k)}_{i(n-1)}\cos 2\alpha)}{p^{(k)2}_{i(n-1)} + x_{ij}^2 + y_{ij}^2 + 2p^{(k)}_{i(n-1)}x_{ij}\cos 2\alpha - 2p^{(k)}_{i(n-1)}y_{ij}\sin 2\alpha}\Bigg] - \frac{2y_{ij}(y_{ij}\cos 2\alpha + x_{ij}\sin 2\alpha)}{x_{ij}^{\,2} + y_{ij}^2} + \\
& \frac{2(y_{ij} - p^{(k)}_{i(n-1)}\sin 2\alpha)(y_{ij}\cos 2\alpha + x_{ij}\sin 2\alpha)}{p^{(k)2}_{i(n-1)} + x_{ij}^2 + y_{ij}^2 + 2p^{(k)}_{i(n-1)}x_{ij}\cos 2\alpha - 2p^{(k)}_{i(n-1)}y_{ij}\sin 2\alpha} + \frac{2y_{ij}(y_{ij}\cos 2\alpha + (p^{(k)}_{j(n-1)} + x_{ij})\sin 2\alpha)}{(p^{(k)}_{j(n-1)} + x_{ij})^2 + y_{ij}^2} - \\
& \frac{2(y_{ij} - p^{(k)}_{i(n-1)}\sin 2\alpha)(y_{ij}\cos 2\alpha + (p^{(k)}_{j(n-1)} + x_{ij})\sin 2\alpha)}{p^{(k)2}_{i(n-1)} + (p^{(k)}_{j(n-1)} + x_{ij})^2 + y_{ij}^2 + 2p^{(k)}_{i(n-1)}(p^{(k)}_{j(n-1)} + x_{ij})\cos 2\alpha - 2p^{(k)}_{i(n-1)}y_{ij}\sin 2\alpha}\Bigg\}\Bigg\},
\end{aligned} \tag{3}$$

where $x_{ij} = (j - i)\delta/\tan\alpha$, $y_{ij} = (j - i)\delta$, and $\delta = a/\sqrt{6}$ is the distance between neighbouring slip planes of partial dislocations.

The interaction energy $E_{n-1}^{\Delta-b}$ is given by the following expression [24]:

$$E_{n-1}^{\Delta-b} = \frac{Db\omega}{2}\sum_{k=1}^{2}\sum_{i=1}^{n-1}\left((h_i - L\cos\alpha)\ln\left[1+\frac{p_{i(n-1)}^{(k)2} + 2p_{i(n-1)}^{(k)}d - 2Lp_{i(n-1)}^{(k)}\sin\alpha}{L^2 + d^2 + h_i^2 - 2Lh_i\cos\alpha - 2Ld\sin\alpha}\right] - h_i\ln\left[1+\frac{p_{i(n-1)}^{(k)2} + 2p_{i(n-1)}^{(k)}d}{d^2 + h_i^2}\right]\right), \tag{4}$$

where $h_i = (i - 1)\delta$.

We now consider the sum energy E_{n-1}^{γ} of the twin boundaries (AD, AF, BN and BE) and adjacent stacking faults of lengths $p_{1(n-1)}^{(k)}$ - $p_{2(n-1)}^{(k)}$. This energy is evidently as follows:

$$E_{n-1}^{\gamma} = \begin{cases} \gamma\sum_{k=1}^{2} p_{1(1)}^{(k)}, & n-1=1; \\ \sum_{k=1}^{2}[\gamma(p_{1(n-1)}^{(k)} - p_{2(n-1)}^{(k)}) + 2\gamma_{TB}p_{2(n-1)}^{(k)}], & n-1\geq 2. \end{cases} \tag{5}$$

The sum of the energies that specify the interaction of the external shear stress τ with $2(n-1)$ dislocation dipoles is given as:

$$E_{n-1}^{\tau} = -b\tau\cos 2\alpha\sum_{k=1}^{2}\sum_{i=1}^{n-1} p_{i(n-1)}^{(k)}. \tag{6}$$

The energies E_n^{b}, E_n^{b-b}, $E_n^{\Delta-b}$, E_n^{γ}, and E_n^{τ} (that characterize the state with $2n$ dislocation dipoles) are calculated in the same way as the energies E_{n-1}^{b}, E_{n-1}^{b-b}, $E_{n-1}^{\Delta-b}$, E_{n-1}^{γ}, and E_{n-1}^{τ}, respectively. In doing so, the energies E_n^{b}, E_n^{b-b}, $E_n^{\Delta-b}$, E_n^{γ}, and E_n^{τ} are given by formulas (2)-(6), where n-1 is replaced by n, and new stable positions $p_{i(n)}^{(k)}$ of previously emitted dislocations are taken into account.

Thus, we calculated all the terms of the energy change $\Delta W_n = W_n - W_{n-1}$ that characterizes formation of twin pairs at GBs. The stable positions $p_{i(i)}^{(k)}$ of the emitted partial dislocations correspond to minimums of the dependences ΔW_n ($p_{i(i)}^{(k)}$) and can be found from equations: $\Delta W_n/\partial p_{i(i)}^{(k)} = 0$, where k = 1,2 In calculation of $p_{i(i)}^{(k)}$, we utilized the following algorithm. The stable positions $p_{1(1)}^{(1)}$ and $p_{1(1)}^{(2)}$ for dislocations of the first pair are calculated using the system of equations: $\partial\Delta W_1/\partial p_{1(1)}^{(k)} = 0$, where ΔW_1 is given by formula (1) at n = 1, and k = 1,2. In the case under our examination, the dislocations of the first pair reach opposite GBs serving as obstacles for further dislocation slip. As a corollary, we have the stable positions $p_{1(1)}^{(1)}$ and $p_{1(1)}^{(2)}$ to be constant. These constant positions are used as an input in further calculations of the stable positions $p_{2(2)}^{(1)}$ and $p_{2(2)}^{(2)}$ of dislocations belonging to the second pair. In doing so, the positions $p_{2(2)}^{(1)}$ and $p_{2(2)}^{(2)}$ represent solutions of the system of equations $\partial\Delta W_2/\partial p_{2(2)}^{(k)}\big|_{p_{1(2)}^{(k)}=p_{1(1)}^{(k)}} = 0$, where ΔW_2 is given by formula (1) at n = 2. With the calculated values of $p_{2(2)}^{(1)}$ and $p_{2(2)}^{(2)}$, from equations $\partial\Delta W_3/\partial p_{3(3)}^{(k)}\big|_{p_{2(3)}^{(k)}=p_{2(2)}^{(k)}} = 0$ we found values of $\tilde{p}_{3(3)}^{(1)}$ and $\tilde{p}_{3(3)}^{(2)}$, in which case ΔW_3 is derived from formula (1) at n = 3.

With values of $\tilde{p}_{3(3)}^{(1)}$ and $\tilde{p}_{3(3)}^{(2)}$ as well as equations $\partial\Delta W_3/\partial p_{2(3)}^{(k)}\big|_{p_{3(3)}^{(k)}=\tilde{p}_{3(3)}^{(k)}} = 0$, corrected values of $\tilde{p}_{2(3)}^{(1)}$ and $\tilde{p}_{2(3)}^{(2)}$ were calculated. In their turn, these corrected values of $\tilde{p}_{2(3)}^{(1)}$ and $\tilde{p}_{2(3)}^{(2)}$ as well as equations $\partial\Delta W_3/\partial p_{3(3)}^{(k)}\big|_{p_{2(3)}^{(k)}=\tilde{p}_{2(3)}^{(k)}} = 0$ were exploited in correction of $\tilde{p}_{3(3)}^{(1)}$ and $\tilde{p}_{3(3)}^{(2)}$. Then, new corrected values of $\tilde{p}_{3(3)}^{(1)}$ and $\tilde{p}_{3(3)}^{(2)}$ were used in a new correction of $\tilde{p}_{2(3)}^{(1)}$ and $\tilde{p}_{2(3)}^{(2)}$, and so on. This iteration procedure has been performed until values of $\tilde{p}_{2(3)}^{(1)}$ and $\tilde{p}_{2(3)}^{(2)}$ as well as $\tilde{p}_{3(3)}^{(1)}$ and $\tilde{p}_{3(3)}^{(2)}$ converge to some constants $p_{2(3)}^{(1)}$ and $p_{2(3)}^{(2)}$ as well as $p_{3(3)}^{(1)}$ and $p_{3(3)}^{(2)}$, respectively. These limiting constants were treated as final values of dislocations belonging to the first and second pairs in the case of n = 3.

The same algorithm was utilized in the case of any finite n. As a result, we calculated stable positions $p_{i(i)}^{(k)}$ (where i = 1,....,n and k = 1,2), for n pairs of partial dislocations emitted from GB AA'.

With formula (1) for the energy change ΔW_n and the above calculation algorithm, from the conditions ΔW_n ($p_{n(n)}^{(k)} = p'$)=0 (where p' = 1 nm), $\Delta W_n\big|_{p_{n(n)}^{(k)}>p'} < 0$, and $\left(\partial\Delta W_n/\partial p_{n(n)}^{(k)}\right)\big|_{p_{n(n)}^{(k)}>p'} \leq 0$ one can calculate the

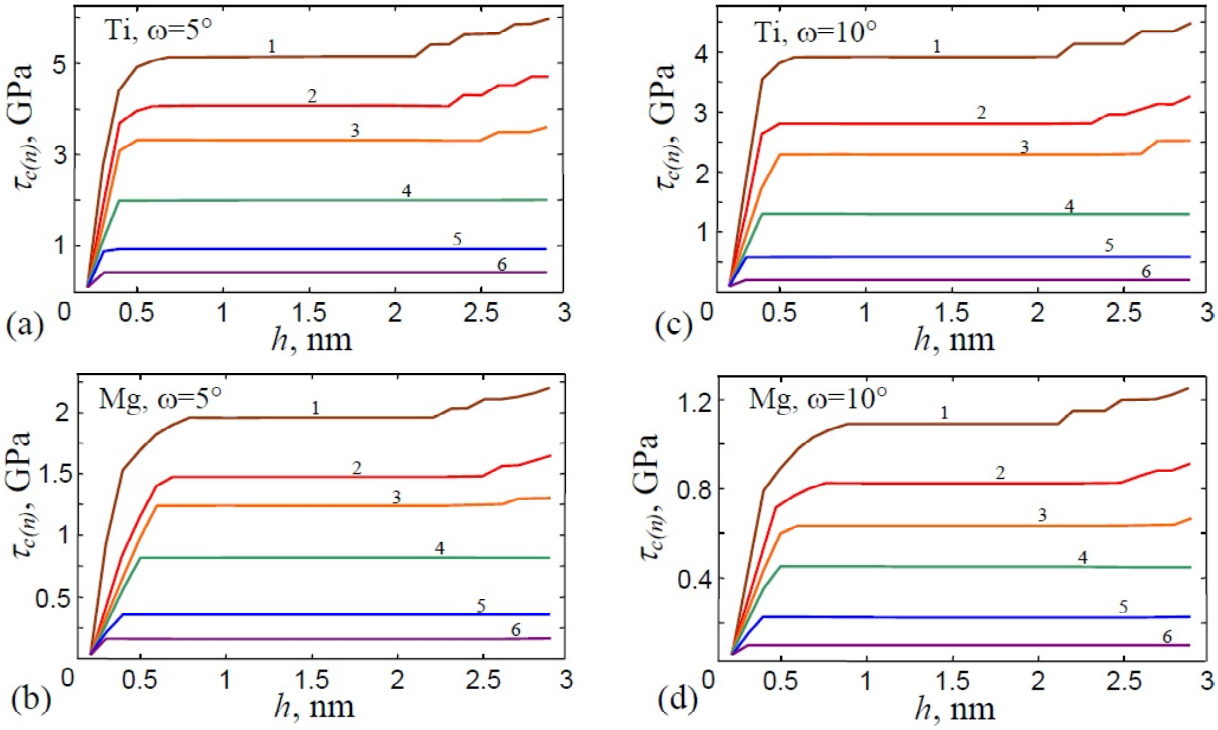

Fig. 3. Dependence of the critical shear stress $\tau_{c(n)}$ on twin thickness h at various values of grain size d = 10 nm (1), 50 nm (2), 100 nm (3), 1 μm (4), 3 μm (5), and 5 μm (6); and disclination strength ω = 5° (a,b) and 10° (c,d).

critical shear stress $\tau_{c(n)}$, the minimum stress at which the nth event of pair dislocation emission is energetically favourable. This stress serves as a key characteristic of the formation of paired twins at GBs.

We now reveal the dependence of the critical stress $\tau_{c(n)}$ on thickness $h = (n - 1)\delta$ of deformation twins ABCD and ABEF in the exemplary cases of titanium (Ti) and magnesium (Mg). In doing so, we exploit the following values of characteristic parameters for Ti: G = 46.7 GPa, ν = 0.31, a = 0.295 nm [31], γ = 0.357J/m^2, and γ_{TB} = 0.273 J/m^2 [32]; and, for Mg: G = 16.4 GPa, ν = 0.31, a = 0.32 nm [31], γ = 0.173 J/m^2, and γ_{TB} = 0.114 J/m^2 [32]. According to the experimental observations [26], the angle α is taken as α = 20°. The GB length L (playing the role of the discclination dipole arm) is in the following relation with the grain size d: $L = d/\sqrt{3}$. This relation corresponds to hexagonal grain shape.

Fig. 3 presents the dependences $\tau_{c(n)}(h)$ at various values of the grain size d and the disclination strength ω. As it follows from Fig. 3, the critical strength $\tau_{c(n)}$ grows with rising the twin thickness h and decreasing the grain size d. The dependence $\tau_{c(n)}(d)$ under consideration is related to the fact that the emitted dislocations in smaller grains are closer to GB that emits new dislocations and thereby more effectively hinder the new emission processes, as compared to the situation with comparatively large grains. In particular, values of the critical stress $\tau_{c(n)}(h,d)$ in the case of metals with small grains (see curves 1-4 in Fig. 3) are very high. They are close to those that initiate fracture processes under conventional quasistatic deformation. At the same time, for polycrystalline titanium and magnesium with comparatively large grains, values of the critical stress $\tau_{c(n)}(h,d)$ (see curves 5 and 6 in Fig. 3) are close to typical stresses operating in these metals in quasistatic deformation regimes [26,33].

Thickening of paired deformation twins is associated with an increase in the number n of emitted dislocations (Fig. 2) and, as a corollary, enhances their hindering effect on new dislocation emission events. In its turn, the enhancement in question gives rise to an increase of the critical stress. This aspect is reflected in the trend that the critical strength $\tau_{c(n)}$ grows with rising the twin thickness h (Fig. 3).

Also, formation of paired deformation twins at GBs can be significantly enhanced due to stress fields created by disclinations located at neighbouring triple junctions of GBs. This effect manifests itself in the trend that the critical stress diminishes, when the disclination strength ω increases (see Figs. 3a and 3b, for ω = 5°, and Figs. 3c and 3d, for ω = 10°).

4. CONCLUDING REMARKS

Thus, we theoretically described a special deformation mechanism realized through formation of paired deformation twins at GBs in nanostructured and coarse-grained polycrystalline metallic materials. In the framework of our model, formation and evolution of paired twins at a GB are mediated by successive emission of partial dislocation pairs from this boundary to adjacent grains (Fig. 2). Our theoretical analysis shows that the critical stress $\tau_{c(n)}$ for formation of paired twins grows with rising the twin thickness h and decreasing the grain size d (Fig. 2). In exemplary cases of titanium and magnesium with small grain sizes, values of the critical stress $\tau_{c(n)}(h,d)$ are very high and can be achieved at only some special schemes of mechanical load, like high-strain-rate deformation, indenter load, diamond anvil cell tests, and high-pressure torsion. At the same time, for coarse-grained polycrystalline titanium and magnesium, values of the critical stress $\tau_{c(n)}(h,d)$ are close to those conventionally achievable in these metals under conventional quasistatic deformation. The theoretical result under discussion is well consistent with the experimental observation [26] of paired deformation twins at GBs in quasistatically deformed polycrystalline titanium.

Also, we theoretically revealed that formation of paired deformation twins at GBs can be significantly enhanced due to stress fields created by disclinations located at neighbouring triple junctions of GBs. (Such triple junction disclinations are typically formed by severe plastic deformation in metals; see, e.g., [27,28]). This effect manifests itself in the trend that the critical stress diminishes, when the disclination strength ω rises (Fig. 3).

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