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CROSSOVER FROM DISLOCATION SLIP TO DEFORMATION TWINNING IN NANOSTRUCTURED AND COARSE-GRAINED METALS

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Abstract. A theoretical model is suggested which describes crossover from dislocation slip to deformation twinning in nanostructured and coarse-grained polycrystalline metals. In the framework of the suggested model, lattice dislocations that mediate dislocation slip in a grain interior are stopped by a grain boundary and form a pile-up configuration. Head dislocations of the pile-up are absorbed by the grain boundary where they split into grain boundary dislocations. A deformation twin is nucleated at these grain boundary dislocations and propagates to the neighbouring grain interior. The energy and stress characteristics of this transformation in nanostructured and coarse-grained polycrystalline metals (Ni, Ti) are calculated. Results of the suggested theoretical model are consistent with experimental data reported in literature.

1. INTRODUCTION

Lattice dislocation slip is the dominant deformation mode in most metallic crystalline materials [1,2]. Also, deformation twinning effectively contributes to plastic flow in metals especially at low temperatures and high strain rates [1,3]. In a metallic polycrystalline specimen, dislocation slip and deformation twinning can concurrently occur in various grains (with various crystal lattice orientations) of the specimen. In doing so, these deformation modes are capable of strongly influencing each other. For instance, following Wang *et al.* [4], the nucleation of deformation twins at grain boundaries (GBs) is induced by lattice dislocation pile-ups stopped by these GBs in neighbouring grains. However, micromechanism(s) of the crossover is (are) unknown. The main aims of this paper are to suggest such a micromechanism and theoretically describe the crossover from lattice slip to deformation twinning at GBs in nanostructured and coarse-grained polycrystalline metallic materials.

Note that, in the experiment [4], the crossover from lattice slip to deformation twinning was observed in coarse-gained polycrystalline titanium. This crossover occurs at GBs which therefore play an important enhancing role in the crossover. In the context discussed, it is logical to expect that the crossover can intensively occur in nanostructured metals where amounts of GBs are extremely large. Also, it is worth noting that deformation twins in nanostructured metals are typically nucleated at

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GBs [5]. At the same time, the formation of lattice dislocation pile-ups (that stimulate the crossover under discussion) is limited in ultrafine grains composing nanostructured metals deformed by lattice slip [2,6-8]. Thus, the two competing structural factors – large amounts of GBs and ultrafine grains – operate in nanostructured metals. This motivates interest in understanding the specific features of the crossover from dislocation slip to deformation twinning in nanostructured metallic materials. We will examine this subject, in parallel with the crossover in coarse-grained polycrystals, in next sections.

2. CROSSOVER FROM LATTICE SLIP TO DEFORMATION TWINNING: GEOMETRIC ASPECTS

We now consider a two-dimensional model of a coarse-grained polycrystalline (or nanostructured) metallic specimen specified by an average grain size d (Fig. 1a). The specimen is under tensile stress σ that initiates plastic flow (Fig. 1a). In the framework of our model, plastic deformation in the grain I occurs by lattice dislocation slip. In doing so, lattice dislocations moving in one crystallographic plane are stopped by a GB and form a pile-up configuration OA (Fig. 1b). Head dislocations of the pile-up reaches the GB at A, where they are absorbed by the GB and split into grain boundary dislocations (Fig. 1 c and d). As a result, a nanoscale wall of densely arranged GB dislocations is formed at local GB fragment AB (Fig. 1d).

Following [9,10], deformation twins are effectively nucleated at such GB fragments specified by high local densities of extrinsic GB dislocations. The twin nucleation occurs through cooperative splitting transformations of the GB dislocations into sessile GB dislocations and partial dislocations that move in the adjacent grain (Fig. 1e). A deformation twin is formed behind the moving partial dislocations (Fig. 1e) (for details, see [10]).

(Generally speaking, the twin nucleation can also occur through successive splitting transformations and through nanoscale ideal shear [9-11]. However, in the examined situation, our analysis showed that the energy and stress characteristics of these twin nucleation micromechanisms are close to those of the twin nucleation through cooperative splitting transformations. Therefore, in this paper, for simplicity, we restrict our consideration to the only the twin nucleation through cooperative splitting transformations.)

We now specify in detail the geometric characteristics of the defect system under examination.

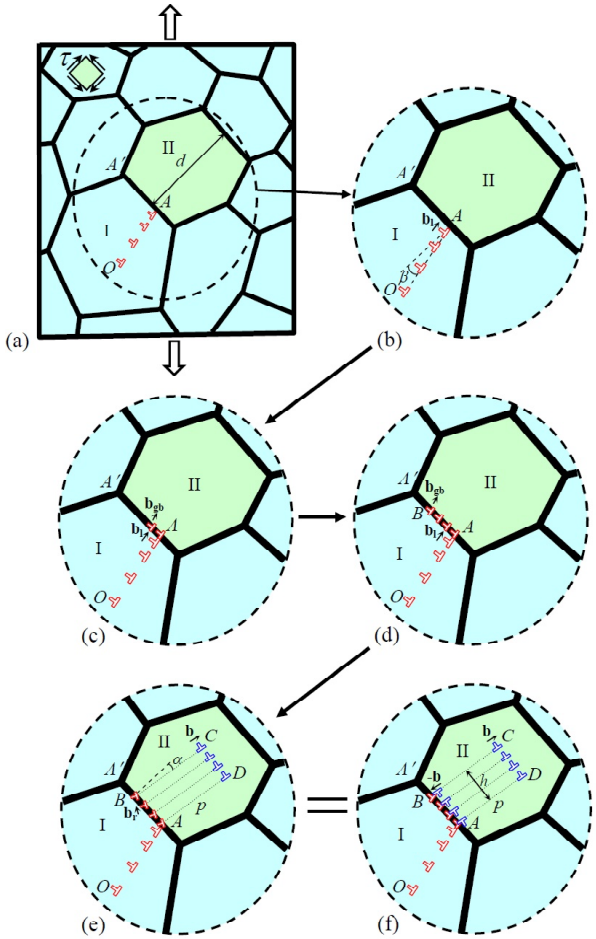

Fig. 1. Crossover from lattice slip to deformation twinning in a metallic specimen. (a) Metallic specimen under tensile load (two-dimensional general view). (b) Pile-up of lattice dislocations in grain I is stopped by grain boundary AA'. (c) Head dislocation of the pile-up is absorbed by the GB AA' where it splits into grain boundary dislocations. (d) Nanoscale wall AB of densely arranged grain boundary dislocations is formed at grain boundary AA'. (e) Grain boundary dislocations cooperatively split into sessile grain boundary dislocations and partial dislocations that move in the adjacent grain II, in which case a deformation twin ABCD is generated behind them. (f) Dislocation configuration consisting of the nanoscale wall of the b_{gb}-dislocations and the wall of dipoles of the partial dislocations with the Burgers vectors ±b. This dislocation configuration is equivalent to the dislocation configuration illustrated in Fig. 1e.

Let n_c be the number of lattice dislocations of the pile-up OA in its initial state (Fig. 1b). The lattice dislocations are characterized by Burgers vectors b_l and hereinafter called b_l-dislocations. When such

dislocations reach the GB AA', they split into GB dislocations characterized by the Burgers vectors b_{gb} (hereinafter called b_{gb}-dislocations) (Figs. 1c and 1d). The b_{gb}-dislocations slowly climb along the GB and form the nanoscale wall configuration *AB* (Fig. 1d). Then, the GB b_{gb}-dislocations cooperatively split into sessile GB dislocations specified by the Burgers vectors b_r and mobile partial twinning dislocations characterized by the Burgers vectors *b* (*b*-dislocations) (Fig. 1e). The *b*-dislocations cooperatively move in the grain II interior, in which case a deformation twin ABCD of length *p* is formed behind them (Fig. 1e).

In terms of the theory of dislocations, the dislocation configuration illustrated in Fig. 1e is equivalent to the configuration consisting of the nanoscale wall of the *b*-dislocations and the wall of dipoles of the partial dislocations with the Burgers vectors ±*b*, as shown in Fig. 1f. Also, the nucleation of the twin ABCD is accompanied by the formation of two twin boundaries AD and BC characterized by the specific (per unit area) energy γ_{TB} (Fig. 1e). The GB plane AA' makes angles α and β with slip planes of the partial *b*-dislocations and perfect lattice b_l-dislocations, respectively (Figs. 1e and 1b, respectively).

3. CROSSOVER FROM LATTICE SLIP TO DEFORMATION TWINNING: ENERGY AND STRESS CHARACTERISTICS

We now consider energy characteristics of the twin nucleation through cooperative generation of *n* dipoles of partial ±*b* -dislocations at the GB AA' near the pile-up of n_c perfect lattice b_l-dislocations stopped by this GB (Fig. 1e). The twin nucleation is specified by the energy change $\Delta W_n=W_n-W$, where *W* is the total energy of the examined defect system in its initial state with the pile-up OA of perfect b_l-dislocations and the wall AB of GB b_{gb}-dislocations (Fig. 1d), and W_n is the total energy of the examined defect system in its final state with *n* dipoles of partial ±*b*-dislocations located at the GB fragment *AB* and at the front of the twin *CD* (Fig. 1f). The twin nucleation is energetically favorable, if $\Delta W_n<0$.

The energy change has the six terms:

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

where $E^b_{\Sigma n}$ is the sum proper energy of *n* dipoles of partial ±*b*-dislocations; $E^{p-b}_{\Sigma n}$ is the energy that characterizes the elastic interaction between the lattice dislocation pile-up *OA* and *n* dipoles of partial ±*b*-dislocations; $E^{w-b}_{\Sigma n}$ is the energy that specifies the elastic interaction between the wall AB of *n* GB b_{gb}-dislocations and *n* dipoles of partial ±*b*-dislocations; $E^{b-b}_{\Sigma n}$ is the sum energy of all pair interactions between *n* dipoles of partial ±*b*-dislocations; E^{γ}_{n} denotes the specific (per unit area) energy of twin boundaries *AD* and *BC*; and $E^{\tau}_{\Sigma n}$ is the energy that characterizes the interaction of the external shear stress τ with *n* dipoles of partial ±*b*-dislocations.

The energy $E^b_{\Sigma n}$ represents the sum of the proper energies of *n* dipoles of partial ±*b*-dislocations in an elastically isotropic solid. It is given as [12]:

$$E^b_{\Sigma n} = nDb^2\left(\ln\frac{p\text{-}r_c}{r_c}+1\right), \tag{2}$$

where $D=G/[2\pi(1-\nu)]$, *G* is the shear modulus, ν is the Poisson' ratio, and $r_c \approx b$ denotes the core radius for partial ±*b*-dislocations.

The interaction energy $E^{p-b}_{\Sigma n}$ is calculated as the work spent to the generation of *n* dipoles of partial ±*b*-dislocations in the shear stress created by the lattice dislocation pile-up *OA* (see, e.g., Ref. [10]) and can be written as follows:

$$\begin{aligned} E^{p-b}_{\Sigma n} = -\sum_{i=2}^{n}\sum_{j=2}^{n_c}\frac{Db_1b}{2}\Bigg(&\cos(\alpha+\beta)\ln\frac{p^2+x_j^2+y_j^2+2px_j\cos(\alpha+\beta)+2py_i\sin(\alpha+\beta)}{x_j^2+y_j^2} \\ &-\frac{2\sin(\alpha+\beta)(y_ix_j+px_j\sin(\alpha+\beta))-2\cos(\alpha+\beta)(y_i^2+py_i\sin(\alpha+\beta))}{p^2+x_j^2+y_j^2+2px_j\cos(\alpha+\beta)+2py_i\sin(\alpha+\beta)} \\ &-\frac{2y_i^2\cos(\alpha+\beta)-2y_ix_j\cos(\alpha+\beta)}{x_j^2+y_j^2}\Bigg). \end{aligned} \tag{3}$$

where n_c and x_j=lag$_j$/τ are the number and coordinates of equilibrium positions of lattice b_l-dislocations belonging to the pile-up OA, lag$_j$ are the Laguerre coefficients [13], y_i=h_i/(cos(α+β), h_i=(i-1)δ, with i=1,2,3…n.

The interaction energy $E_{\Sigma n}^{w-b}$ is calculated as the work spent to the generation of n dipoles of partial ±b-dislocations in the shear stress field created by GB b_{gb}-dislocations (see, e.g., Ref. [14]), in which case we have:

$$E_{\Sigma n}^{w-b} = \frac{Db_{gb}b}{2}\sum_{j=1}^{n}\sum_{i=1}^{n}\left((y_i - y_{ij}\cos(\alpha+\beta))\ln\left[1+\frac{p^2-2y_{ij}p\sin(\alpha+\beta)}{y_{ij}^2+y_i^2-2y_{ij}y_i\cos(\alpha+\beta)}\right] - y_i\ln\left[1+\frac{p^2}{y_i^2}\right]\right), \quad (4)$$

where y_{ij}=h_j-h_i.

The energy $E_{\Sigma n}^{b-b}$ represents the sum of the energies that specify all pair interactions between n dipoles of partial ±b-dislocations and can be written as the following double sum over indices i and j (see, e.g., Ref. [14]):

$$E_{\Sigma n}^{b-b} = \frac{Db^2}{2}\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\left\{-2y_{ij}^2\left(\frac{p^2+2px_{ij}}{\left(p^2+x_{ij}^2+y_{ij}^2+2px_{ij}\right)\left(x_{ij}^2+y_{ij}^2+2px_{ij}-2px_{ij}\right)} - \frac{p^2-2px_{ij}}{\left(x_{ij}^2+y_{ij}^2\right)\left(p^2+x_{ij}^2+y_{ij}^2-2px_{ij}\right)}\right) + \ln\left[1+\frac{p^2-2px_{ij}}{x_{ij}^2+y_{ij}^2}\right] - \ln\left[1-\frac{p^2+2px_{ij}}{p^2+x_{ij}^2+y_{ij}^2+2px_{ij}}\right]\right\}, \quad (5)$$

where x_{ij}=(h_i-h_j)tanα.

The energy of twin boundaries is given by the following standard formula:

$$E_n^{\gamma} = 2\gamma_{TB}p,\ n \geq 2. \quad (6)$$

The energy that characterizes the interaction of the external shear stress τ with n dipoles of partial ±b-dislocations is as follows:

$$E_{\Sigma n}^{\tau} = -npb\tau\cos2\alpha, \quad (7)$$

Formulas (1)-(7) allow us to calculate the energy change ΔW_n. With these calculations, we obtained the dependence of ΔW_n on the twin length p, for various values of the external shear stress τ, in the exemplary cases of nanostructured nickel (Ni) and titanium (Ti). In doing so, we used the following characteristic values of their parameters: for Ni, G =73 GPa, ν=0.34, a=0.352 nm, b_l=$a\sqrt{2}$/2, b=a/$\sqrt{6}$, δ=a/$\sqrt{3}$ [1], $b_{gb}\approx$ 0.1 nm and γ_{TB}=0.110 J/m^2 [15]; and, for Ti, G =46.7 GPa, ν=0.31, a=0.295 nm, b_l=$a\sqrt{2}$/3, b=a/$\sqrt{3}$, δ=a/$\sqrt{6}$ [16], $b_{gb}\approx$ 0.1 nm and γ_{TB}=0.273 J/m^2 [17]. The dependence $\Delta W_n(p)$ is presented in Fig. 2, for d=50 nm, n_c=7, n=10, α=β=10° and various values of the external shear stress τ.

As it follows from Fig. 2, there are the two basic types of functions $\Delta W_n(p)$, depending on the external stress τ. For low values of τ, when p increases, the energy change ΔW_n fist increases, reaches its maximum, and then decreases. This means that the generation and growth of the deformation twin needs to overcome an energy barrier. With rising the external stress τ, the energy barrier diminishes and disappears at some critical value τ_c of the stress (Fig. 2). In the situation where $\tau > \tau_c$, for $p \leq d$, the energy change ΔW_n is always negative so that the twin nucleation and growth are energetically favorable. In the discussed situation with high external stresses, the twin nucleated at a GB propagates across a grain and reaches an opposite GB.

The critical external stress τ_c is defined as the minimum shear stress at which the twin nucleation through cooperative emission of partial dislocations from a GB (Fig. 1e) is energetically favorable. Using the function $\Delta W_n(p)$, the critical shear stress τ_c can found from the following conditions: $\Delta W_n(p=p')$, where p'=1 nm, $\Delta W_n\big|_{p>p'} < 0$, and $\left.\frac{\partial \Delta W}{\partial p}\right|_{p>p'} \leq 0$.

The twin length p is chosen as p=1 nm, because it is the minimum twin length at which the notion/definition of twin has sense.

We now calculate the dependence of the critical shear stress τ_c on the twin thickness h in the exemplary cases of nanostructured and coarse-grained polycrystalline Ni and Ti at various values of the number n_c of lattice dislocations composing the pile-up configuration (Fig. 3). The dependences $\tau_c(h,n_c)$ demonstrate that the critical stress τ_c increases, when the twin thickness h increases and/or the number n_c decreases (Fig. 3).

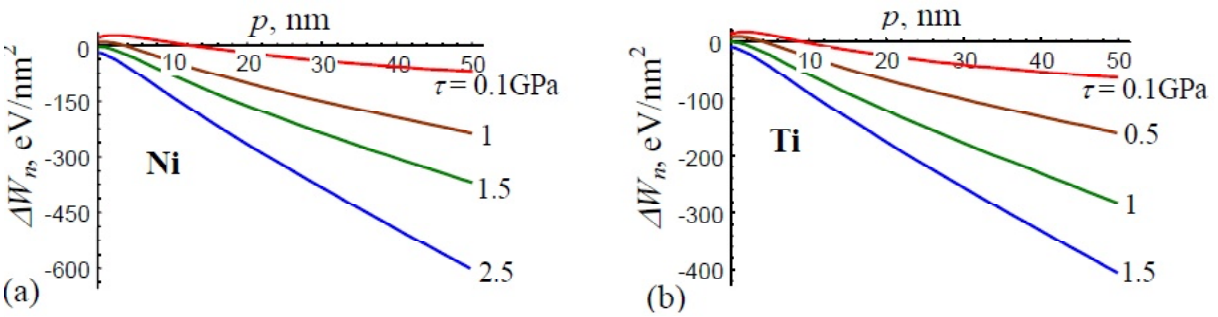

Fig. 2. Dependences of the energy change ΔW_n on the twin length p at various values of the external shear stress τ, for nanostructured (a) Ni and (b) Ti.

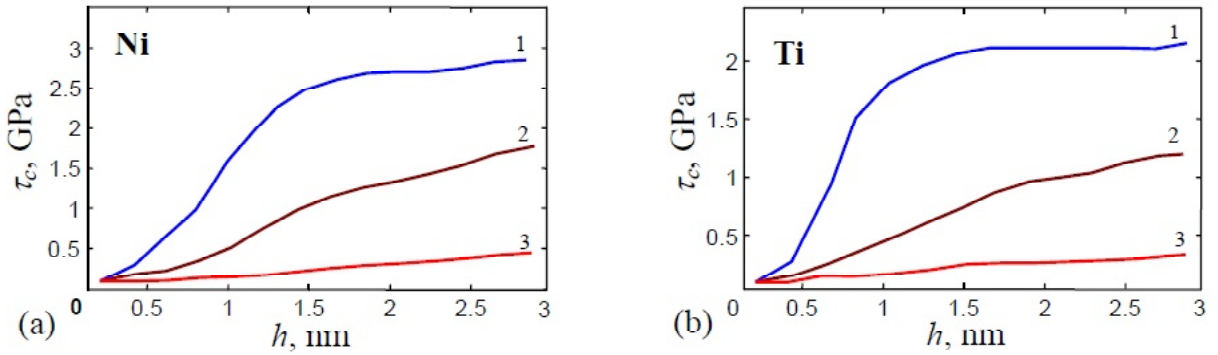

Fig. 3. Dependences of the critical shear stress τ_c on twin thickness *h*, for nanostructured (a) Ni and (b) Ti, at various numbers of lattice dislocations in the pile-up n_c=5, 10, and 20 (curves 1, 2, and 3, respectively).

For low enough number n_c (= 5 and 10) of lattice dislocations in the pile-up, values of τ_c are high (see curves 1 and 2 in Fig. 3) 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. Note that, for geometric reasons, values of the number n_c of lattice dislocations in one pile-up configuration are low in nanostructured materials [2,6-8]. In the context discussed, we conclude that the crossover from dislocation slip to deformation twinning can occur in nanostructured metals at only special deformation regimes characterized by high applied stresses.

At the same time, in the case of large number n_c = 20 of lattice dislocations in the pile-up (see curves 3 in Fig. 3), values of the critical shear stress τ_c are close to those typically measured in quasistatic deformation tests of coarse-grained polycrystalline nickel and titanium. This is well consistent with both numerous experimental observations of large dislocation pile-ups in coarse-grained polycrystalline metals (for a review, see [18,19]) and experimental observation [4] of the crossover from dislocation slip to deformation twinning in coarse-grained Ti.

4. CONCLUDING REMARKS

Thus, we theoretically described the experimentally observed [4] crossover from lattice slip to deformation twinning in metallic materials. In the framework of our description, lattice dislocations that mediate dislocation slip in a grain interior are stopped by a GB and form a pile-up (Fig. 1b). Head dislocations of the pile-up are absorbed by the GB where they split into GB dislocations (Figs. 1c and 1d). As a result, a nanoscale wall of densely arranged GB dislocations is formed at local GB fragment (Fig. 1d). The twin nucleation occurs through cooperative splitting transformations of the GB dislocations into sessile GB dislocations and partial dislocations that move in the adjacent grain, in which case a deformation twin is formed behind them (Fig. 1e).

The energy and stress characteristics of this transformation in nanostructured and coarse-grained polycrystalline metals (Ni, Ti) are calculated. It is shown that the critical stress τ_c increases, when the twin thickness *h* increases and/or the number n_c of lattice dislocations in the pile-up decreases (Fig. 3). This theoretical result is important for understanding the specific features of the crossover

from dislocation slip to deformation twinning in nanostructured and coarse-grained polycrystalline metals, because, for geometric reasons, values of the number n_c of lattice dislocations in one pile-up configuration are low in nanostructured materials, in contrast to their coarse-grained counterparts where n_c can be large.

More precisely, for low enough number n_c (= 5 and 10) of lattice dislocations in the pile-up, values of t_c are high (see curves 1 and 2 in Fig. 3) 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. In the context discussed, we conclude that the crossover from dislocation slip to deformation twinning can occur in nanostructured metals at only special deformation regimes characterized by high applied stresses.

At the same time, in the case of large number n_c= 20 of lattice dislocations in the pile-up (see curves 3 in Fig. 3), values of the critical shear stress τ_c are close to those typically measured in quasistatic deformation tests of coarse-grained polycrystalline nickel and titanium. This is well consistent with both numerous experimental observations of large dislocation pile-ups in coarse-grained polycrystalline metals and experimental observation [4] of the crossover from dislocation slip to deformation twinning in coarse-grained Ti.

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