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MECHANISM OF STRESS-DRIVEN GRAIN BOUNDARY MIGRATION IN NANOTWINNED MATERIALS

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Abstract. Stress-driven grain boundary (GB) migration in ultrafine-grained materials with nanotwinned structure is theoretically described. In the framework of the theoretical model, the stress-driven high-angle GB migration is accompanied by migration of twin boundaries which adjoin this GB. Energetic characteristics and critical stresses of the GB migration accompanied by the twin boundary migration are calculated.

1. INTRODUCTION

Nanostructured materials often exhibit the outstanding physical and mechanical properties such as high strength and hardness, but, in most cases, at the expense of low ductility and low fracture toughness. However, recently, several examples of functional ductility and good toughness have been reported [1-7]. For example, novel nanotwinned metals (ultrafine-grained metallic materials with high-density ensembles of nanoscale twins within grains) exhibit simultaneously high strength and good ductility at room temperature [1-7]. From a microscopic viewpoint, the properties of nanostructured materials are dramatically influenced by specific deformation mechanisms which effectively operate in these materials. 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 due to stress-driven migration of twin boundaries [1,8-12]. Another mode that causes a special interest is stress-driven migration of GB [13-17]. Existing theoretical models [18-22] describe the stress-driven GB migration in nanostructured materials without taking into account the presence of nanoscale twins in grains. However, twin boundary migration coupled to the stress-driven GB capable of reducing the twin length. It is assumed that decrease in the length of twins facilitates the process of the GB migration as compared to the GB migration in the absence of twins. Thus, the main aim of this paper is to theoretically describe the stress-driven high-angle GB migration accompanied by the twin boundary migration in ultrafine-grained materials with nanotwinned structure.

2. MODEL OF STRESS-DRIVEN GB MIGRATION ACCOMPANIED BY TWIN BOUNDARY MIGRATION

Consider a two-dimensional model of an ultrafine-grained specimen containing ensembles of nanotwins bounded by coherent twin boundaries and grain boundaries. We assume that the nanotwinned

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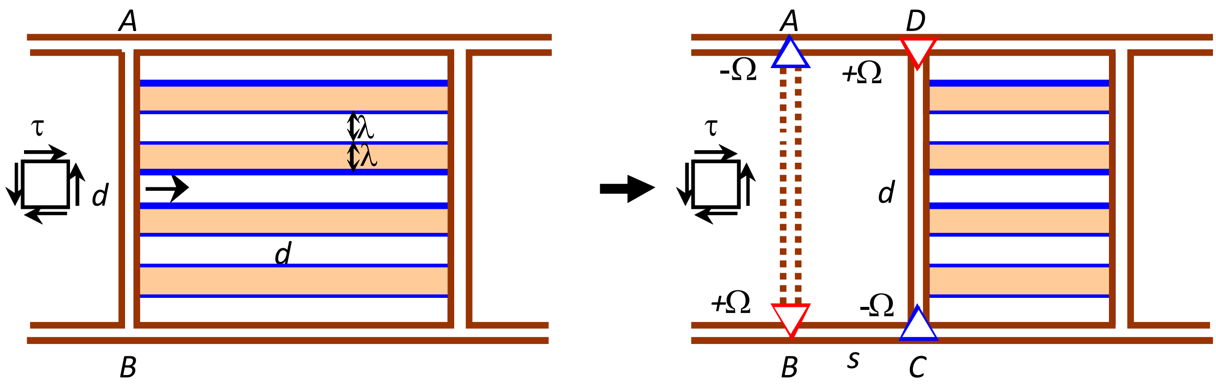

Fig. 1. Model of the stress-driven GB migration accompanied by the twin boundary migration in ultrafine-grained materials with nanotwinned structure. (a) An initial defect configuration containing high-angle GB *AB* and nanoscale twins which adjoin the GB *AB*. (b) Migration GB *AB* to a distance *s* in a new position *CD*.

specimen has rectangular grains with an average size *d* (Fig. 1a). Let us consider an individual grain containing n identical growth nanotwins of the same thickness λ and length *d* distributed periodically and restricted by twin boundaries, with the same distance λ in between (Fig. 1a). The nanotwins adjoin the GB *AB* representing a high-angel tilt boundary which characterized by the tilt misorientation parameter Ω. It is assumed that under action of an external shear stress τ, the grain boundary *AB* migrates to a distance *s* in a new position *CD* (Fig. 1b). It is well known [18] that stress-driven GB migration is accompanied by formation of wedge disclinations at GB junctions (Fig. 1b). Consider this process in detail. In the initial state (Fig. 1a), triple junctions *A* and *B* are supposed to be geometrically compensated. In other words, the sum of GB misorientation angles at each of these junctions is equal to zero. After GB *AB* migration the angel gaps $\pm\Omega$ appear at the GB junctions *A* and *B*, and at two new GB junctions *C* and *D*. In the theory of defects in solids, these angel gaps are defined as partial wedge disclinations having strength $\pm\Omega$ (Fig. 1b). Thus, stress-induced migration of high-angle tilt GB *AB* results in the formation of a quadrupole of wedge disclinations *ABCD* with strength $\pm\Omega$ (quadrupole $\pm\Omega$-disclinations) (Fig. 1b).

In the frame of the work, the GB *AB* migration is accompanied by migration of twin boundaries which adjoin the GB *AB* (Fig. 1b). The migration of the twin boundaries leads to a decrease in the length of nanotwins by a value which equal to the distance *s* of the GB *AB* migration (Fig. 1b). Decrease in the length of nanotwins reduces elastic energy of the defective system and, therefore, facilitates the process of the GB *AB* migration. In other words, the GB migration accompanied by the twin boundary migration becomes possible at lower values of the external shear stress τ in comparison with the stresses necessary for GB migration in the absence of nanotwins.

Further, consider the energy characteristics and estimate the critical stresses of the stress-driven GB migration in ultrafine-grained materials with nanotwinned structure.

3. ENERGETIC CHARACTERISTICS AND CRITICAL STRESSES OF THE GB MIGRATION ACCOMPANIED BY THE TWIN BOUNDARY MIGRATION

Let us calculate the energy difference ΔW specifying the GB migration (Figs. 1a,b) under consideration. To do so, we assume that the ultrafine-grained specimen represents an isotropic solid characterized by the shear modulus *G* and the Poisson ratio ν. The GB *AB* migration is characterized by the energy change $\Delta W = W_2 - W_1$ where W_1 is the energy of the defect configuration in its initial state (Fig. 1a), and W_2 is the energy of the defect configuration in its final state after GB *AB* migration (Fig. 1b). The transformation is energetically favorable, if $\Delta W<0$. In terms of the theory of defects in solids, the energy change ΔW is written as follows:

$$\Delta W = E_s^{\Omega} + \Delta E_{TB} - A_{\tau}, \tag{1}$$

E_s^{Ω} is the proper energy of the quadrupole $\pm\Omega$-disclination; ΔE_{TB} is the difference in the energy of twin boundaries between the final and initial states; A_{τ} is the work spent by the external shear stress τ on movement of the GB *AB* over the distance *s*.

The proper energy of the disclination quadrupole is given by the following standard expression [23]:

$$E_s^{\Omega} = \frac{D\Omega^2 d^2}{2}\left[\left(1+\frac{s^2}{d^2}\right)\ln\left(1+\frac{s^2}{d^2}\right)-\frac{s^2}{d^2}\ln\frac{s^2}{d^2}\right], \tag{2}$$

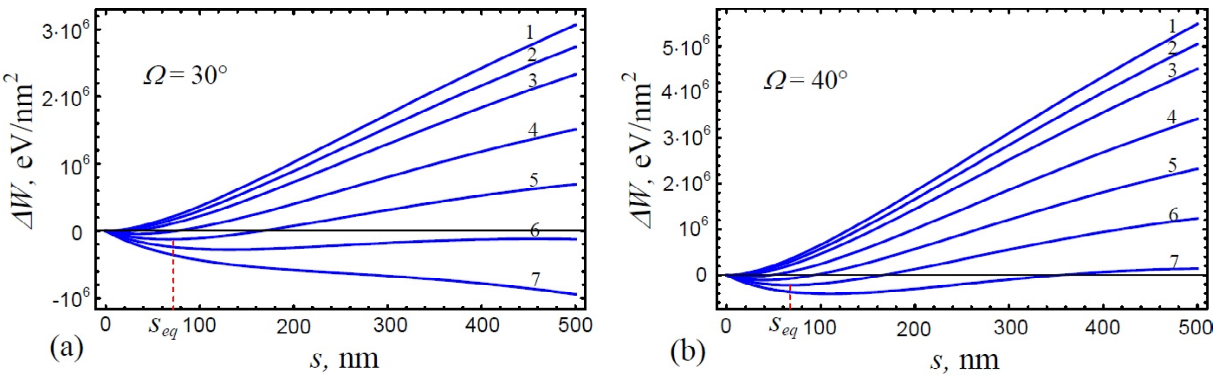

Fig. 2. Dependences the energy change ΔW on the migration distance s, for misorientation parameter W=30° (a) and 40° (b), at various values of the external shear stress τ = 0.1,0.5,1,2,3,4, and 5 GPa (curves 1, 2, 3, 4, 5, 6, and 7, respectively).

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

The twin boundary energy difference ΔE_{TB} is given by formula:

$$\Delta E_{TB} = n\gamma_{TB}(s-d), \tag{3}$$

where γ_{TB} is the specific energy (per unit area) of twin boundaries, $n = \lfloor (d/\lambda - 1)/2 \rfloor$ is the number of nanotwins, where $\lfloor X \rfloor$ means an integer part of a rational number X.

The work A_τ spent by the external shear stress τ on movement of the GB AB over the distance s is as follows:

$$A_\tau = \Omega\tau s d. \tag{4}$$

With help of formulas (1)-(4), we obtain the expressions for total energy change ΔW. Let us use these formulas in order to calculate the dependence of the energy difference ΔW on the GB AB migration distance s in exemplary case of ultrafine-grained nanotwinned copper (Cu) characterized by the following parameter values: G=48 GPa, ν=0.34, and γ_{TB}=24 mJ/m^2 [24]. The twin thickness λ and the grain size d are taken as λ =15 nm and d = 500 nm. The dependences $\Delta W(s)$ are presented in Fig. 2, for various values of the external shear stress t and of the misorientation parameter W = 30° (the strength of quadrupole of ± Ω-disclinations) (Fig. 2a) and 40° (Fig. 2b). These values of Ω correspond to the case of high-angle GB AB. As it follows from Fig. 2, there are three ways of function $\Delta W(s)$ behavior, depending on the external stress τ. For low values of the external shear stress τ, the energy change $\Delta W(s)$ fist decreases, reaches its minimum, and then grows monotonously with rising the distance s (Fig. 2a, curves 1-5 and Fig. 2b, curves 1-7). In this case the initial stage of the GB AB migration is energetically favorable (the energy change is negative $\Delta W(s)$<0 and monotonically decreases) at some critical value τ_{c1} of the external shear stress (Fig. 2). Thus, the critical stress τ_{c1} is the lowest stress at which stable migration of GB AB starts to occur. The GB AB can migrate until the point of minimum which determines the equilibrium migration distance s_{eq} (Fig. 2). The distance s_{eq} of the equilibrium migration of the GB AB is set by the level of the external stress τ, than higher value of the external shear stress τ the more equilibrium GB migration distance s_{eq} (Fig. 2). With rising the external shear stress τ, the energy change $\Delta W(s)$, after reaching its minimum, increases and achieves its maximum, and then decreases monotonously (see Fig. 2a, curve 6). The point of maximum determines the energy barrier for further GB migration. When the external shear stress τ is high enough, the energy change is always negative and decreases monotonously with increasing the migration distance s at some critical value τ_{c2} of the shear stress (Fig. 2a, curve 7). For the external shear stress $\tau > \tau_{c2}$, there exist no stable equilibrium position and/or energy barriers for GB migration. In this situation where $\tau > \tau_{c2}$, unstable migration of GB AB is occurred. Thus, the critical stress τ_{c2} determines the transition from stable to unstable GB migration. As it can be seen from the curves in Fig. 2, the decrease in the misorientation parameter Ω (the strength of quadrupole of ± Ω -disclinations) reduces the level of the external shear stress τ required for the GB AB migration.

Let us calculate the values of the critical stresses τ_{c1} and τ_{c2} which determine stable and unstable GB migration, respectively. The start of GB AB migration is possible, if $\Delta W(s=s')$, where s'= 1 nm. Thus, the equation $\Delta W(s=s')$=0 determines the critical stress τ_{c1} as the stress required to start process of the GB AB migration.

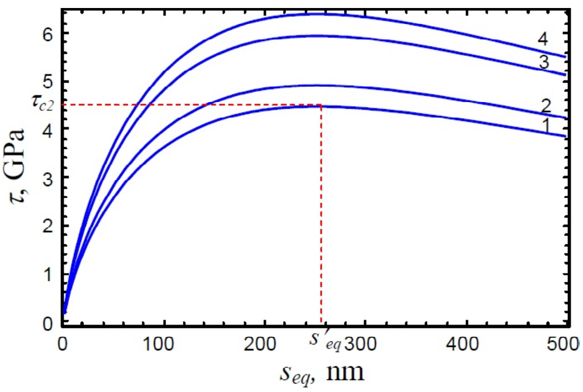

Fig. 3. Dependences of the external shear stress τ on the equilibrium migration length s_{eq} in the case of GB migration accompanied by twin boundary migration (curves 1 and 3) and GB migration in absence of nanotwins (curves 2 and 4), at various values of misorientation parameter $W = 30°$ (curves 1 and 2) and 40° (3 and 4). Correspondence τ and s_{eq} is correct to the left of the point (s'_{eq}, τ_{c2}).

The equilibrium migration length, which characterizes the stable GB migration, corresponds to the minimum points on the dependences $\Delta W(s)$ (Fig. 2). The minimum points (which specify the equilibrium migration length) can be found from equation for the energy change $\Delta W(s)$ and the mathematical conditions $\partial \Delta W(s)/\partial s = 0$ and $\partial^2 \Delta W(s)/\partial s^2 > 0$. Using these mathematical conditions and the formula for the energy change $\Delta W(s)$ (formulas (1)-(4)), let us write the dependence of the external shear stress on the equilibrium GB *AB* migration length s_{eq} in the following form:

$$\tau(s_{eq}) = \frac{F(s_{eq})}{\Omega d}, \quad (5)$$

where

$$F(s_{eq}) = \partial\left(E_S^{\Omega} - \Delta E_{TB}\right)/\partial s\Big|_{s=s_{eq}} .$$

Let us calculate the dependences $\tau(s_{eq})$ in exemplary case of nanotwinned copper (Cu). The dependences $\tau(s_{eq})$ are presented in Fig. 3, for various values of the misorientation parameter Ω. The point of maximum on dependencies $\tau(s_{eq})$ corresponds to the maximum stress $\tau = \tau_{c2}$ at which stable GB migration is realized, and the distance s'_{eq} is the maximum equilibrium migration length of the GB *AB* (Fig. 3). Thus, in the situation where $\tau > \tau_{c2}$, the GB migration becomes unstable and the GB *AB* can migrate until it reaches the opposite GB. Fig. 3 illustrates a comparison of dependences $\tau(s_{eq})$ (curves 1 and 3) corresponding to the stress-driven GB *AB* migration accompanied by the twin boundary migration with dependences $\tau(s_{eq})$ (curves 2 and 4) corresponding to the stress-driven GB *AB* migration in the absence of nanotwins (in the case γ_{TB}=0). From Fig. 3, it follows that the presence of nanoscale twins facilitates the process of the GB *AB* migration.

4. CONCLUSIONS

Thus, in this paper, a theoretical model which describes the stress-driven GB migration accompanied by the twin boundary migration in ultrafine-grained materials has been suggested. It has been shown that there are two main regimes of GB migration depending on the level of the external shear stress τ: stable and unstable regime. When the external shear stress $\tau_{c1} \leq \tau < \tau_{c2}$, the GB migrates in a stable regime characterized by the equilibrium migration length s_{eq} which is determined by the level of τ. If $\tau > \tau_{c2}$, the GB migration becomes unstable and GB can migrate until it reaches the opposite GB. In the framework of the model, the critical stresses τ_{c1} and τ_{c2} have been determined. A comparison of the GB migration accompanied by the twin boundary migration with the GB migration in the absence of nanoscale twins has been performed. Also, it has been shown that the presence of nanoscale twins facilitates the process of the GB migration.

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