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Twinning propensity in nanocrystalline face-centered cubic, body-centered cubic, and hexagonal close-packed metals

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ABSTRACT

The nanotwinned structures in metals exhibit the unique combination of physical properties. The unifying approach is developed that can be applied to nanocrystalline (nc) materials with different crystal structures. It is used to make a bridge between microscopical mechanisms of twin nucleation and macroscopic characteristics of the twinning and calculate them. The grain size range of the nanotwinning propensity, the grain size of its peak, and the requisite external twinning stress are calculated for the nc face-centered cubic metals *Al*, *Cu*, *Ni*, *Pd*, *Au*, *Ag*, for nc body-centered cubic metals *Ta*, *Fe*, *Nb*, *Mo*, and for hexagonal close-packed nc metals *Co*, *Zr*, *Mg*, *Ti*.

1. Introduction

Mechanical properties related to twinning have been important materials' issues [1]. Nanotwinned structures were observed last decade in nc metals *Al*, *Cu*, *Ni*, *Pd*, *Ta*, (see, for example, papers [2–10] and reviews [11,12]). It was reported in Refs. [13–16] that with the decreasing grain size the number of grains containing twins first increases and then decreases demonstrating inverse grain size effect. The nanotwinned structures provide unique mechanism to increase the strength and ductility of nc metals [17,11]. They also exhibit combination of high strength, high electrical conductivity [17,18] and high stability [17,19] of face-centered cubic (fcc) nc metals. The nanotwinning as the deformation mechanism of the body-centered cubic (bcc) nc *Ta* was experimentally observed in Ref. [7]. There are the experimental observations of twinning in nc hexagonal close-packed (hcp) metals: *Zr* [20], *Co* [21], the ultrafine-grained hcp *Ti* [22,23], nc hcp *Mg* [24,25], and hcp *Mg* alloy [26,27]. Thus, the development of principles of nanotwin engineering, such as selection of the nanotwinned structures in wide range of nc materials with different types of crystal lattices, becomes actually important problem. In this paper, we develop the unifying approach that can be used for this purpose.

A high concentration of stress in the course of formation of twin inclusion is necessary for the stage of a twin nucleation. This important stage that determines possibility of twinning in the nc materials mainly attracted attention and was analyzed thoroughly (see, for example, Refs. [3,28–30]). In Ref. [31], the next stages of twinning that is the growth of the wedge shaped twin in the grain and a propagation of twinning through the polycrystalline nc materials were analyzed. Approach developed in the current paper is based on the results obtained in Ref. [31].

This paper is organized in the following way. In Section 2, we obtain the low limit for a critical grain size for nc materials below which the twinning does not occur and the upper limit for the grain size above which the slip prevails over the twinning. Results of calculations for the grain size range of the nanotwinning propensity, the grain size of its peak, and the requisite external stress for twinning propagation in nc materials with different crystal structures are presented and discussed in Section 3. Conclusions follow in Section 4.

2. Method

The twin growth stage of twinning in nc fcc materials is analyzed in Ref. [31] by using the consistent application of the dislocation theory of twins [32,33]. The theoretical consideration of both statics [32] and dynamics [34] of twins was made. Experimental studies show the validity of the dislocation theory of twins for the description of twins in metals, minerals [33], in the high-temperature superconductor $YBa_2Cu_3O_{7-\delta}$ [35,36], and in the natural diamond [37]. The real situation in the nc materials is very complicated and substantially influenced by the presence of

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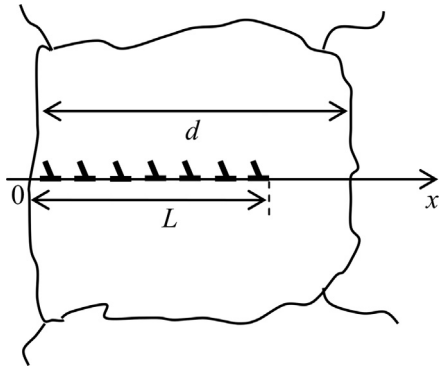

Fig. 1. A schematic representation of the twin growth stage in the grain of a nanocrystalline metal under influence of the external elastic field. The twin formed by a pile-up of twinning dislocations is positioned along the x-axis from a point $x=0$ to a point $x=L$. L is the twin length and d is the grain size.

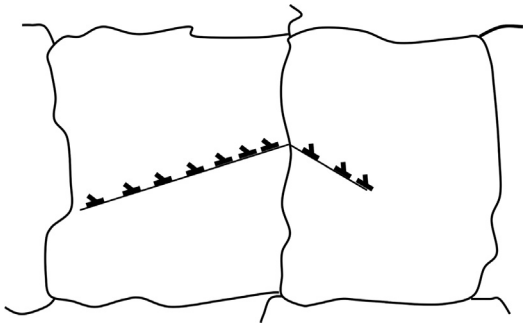

Fig. 2. A schematic representation of the twinning propagation in a polycrystalline nc metal. The twin growth stage in the grain leads to the situation in which it runs in the opposite GB and becomes pinned there. This leads to the concentration of stress and related dislocation activity that helps to nucleate a twin in the adjacent grain.

the grain boundaries (GBs). Nanocrystalline materials often have non-equilibrium GBs with high densities of dislocations [11]. A typical non-equilibrium GB was modeled in Ref. [38] as a low-angle GB formed by the vertical wall of dislocations. Dislocation models are applicable for low-angle GBs [39]. These GBs create a long-range elastic field. It is stated in Ref. [11] that the non-equilibrium GBs would make twinning easier. In Ref. [31] the growth of a horizontal twin is considered in the presence of the long-range elastic field of the vertical wall of dislocations. Equations usually used to describe the long-range elastic field of dislocations are still valid inside grains of nc materials. Following Ref. [28], we suppose that these equations are still valid inside grains of the nc materials at the grain sizes down to 2 nm.

In the framework of the dislocation theory of twins [33,31], the length of the wedge shaped twin nucleated at the GB located at the origin of coordinate and growing inside grain in the direction of the another GB located at $x=d$ (d is the size of the grain) along x-axis (see Fig. 1) in the elastic field can be determined from the following equation:

$$\frac{2}{\pi}\int_0^L \frac{\sigma_e(x)\,dx}{\sqrt{L^2-x^2}} = \sqrt{\frac{G\gamma_{tw}}{\pi(1-\nu)}}\frac{1}{\sqrt{L}}. \tag{1}$$

In Eq. (1), G is the shear modulus, ν is the Poisson's ratio, γ_{tw} is the twin boundary energy, σ_e is the external elastic stress and L is the twin length. When the length of the growing twin L becomes comparable to the grain size d, the twin exhibits a loss of stability and reaches the grain size by a jump [33]. Taking into account this circumstance, one can estimate from Eq. (1) the stress needed for formation of the twin completely intersecting the grain with size d. The relationship (1) can also be used to estimate d in which the twin intersects the grain when the external uniform elastic stress stress σ_e is applied. In proportion to decrease of the grain size, subgrains were first formed with small-angle GBs followed by the subsequent small-angle to large-angle transformations of the GBs [5]. The special large-angle GBs usually do not create a long-range elastic field, and the nucleation of a twin could be done only by a uniform stress created by an external load applied to the material without the assistance of the long-range elastic stress of the GB. In this case the external uniform elastic stress σ_e at which the twin appears, equals to the twin nucleation stress σ_n: $\sigma_e=\sigma_n$. The corresponding grain size d_{crit1} can be found now from Eq. (1). The stress σ_n usually is very high and one can expect that when σ_e is approaching σ_n, the twinning seized to be the leading mechanism of the plastic deformation of material with the grain sizes $d \geq d_{crit1}$. Therefore d_{crit1} can be treated as the lower limit of twinning propensity below which the nanotwinning does not occur. From Eq. (1) it can be estimated as follows:

$$d_{crit1} \geq \frac{G\gamma_{tw}}{\pi(1-\nu)\sigma_n^2}. \tag{2}$$

The next step is the propagation of twinning through the polycrystalline nc material under the external macroscopic elastic stress σ_T. The twin growth stage in the grain leads to the situation in which the twin (pile-up of twinning dislocations) runs in the opposite GB and becomes pinned there. This leads to the concentration of stress and related dislocation activity that helps nucleate a twin in the adjacent grain, as shown in Fig. 2. Following Ref. [39], the force per unit length acting at the tip of the initial twin pinned at the GB, when the requisite external stress σ_T is applied, can be estimated as $f=(\pi(1-\nu)\sigma_T^2 d)/4G$. The corresponding requisite external stress σ_T for a twinning propagation in a polycrystalline nc material can be found by equating the critical value of the force per unit length $f^*=\sigma_n b_T$ and the force per unit length f acting at the tip:

$$\sigma_T = \sqrt{\frac{4Gb_T}{\pi(1-\nu)\,d}}\sigma_n. \tag{3}$$

where b_T is the Burgers vector of the twinning dislocation. The process of twin nucleation has been analyzed many times elsewhere. The corresponding expression of the twin nucleation stress σ_n for different possible dislocation mechanisms of nucleation can be substituted in (3). For the other hand, the slip nucleation stress can be estimated by analogy with Ref. [3] using results of Ref. [39] for nucleation of a slip dislocation with the Burgers vector of the slip dislocation and taking into account a lattice friction stress (Peierls stress) that is needed to set the slip dislocation in motion after nucleation. The result is

$$\sigma_S = \sqrt{\frac{4G}{\pi(1-\nu)}\left[\frac{Gb_S^2}{d^2}+\frac{S_{Sfr}b_S}{d}\right]}, \tag{4}$$

where σ_S is the requisite external stress for slip propagation in polycrystalline nc material, b_S is the Burgers vector of the slip dislocation, and S_{Sfr} is the Peierls stress for slip dislocation. The value of S_{Sfr} in Eq. (4) can be estimated according to Ref. [39] as follows: $S_{Sfr} \propto 10^{-4}G$ (it is much greater than a lattice friction stress for the twinning dislocation and could not be neglected). Eqs. (3) and (4) allow to obtain the upper critical grain sizes d_{crit2} above which the nanotwinning does not occur that can be estimated from the condition $\sigma_T=\sigma_S$. If $S_{Sfr}d/Gb_S \ll 1$ (usually this demand is fulfilled in the nc materials), one can get the following