

NUCLEATION OF NANOGRAINS THROUGH STRESS-DRIVEN MIGRATION AND SPLITTING OF GRAIN BOUNDARIES IN NANOMATERIALS AND GUM METALS

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Abstract. A theoretical model is suggested which describes the generation of nanoscale grains due to stress-driven splitting and migration of grain boundaries in nanomaterials and Gum metals. In the framework of the suggested model, the stress-driven splitting and migration of grain boundaries are described as those related to transformations of grain boundary disclinations. The energy and stress characteristics for generation of nanoscale grains through stress-driven splitting and migration of grain boundaries in nanocrystalline aluminium, nanocrystalline nickel, and Gum metal with the Ti–Nb–Ta–Zr–O composition are calculated.

1. INTRODUCTION

Nanocrystalline and ultrafine-grained materials (hereinafter called nanomaterials) exhibit excellent mechanical properties due to the nanoscale and interface effects; see, e.g., reviews [1–7]. In particular, following experimental data, computer simulations and theoretical models, ultrasmall sizes of grains and extremely large amounts of grain boundaries (GBs) in nanomaterials are responsible for the operation of specific GB deformation mechanisms in such materials; see, e.g., [1–20]. One of such specific deformation mechanisms is the stress-driven GB migration that typically leads to grain growth [21–33]. However, theoretical studies [34,35] demonstrated that stress-driven GB migration can lead to the formation of new nanoscopic grains in nanomaterials, but not only to the growth of the existing grains.

The results of these studies are well consistent with the experimental observations [36–39] of the deformation-induced formation of finest nanograins,

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their chains and other groups in nanomaterials (see also computer simulations [40,41]). Previous theoretical works [34,35] examined the situation where nanograin nucleation is initiated by preceding GB sliding, which creates disclination dipoles that split in the course of nanograin nucleation. However, disclination ensembles capable of initiating the nanograin nucleation can also be resulted from the preceding stress-driven GB migration, but not only GB sliding. The main aim of this paper is to suggest a theoretical model describing the nucleation of new nanograins near the disclination quadrupoles generated due to the stress-driven GB migration in nanomaterials.

2. NANOGRAIN NUCLEATION INDUCED BY GRAIN BOUNDARY MIGRATION

We now consider a two-dimensional model of the deformed nanocrystalline solid with model rectan-

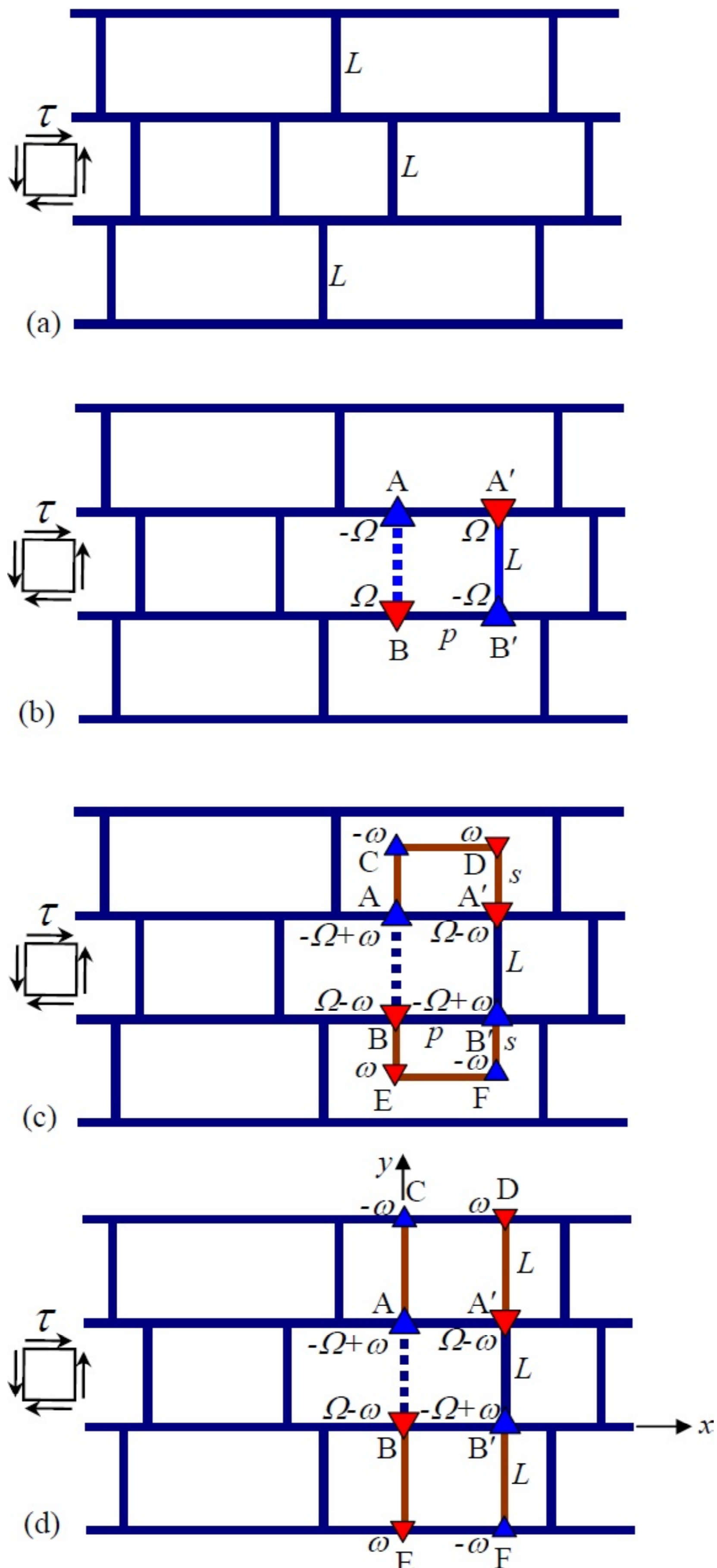


Fig. 1. Stress-driven migration of grain boundaries and generation of new nanograins in a nanocrystalline solid. (a) Model nanocrystalline specimen with rectangular grains. (b) Tilt boundary AB migrates to a new position $A'B'$, resulting in the formation of a quadrupole of wedge disclinations with the strengths $\pm\Omega$. (c) Grain boundaries AA' and BB' split into new immobile grain boundaries AA' and BB' and moving grain boundaries CD and EF . The splitting process is accompanied by the splitting of the disclination dipoles AA' and BB' (into two new immobile disclination dipoles AA' and BB' of the $\pm(\Omega - \omega)$ -disclinations and two moving dipoles, CD and EF , of the $\pm\omega$ -disclinations) and results in the formation of the new nanograins $ACDA'$ and $BEFB'$. (d) Grain boundaries CD and EF migrate further, leading to nanograin expansion, until they stop at other GBs.

gular grains of the width L (Fig. 1a). Let us assume that GB AB (that is supposed to be a tilt boundary) migrates over a distance p to its new position $A'B'$ under the action of a high uniform shear stress τ acting in the nanocrystalline solid (Fig. 1b). Following Refs. [23,28], the migration of a tilt boundary leads to the formation of a quadrupole of wedge disclinations at the points A, B, A' , and B' , whose strengths $\pm\Omega$ depend on the misorientation of the migrating boundary (Fig. 1b). In the case illustrated in Fig. 1b, the arms of the quadrupole $ABB'A'$ are equal to L and p . In the examined situation, the GB $A'B'$ is supposed to migrate until it either reaches its equilibrium position or approaches an opposite GB that can retard its further migration.

We also assume that the GB AA' (supposed to be a tilt boundary) under the action of the shear stress τ splits into two GBs: an immobile GB at the line AA' , and a migrating GB CD . Similarly, we suppose that the shear stress τ causes the tilt boundary BB' to split into a new immobile GB BB' and a migrating GB EF . As it has been shown previously [34,35], such a splitting process should be accompanied by a splitting of the wedge disclinations at the points A, B, A' , and B' , resulting in the formation of four wedge disclination dipoles: two immobile disclination dipoles, AA' and BB' , containing the disclinations with the strengths $\pm(\Omega - \omega)$ and two mobile disclination dipoles, CD and EF , comprising the disclinations with the strengths $\pm\omega$ (Fig. 1c). The mobile GBs, CD , and EF , can migrate until they either reach their equilibrium positions (Fig. 1c) or approach the opposite GBs (Fig. 1d) that block their further motion.

Let the distance traveled by the GBs CD and EF be the same and equal to s . Then the migration of the GBs CD and EF leads to the formation of four new GBs, $AC, A'D, BE$, and $B'F$ of length s (Fig. 1c). For simplicity, we assume that the GBs AA' and BB' are high-angle ones (both prior to and after their splitting), and their specific inelastic energy (per unit area) does not change due to their splitting. We also assume that the mobile GBs CD and EF are low-angle ones. (This assumption corresponds to the experimental observations [37,38] of the generation of nanograins and nanograin chains with low-angle GBs inside nanograins with high-angle GBs in nanocrystalline solids.) Then the GBs $AC, A'D, BE$, and $B'F$ are also low-angle ones, and the energy of all the above low-angle GBs, including the GBs CD and EF , does not incorporate any inelastic terms.

Thus, due to the splitting of the GBs AA' and BB' , followed by the migration of GBs CD and EF , two new nanograins $ACDA'$ and $BEFB'$ are gener-

ated (Figs. 1c and 1d). The nucleation of these new nanograins is accompanied by the formation of the defect configuration that comprises two quadrupoles, $ABB'A'$ and $CEFD$, of wedge disclinations with the strengths $\pm(\Omega-\omega)$ and $\pm\omega$, respectively (Figs. 1c and 1d).

3. ENERGY AND CRITICAL STRESSES FOR NANOGRAIN NUCLEATION

Let us calculate the energy specifying the formation of two new nanograins, $ACDA'$ and $BEFB'$ (Figs. 1c and 1d). The splitting of the disclination dipoles AA' and BB' and associated formation of new nanograins are characterized by the energy change $\Delta W = W_2 - W_1$, where W_1 and W_2 are the energies of the specimen before and after the splitting of the disclination dipoles AA' and BB' , respectively, that is, the energies of the specimen containing the disclination quadrupole $ABB'A'$ (Fig. 1b) and that containing two disclination quadrupoles, $ABB'A'$ and $CEFD$ (Figs. 1c and 1d), respectively. For simplicity, we assume that the specific energy (per unit area) of the GBs AA' and BB' does not change after their splitting. Then the expression for the energy variation ΔW can be presented as follows:

$$\Delta W = E_s^\omega + E_s^{\Omega-\omega} - E_s^\Omega + E_i^{\omega-(\Omega-\omega)} - A_\Sigma^\tau, \quad (1)$$

where E_s^Ω , E_s^ω , and $E_s^{\Omega-\omega}$ are the self-energies of the quadrupoles of the disclinations with the strengths $\pm\Omega$, $\pm\omega$, and $\pm(\Omega-\omega)$, respectively, $E_i^{\omega-(\Omega-\omega)}$ is the energy of the elastic interaction between the quadrupoles of the disclinations with the strengths $\pm\omega$ and $\pm(\Omega-\omega)$, and A_Σ^τ is the sum work spent by the external stress τ to the motion of the disclination dipoles CD and EF over the distance s .

In the isotropic approximation, the self-energies E_s^Ω , E_s^ω , and $E_s^{\Omega-\omega}$ of the disclination quadrupoles are given by [42]:

$$E_s^\Omega = \frac{D\Omega^2 L^2}{2} \left[\left(1 + \frac{\rho^2}{L^2} \right) \ln \left(1 + \frac{\rho^2}{L^2} \right) - \frac{\rho^2}{L^2} \ln \frac{\rho^2}{L^2} \right], \quad (2)$$

$$E_s^\omega = \frac{D\omega^2 (2s+L)^2}{2} \left[\left(1 + \frac{\rho^2}{(2s+L)^2} \right) \times \ln \left(1 + \frac{\rho^2}{(2s+L)^2} \right) - \frac{\rho^2}{(2s+L)^2} \ln \frac{\rho^2}{(2s+L)^2} \right], \quad (3)$$

$$E_s^{\Omega-\omega} = \frac{D(\Omega-\omega)^2 L^2}{2} \times \left[\left(1 + \frac{\rho^2}{L^2} \right) \ln \left(1 + \frac{\rho^2}{L^2} \right) - \frac{\rho^2}{L^2} \ln \frac{\rho^2}{L^2} \right], \quad (4)$$

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

The energy $E_s^{\omega-(\Omega-\omega)}$ of the elastic interaction between the disclination quadrupoles $ABB'A'$ and $CEFD$ can be presented [42] as

$$E_s^{\omega-(\Omega-\omega)} = -(\Omega-\omega) \int_0^{\rho} \int_0^L \sigma_{xy}^\omega(x,y) dy dx, \quad (5)$$

where $\sigma_{xy}^\omega(x,y)$ is the xy -component of the stress field created by the disclination quadrupole $CEFD$ shown in Fig. 1c in the Cartesian coordinate system (x,y) shown in Fig. 1d. The expression for the stress $\sigma_{xy}^\omega(x,y)$ follows [42] as

$$\sigma_{xy}^\omega = D\omega \left(\frac{x(y-s-L)}{x^2 + (y-s-L)^2} + \frac{(x-\rho)(y+s)}{(x-\rho)^2 + (y+s)^2} - \frac{(x-\rho)(y-s-L)}{(x-\rho)^2 + (y-s-L)^2} - \frac{x(y+s)}{x^2 + (y+s)^2} \right). \quad (6)$$

The sum work A_Σ^τ spent by the external shear stress τ on the motion of the disclination dipoles CD and EF over the distance s is given [42] as

$$A_\Sigma^\tau = 2\tau\omega\rho s. \quad (7)$$

Formulas (1) to (7) allow one to get an expression for the energy change ΔW . The generation and growth of new nanograins (resulting in an increase of the parameter s from zero to its maximum value) is favored, if the relation $\partial\Delta W(s)/\partial s < 0$ is valid. Our calculations demonstrated that, if the relation is satisfied at $s = 0$, it continues to be valid at any larger values of s , for any values of other parameters. This means that, if the new grains are energetically favored to nucleate, they are always favored to grow further. Therefore, the nucleated grains expand until their migrating GBs CD and EF reach the pre-existent immobile GBs, which are assumed to block migration of GBs CD and EF . That is, the motion of the GBs CD and EF stops at $s = L$ (Fig. 1d). Thus, the relation $(\partial\Delta W(s)/\partial s)|_{s=0} < 0$ gives the criterion for both the nucleation of two new nanograins

and their growth until their characteristic size (equal to the migration distance of GBs CD and EF) s reaches value of $s = L$.

With formulas (1)–(7), the relation $(\partial\Delta W(s)/\partial s)|_{s=0} < 0$ can be rewritten as $\tau > \tau_{c1}$, where

$$\tau_{c1} = \frac{1}{2\omega\rho} \frac{\partial}{\partial s} \left(E_s^\omega + E_i^{\omega-(\Omega-\omega)} \right) \Big|_{s=0}. \quad (8)$$

Formula (8) demonstrates that the critical stress τ_{c1} depends on the distance p of the GB AB migration (Fig. 1b) which precedes the splitting and migration of the GBs CD and EF . Previous calculations [23] demonstrated that a migrating GB can stop at its equilibrium position, if $p/L < 0.505$. When $p/L > 0.505$, such a GB exhibits the "unlimited" migration, in which case its motion can only be stopped by other GBs. For simplicity, here we focus our examination on the case situation where the migrating GB AB stops at its equilibrium position, that is, the situation where $p/L < 0.505$. In this situation, the stress τ needed to move the GB AB over a distance p follows [23] as $\tau = \tau_{c2}$, where

$$\tau_{c2} = \frac{D\Omega p}{L} \ln \left(1 + \frac{L^2}{p^2} \right). \quad (9)$$

With formulas (8) and (9), we now plot the dependences $\tau_{c1}(p)$ and $\tau_{c2}(p)$ in the exemplar cases of nanocrystalline metals (Al and Ni) and nanocrystalline Ti alloy (Ti–Nb–Ta–Zr–O) called "Gum metal". These materials are characterized by the following elastic moduli: for Al, $G = 27$ GPa and $\nu = 0.34$ [43]; for Ni, $G = 73$ GPa and $\nu = 0.31$ [43]; for Gum metal, $G = 9$ GPa and $\nu = 0.3$ [44]. The dependences $\tau_{c1}(p)$ and $\tau_{c2}(p)$ are shown in Fig. 2, for $L = 50$ nm, $\Omega = 10^\circ$ and various values of ω . As it follows from Fig. 2, the critical stresses τ_{c1} and τ_{c2} increase with an increase in p . Fig. 2 also clearly demonstrates that, for Al, Ni and Gum metal, we always have: $\tau_{c1} < \tau_{c2}$. This implies that, if a tilt GB migrates under the applied shear stress, it can lead to the formation and motion of new low-angle GBs resulting in the generation and expansion of new nanograins.

4. CONCLUDING REMARKS

Thus, in this paper, we have suggested a theoretical model of stress-driven nanograin nucleation in nanocrystalline solids and Gum metals, resulting from preceding GB migration. We have calculated the critical parameters for nanograin nucleation and expansion. It is found that, if new nanograins nucle-

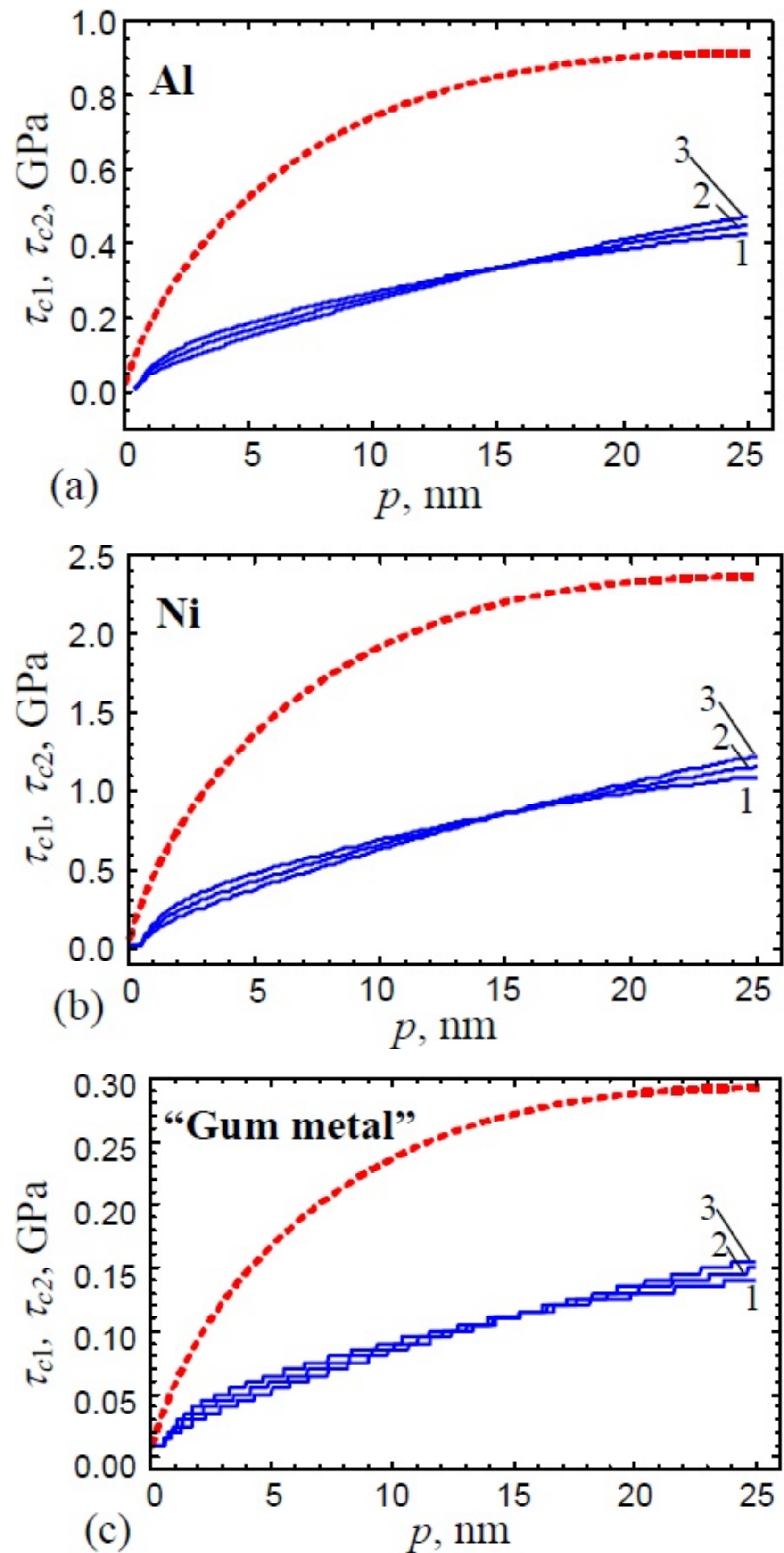


Fig. 2. Dependences $\tau_{c1}(p)$ (solid curves) and $\tau_{c2}(p)$ (dashed curves) for nanocrystalline Al (a), Ni (b) and Ti alloy "Gum metal" (c) at $\omega = 3, 5,$ and 7° (curves 1, 2, and 3, respectively, in figures (a-c)).

ate, they expand until their moving GBs reach the pre-existent GBs that block them and thereby stop expansion of the new nanograins. Also, our calculations demonstrated that the critical stress for the formation of new nanograins with the migrating low-angle tilt boundaries is always smaller than the critical stress for GB migration that precedes nanograin nucleation. Thus, if a tilt GB migrates under the applied shear stress, it can also result in the formation of new nanograins. This result explains the experimental observations [36–39] of the deformation-induced formation of nanograins and their groups in nanomaterials.

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