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Emission of partial dislocations from triple junctions of grain boundaries in nanocrystalline materials

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Abstract
A theoretical model is suggested that describes emission of partial Shockley dislocations from triple junctions of grain boundaries (GBs) in deformed nanocrystalline materials. In the framework of the model, triple junctions accumulate dislocations due to GB sliding along adjacent GBs. The dislocation accumulation at triple junctions causes partial Shockley dislocations to be emitted from the dislocated triple junctions and thus accommodates GB sliding. Ranges of parameters (applied stress, grain size, etc) are calculated in which the emission events are energetically favourable in nanocrystalline Al, Cu and Ni. The model accounts for the corresponding experimental data reported in the literature.

1. Introduction

Nanocrystalline materials (NCMs) exhibit outstanding mechanical properties that represent the subject of rapidly growing research efforts in applied physics, materials science and technology, e.g. [1–24]. The unique deformation behaviour of NCMs is strongly influenced by grain boundaries (GBs) whose volume fraction is extremely high in these materials. For example, GBs serve as channels for such deformation modes as GB sliding [9–15], Coble creep [16–18], triple junction diffusional creep [19] and rotational deformation [20–26] in NCMs with the finest grains. As shown in recent experiments [4–8], GBs generate partial dislocations which carry twin deformation in nc-metals. Experimental data [5–8] are indicative that twinning plays the dominant role in plastic flow in nc-metals fabricated by the cryomilling method. Chen *et al* [4] reported that the partial dislocation slip occurs at lower shear stresses compared with the perfect dislocation slip in grains having a size smaller than some critical value. In this case, the shear stress needed to activate the partial dislocation sources at GBs controls the flow stress in NCMs deformed through emission and movement of partial dislocations, carriers of deformational twinning. Therefore, it is important to identify the nature of GB sources of partial dislocations in deformed NCMs. Recent theoretical models [27,28] have described such sources as both GB disclinations and intrinsic GB dislocations. Besides GB disclinations and intrinsic GB dislocations responsible for misorientation mismatch at high-angle GBs, mobile GB dislocations often exist in GBs and carry GB sliding in deformed NCMs. Mobile GB dislocations are stopped by and stored at triple junctions of GBs. In these circumstances, dislocated triple junctions whose density is extremely high in NCMs can serve as effective sources of lattice dislocations. The main aim of this paper is to suggest a theoretical model describing emission of partial lattice dislocations from triple junctions of GBs as a process occurring due to GB sliding and providing its effective accommodation in deformed NCMs.

2. Model

GB sliding is treated as very essential in NCMs with the finest grains [3, 9–15] and even dominant in NCMs showing superplasticity [3, 13, 29, 30]. The evolution of defect ensembles at GBs and their triple junctions crucially affects GB sliding and its accommodation. For illustration, let us consider a fragment of GB ensemble (figure 1(*a*)) in a mechanically loaded NCM where GB sliding contributes highly to plastic deformation. This fragment contains three triple junctions A, O and B of GBs. Following a theoretical description [13] of GB sliding in NCMs, the triple junction O is an obstacle for GB sliding along the boundaries AO and OB. As a corollary,

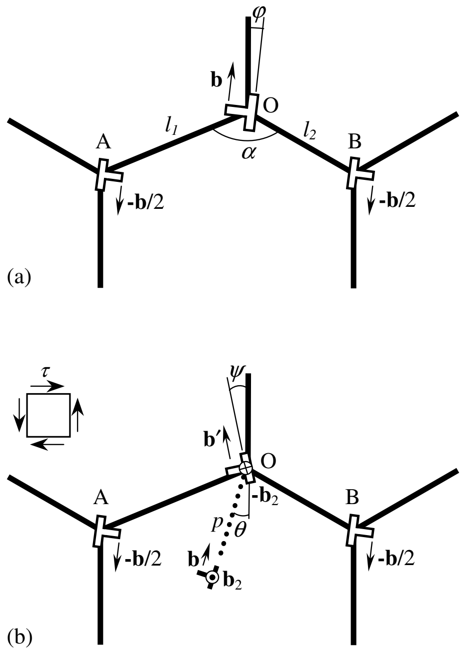

Figure 1. Dislocation configurations in a NCM where GB sliding occurs. (*a*) Initial configuration with sessile dislocations (resulted from GB sliding) at the triple junctions A, O and B. (*b*) Shockley partial dislocation is emitted from the triple junction O.

the GB sliding induces the formation of a sessile dislocation at the triple junction O. The dislocation has the Burgers vector $\boldsymbol{b}$ with orientation specified by the angle φ. Hereinafter the triple junction dislocation is called $\boldsymbol{b}$-dislocation. The triple junction geometry is characterized by the angle α between the boundaries AO and OB having the lengths l_1 and l_2, respectively. For definiteness, the latter are assumed to be equal, i.e. $l_1 = l_2$.

The triple junctions A and B (figure 1(*a*)) also conduct GB sliding and thereby contain dislocations formed due to GB sliding. In the framework of our model, GB sliding is enhanced at the triple junction O (because of its geometry and/or other factors), in which case the Burgers vector magnitude b of its dislocation is larger than the Burgers vector magnitudes of the dislocations formed at the triple junctions A and B. For simplicity of our further calculations, we assume that the dislocations at the triple junctions A and B are characterized by identical Burgers vectors $-\boldsymbol{b}/2$, whose sum is equal by magnitude and opposite in sign to the Burgers vector $\boldsymbol{b}$. Therefore the sum stress fields of the dislocations shown in figure 1(*a*) are screened at the screening length R of the order of a grain size. This statement corresponds to the common viewpoint that the grain size d is a characteristic length scale in nc-structures.

GB sliding leads to both a gradual increase of the Burgers vector $\boldsymbol{b}$ and thereby an increase in the total energy of the defect system (figure 1(*a*)). One of the effective channels of the energy relaxation is the transformation of the $\boldsymbol{b}$-dislocation through emission of a dislocation into the adjacent grain interior (figure 1(*b*). This relaxation mechanism competes with the nanocrack generation at triple junctions (see experimental data [31] and a theoretical model [32]) and thereby enhances the ductility of an NCM. In addition, such a relaxation mechanism accounts for experimental observation [4–8] of partial dislocations carrying deformation twinning in NCMs.

In the framework of our model, the $\boldsymbol{b}$-dislocation splits into an immobile triple junction dislocation with the Burgers vector $\boldsymbol{b}-\boldsymbol{b}_e$ and a mobile Shockley partial dislocation with the Burgers vector $\boldsymbol{b}_e = a\,[112]/6$ (here a is the fcc crystal lattice parameter) and moves into the grain interior (figure 1(*b*)). As a result, a new defect configuration is formed at and near the triple junction O. For convenience of our further calculations, it is represented as an edge dislocation with the Burgers vector $\boldsymbol{b}'$ at the triple junction O, an edge partial dislocation with the Burgers vector $\boldsymbol{b}_1$ and a dipole of screw partial dislocations with the Burgers vectors $\pm\boldsymbol{b}_2$. The edge $\boldsymbol{b}'$- and screw $-\boldsymbol{b}_2$-dislocations form a residual triple junction dislocation with the Burgers vector $\boldsymbol{b} - \boldsymbol{b}_e$. The edge $\boldsymbol{b}_1$- and screw $\boldsymbol{b}_2$-dislocations form a moving Shockley dislocation. The stacking fault of the length p is formed behind the Shockley partial dislocation moved by the distance p. The dislocation slip plane orientation is characterized by the angle θ made by the slip plane and plane of the 'upper' GB adjacent to the triple junction O. Notice that the sum Burgers vector of the dislocation configuration shown in figure 1(*b*) is zero-vector, as is the case with the initial dislocation configuration shown in figure 1(*a*).

Consider the energy difference that characterizes emission of a Shockley partial dislocation from a triple junction. The emission is energetically favourable if the total energy (per unit length of a dislocation) W_2 of the defect system after the emission (figure 1(*b*)) is lower than the total energy W_1 before the emission (figure 1(*a*)): $\Delta W = W_2 - W_1 < 0$.

The total energy W_1 of the defect system in its initial state (figure 1(*a*)) consists of the five terms:

$$W_1 = E^b_{\text{self}} + 2E^{b/2}_{\text{self}} + E^{b-(b/2)}_{\text{int A}} + E^{b-(b/2)}_{\text{int B}} + E^{(b/2)-(b/2)}_{\text{int}}, \quad (1)$$

where E^b_{self} and $E^{b/2}_{\text{self}}$ are the self energies of the $\boldsymbol{b}$- and $(\boldsymbol{b}/2)$-dislocations, respectively; $E^{b-(b/2)}_{\text{int A}}$ and $E^{b-(b/2)}_{\text{int B}}$ are the energies of elastic interaction of the $\boldsymbol{b}$-dislocation with the $(\boldsymbol{b}/2)$-dislocations located at the triple junctions A and B, respectively; and $E^{(b/2)-(b/2)}_{\text{int}}$ is the energy of elastic interaction between these $(\boldsymbol{b}/2)$-dislocations. The self energies of the $\boldsymbol{b}$- and $(\boldsymbol{b}/2)$-dislocations are given by the following standard expressions [33]:

$$E^b_{\text{self}} = \frac{Db^2}{2}\left(\ln\frac{R}{r} + 1\right), \qquad E^{b/2}_{\text{self}} = \frac{Db^2}{8}\left(\ln\frac{R}{r/2} + 1\right). \quad (2)$$

Here $D = G/[2\pi(1-\nu)]$, G is the shear modulus, ν is the Poisson ratio, $r \approx b$ is the core radius of the $\boldsymbol{b}$-dislocation, R is the screening length for the dislocation stress fields. Since the sum Burgers vector of the dislocation configuration shown in figure 1(*a*) is zero-vector, R is of the order of the grain size d. For definiteness, we assume that $R \approx 2d$.

Each of the interaction energies $E^{b-(b/2)}_{\text{int A}}$, $E^{b-(b/2)}_{\text{int B}}$ and $E^{(b/2)-(b/2)}_{\text{int}}$ is calculated in the standard way [34] as the work spent to generate one dislocation in the stress field of the other. In doing so, we find

$$\begin{aligned} E^{b-(b/2)}_{\text{int A}} &= -Db^2\,\Phi(x_1, y_1)/4, \\ E^{b-(b/2)}_{\text{int B}} &= -Db^2\,\Phi(x_2, y_2)/4, \\ E^{(b/2)-(b/2)}_{\text{int}} &= Db^2\,\Phi(x_3, y_3)/8, \end{aligned} \quad (3)$$

where

$$\Phi(x,y) = \ln\frac{(R+x)^2+y^2}{x^2+y^2} - \frac{2R(R+2x)y^2}{((R+x)^2+y^2)(x^2+y^2)},$$

$x_1 = l_1\cos(\alpha/2-\varphi)$, $y_1 = l_1\sin(\alpha/2-\varphi)$, $x_2 = l_2\cos(\alpha/2+\varphi)$, $y_2 = l_2\sin(\alpha/2+\varphi)$, $x_3 = x_1 - x_2$, $y_3 = y_1 + y_2$.

The total energy of the defect system after emission of the Shockley dislocation (figure 1(*b*)) consists of the twelve terms:

$$W_2 = E^{b'}_{\rm self} + 2E^{b/2}_{\rm self} + E^{b_1}_{\rm self} + E^{b_2}_{\rm self} + E^{b'-(b/2)}_{\rm int\,A} + E^{b'-(b/2)}_{\rm int\,B} + E^{(b/2)-(b/2)}_{\rm int} + E^{b_1-(b/2)}_{\rm int\,A} + E^{b_1-(b/2)}_{\rm int\,B} + E^{b_1-b'}_{\rm int} + E_\tau + E_\gamma. \quad (4)$$

Here $E^{b'}_{\rm self}$, $E^{b/2}_{\rm self}$, $E^{b_1}_{\rm self}$ and $E^{b_2}_{\rm self}$ are the self energies of the $\boldsymbol{b}'$-dislocation, $(\boldsymbol{b}/2)$-dislocation, $\boldsymbol{b}_1$-dislocation and the dipole of screw $\pm\boldsymbol{b}_2$-dislocations, respectively; $E^{b'-(b/2)}_{\rm int\,A}$, $E^{b'-(b/2)}_{\rm int\,B}$ are the energies of elastic interaction between the $\boldsymbol{b}'$-dislocation and $(\boldsymbol{b}/2)$-dislocations located at the triple junctions A and B, respectively; $E^{(b/2)-(b/2)}_{\rm int}$ is the energy of elastic interaction between these $(\boldsymbol{b}/2)$-dislocations; $E^{b_1-b'}_{\rm int}$, $E^{b_1-(b/2)}_{\rm int\,A}$ and $E^{b_1-(b/2)}_{\rm int\,B}$ are the energies of elastic interaction of the emitted Shockley $\boldsymbol{b}_1$-dislocation with the $\boldsymbol{b}'$- and $(\boldsymbol{b}/2)$-dislocations; E_τ is the external shear stress τ work spent to move the Shockley dislocation by the distance p; and E_γ is the specific energy of the stacking fault formed behind the Shockley partial dislocation. The magnitude b' and orientation angle ψ of the Burgers vector $\boldsymbol{b}'$ of the residual triple junction dislocation are given by $b' = \sqrt{b^2+b_1^2-2bb_1\cos(\theta-\varphi)}$ and $\psi = \arcsin\{(b_1/b')\sin(\theta-\varphi)\} - \varphi$. The self energy $E^{b/2}_{\rm self}$ is still determined by equation (2). The self energies $E^{b'}_{\rm self}$ and $E^{b_1}_{\rm self}$ read [33]

$$E^{b'}_{\rm self} = \frac{Db'^2}{2}\left(\ln\frac{R}{r'}+1\right), \qquad E^{b_1}_{\rm self} = \frac{Db_1^2}{2}\left(\ln\frac{R}{r_1}+1\right), \quad (5)$$

where $r' \approx b'$ and $r_1 \approx b_1$ are the core radii of the $\boldsymbol{b}'$- and $\boldsymbol{b}_1$-dislocations, respectively. The self energy of the dipole of screw $\pm\boldsymbol{b}_2$-dislocations is calculated as the work spent to generate the dipole in its proper stress field. As a result, we have

$$E^{b_2}_{\rm self} = D(1-\nu)b_2^2\left(\ln\frac{p-r_2}{r_2}+1\right), \quad (6)$$

where $r_2 \approx b_2$ is the core radius of the $\boldsymbol{b}_2$-dislocation.

The interaction energies $E^{b'-(b/2)}_{\rm int\,A}$, $E^{b'-(b/2)}_{\rm int\,B}$, $E^{b_1-b'}_{\rm int}$, $E^{b_1-(b/2)}_{\rm int\,A}$ and $E^{b_1-(b/2)}_{\rm int\,B}$ are calculated in a similar way as formulae (3). In doing so, we find

$$E^{b'-(b/2)}_{\rm int\,A} = -\frac{Db'b}{2}\Psi(x_1', -y_1', \varphi+\psi),$$
$$E^{b'-(b/2)}_{\rm int\,B} = -\frac{Db'b}{2}\Psi(x_2', y_2', \varphi+\psi),$$
$$E^{b_1-b'}_{\rm int} = Db'b_1\Psi(x', -y', \theta+\psi), \quad (7)$$
$$E^{b_1-(b/2)}_{\rm int\,A} = -\frac{Dbb_1}{2}\Psi(-\tilde{x}_1, -\tilde{y}_1, \theta-\varphi),$$
$$E^{b_1-(b/2)}_{\rm int\,B} = -\frac{Dbb_1}{2}\Psi(\tilde{x}_2, \tilde{y}_2, \theta-\varphi),$$

where

$$\Psi(x,y,\tilde\theta) = \frac{\cos\tilde\theta}{2}\ln\frac{(R+x)^2+y^2}{x^2+y^2} - \frac{y(x\sin\tilde\theta + y\cos\tilde\theta)}{x^2+y^2} + \frac{y[(R+x)\sin\tilde\theta + y\cos\tilde\theta]}{(R+x)^2+y^2},$$

$x_1' = x_1(\varphi\to-\psi)$, $y_1' = y_1(\varphi\to-\psi)$, $x_2' = x_2(\varphi\to-\psi)$, $y_2' = y_2(\varphi\to-\psi)$, $x' = p\cos(\theta+\psi)$, $y' = p\sin(\theta+\psi)$, $\tilde{x}_1 = x'(\psi\to-\varphi) - x_1$, $\tilde{y}_1 = y_1 - y'(\psi\to-\varphi)$, $\tilde{x}_2 = x_2 - x'(\psi\to-\varphi)$, $\tilde{y}_2 = y_2 + y'(\psi\to-\varphi)$. The energy terms E_τ and E_γ are given by evident formulae

$$E_\tau = -bp\tau\cos 2\theta, \qquad E_\gamma = p\gamma. \quad (8)$$

3. Results

Formulae (1)–(8) allow us to calculate the characteristic energy difference ΔW and its dependence on p, the distance moved by the Shockley partial dislocation emitted from a dislocated triple junction (figure 1(*b*)). The partial dislocation emission is energetically favourable if $\Delta W < 0$. The dependences $\Delta W(p)$ for different values of the shear stress τ are shown in figure 2, for Al, Cu and Ni. We used the following characteristic values of parameters [24, 33]. For Al: $G = 27$ GPa, $\nu = 0.31$, Burgers vector magnitudes $b_1 \approx 0.143$ nm and $b_2 \approx 0.022$ nm, and the stacking fault energy $\gamma = 120\,\mathrm{mJ\,m^{-2}}$. For Cu: $G = 44$ GPa, $\nu = 0.38$, $b_1 \approx 0.128$ nm, $b_2 \approx 0.02$ nm and $\gamma = 45\,\mathrm{mJ\,m^{-2}}$. For Ni: $G = 73$ GPa, $\nu = 0.34$, $b_1 \approx 0.125$ nm, $b_2 \approx 0.019$ nm and $\gamma = 183\,\mathrm{mJ\,m^{-2}}$. The Burgers vector magnitude b of the triple junction dislocation was taken as the minimum critical magnitude $b_{\rm crit}$ at which the emission is energetically favourable. In the case under consideration, for nanocrystalline Al, Cu and Ni, we used $b_{\rm crit} \approx 0.25$ nm at the angle $\varphi = 0°$. The triple junction angle α and GB lengths were taken as $\alpha = 120°$ and $l_1 = l_2 = 30$ nm. The angle θ of orientation of the $\boldsymbol{b}_1$-dislocation glide plane was chosen as that corresponding to the most favourable emission of this dislocation ($\theta \approx 5°$).

As follows from the dependences $\Delta W(p)$ shown in figure 2, the energy gain due to the Shockley dislocation emission (figure 1(*b*)) in Cu is larger than that in Ni, which in its turn is larger than that in Al at the same level of τ. In most cases, there is an equilibrium distance $p_{\rm eq}$ moved by the Shockley dislocation; it corresponds to the minimum of the function $\Delta W(p)$. The only exception is the case of Cu at $\tau_{\rm crit} \approx 450$ MPa (figure 2(*b*), curve 5), in which $\Delta W(p)$ gradually decreases with rising p and, as a corollary, the Shockley dislocation moves across the grain interior towards a GB opposite the triple junction O. Also, in Cu, the partial dislocation is characterized by the largest values of the equilibrium distance $p_{\rm eq}$ for $\tau = 50$, 150, 250 and 350 MPa, compared with the corresponding distances in Al and Ni (figures 2(*a*) and (*c*), respectively). It is explained by the fact that Cu is characterized by the lowest value of the stacking fault energy specifying the hampering force for the Shockley dislocation emission.

It is evident that the equilibrium distance $p_{\rm eq}$ grows with rising τ. We have calculated the dependences of $p_{\rm eq}$ on the grain size d for different levels of τ (figure 3). In the framework

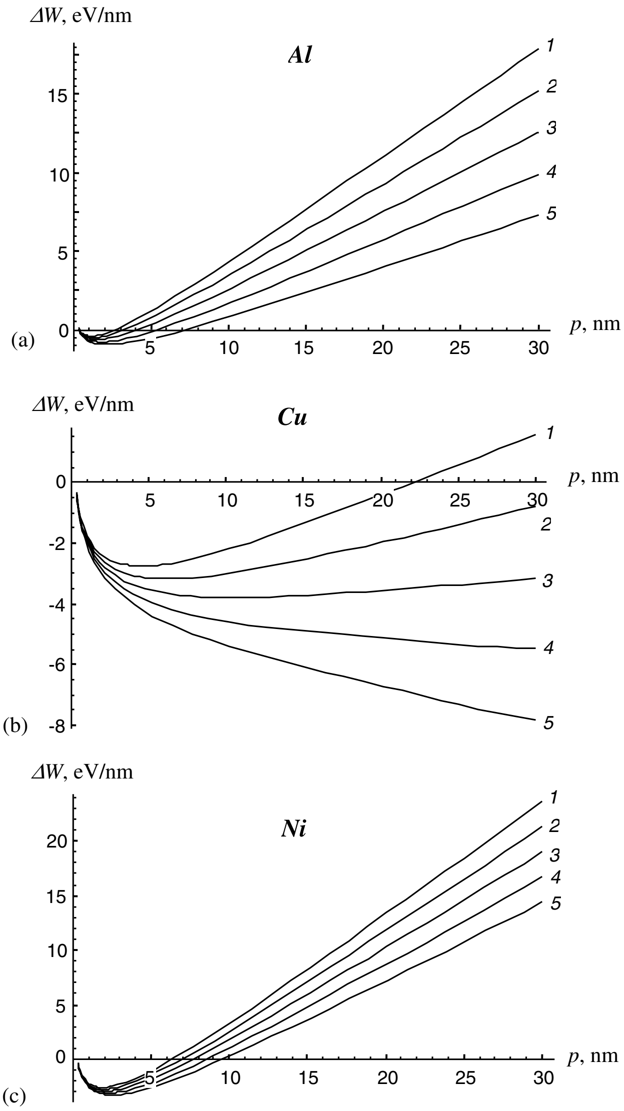

Figure 2. Dependence $\Delta W(p)$ at the shear stress values $\tau = 50$ (curve 1), 150 (2), 250 (3), 350 (4) and 450 MPa (5) for (*a*) Al, (*b*) Cu and (*c*) Ni.

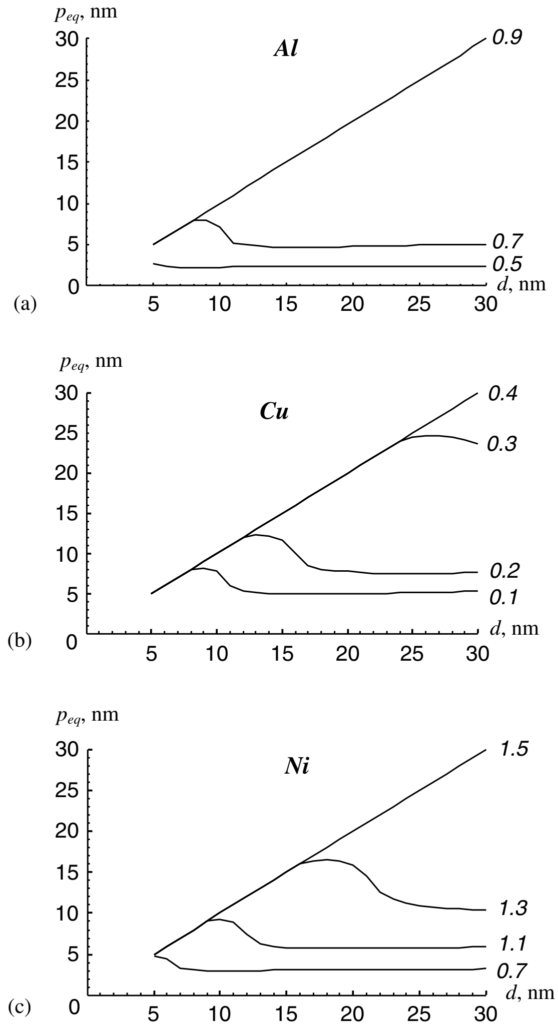

Figure 3. Dependences of the equilibrium distance p_{eq} (moved by the emitted partial dislocation) on the grain size d at the different shear stress τ values shown in gigapascal units at the curves for (*a*) Al, (*b*) Cu and (*c*) Ni.

of our model, d plays the role of the effective screening length for the dislocation configuration under consideration (figure 1) and thus is involved in consideration. As is shown in figure 3, the emitted partial dislocation can achieve the opposite GB (thus crossing the grain body, when $p_{\text{eq}} = d$) under the following minimal values of the external shear stress: $\tau \approx 900$ MPa in Al, 400 MPa in Cu and 1500 MPa in Ni.

4. Concluding remarks

In this paper, it has been shown theoretically that the emission of partial dislocations from triple junctions of GBs is energetically favourable in NCMs where GB sliding contributes to plastic flow. In such NCMs, GB sliding leads to storage of GB dislocations at triple junctions (figure 1(*a*)) and gradual increase of the system strain energy. The energy can effectively relax through the emission of Shockley partial dislocations into the adjacent grain interior (figure 1(*b*)). This theoretical statement accounts for experimental observations [4–8] of partial dislocations carrying deformation twinning in NCMs. Following the results of our model, the partial dislocation emission from triple junctions is enhanced in nc-Cu, compared with nc-Ni and Al (figures 2 and 3). It is naturally explained by the fact that Cu is characterized by the very low stacking fault energy specifying the hampering force for the emission.

It is worth noting that this conclusion does not mean that nc-Cu is more plastically deformable than nc-Al. It concerns only the possibility of deforming through generation and propagation of partial dislocations. Under the shear stress $\tau < 900$ MPa, our model nc-Al should deform due to other mechanisms (say the motion of perfect dislocations) which can provide its relatively higher plasticity.

Emission of partial dislocations from triple junctions (figure 1(*b*)) competes with the generation of nanocracks there (see experimental data [31] and theoretical model [32]) and thereby enhances the ductility of an NCM. When the partial dislocation emission is enhanced, the emission events cause a decrease in the rate of the dislocation accumulation at triple junctions. As a result, the partial dislocation emission from triple junctions hampers the nanocrack generation and growth in the vicinities of triple junctions. This effect is worth being taken into account in the explanation of the experimentally observed [5–8] good ductility of NCMs (fabricated by the cryomilling method) showing the enhanced emission of partial dislocations from GBs.

Acknowledgments

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