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GRAIN BOUNDARY DISLOCATION STRUCTURES NEAR TRIPLE JUNCTIONS IN NANO- AND POLYCRYSTALLINE MATERIALS

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Abstract. A theoretical model is suggested which describes structural and behavioral features of grain boundary dislocation configurations near triple junctions in nano- and polycrystalline materials. With the elastic interaction between grain boundary dislocations taken into account, we have theoretically examined deviations of spatial arrangement of boundary dislocations near triple junctions, from a periodic arrangement. Also, the local migration of grain boundaries near their triple junctions has been theoretically described, induced by grain boundary sliding in mechanically loaded nano- and polycrystalline materials. In the framework of the model, the key driving force for the local migration is a release of the elastic energy of ensemble of gliding boundary dislocations (carriers of grain boundary sliding) and immobile boundary dislocations (associated with grain boundary misorientation). It is shown that migration is capable of effectively enhancing grain boundary sliding, in which case the combined effects of grain boundary sliding and migration near triple junctions cause plastic flow localization in fine-grained materials, reported in the literature.

1. INTRODUCTION

Grain boundaries (GBs) represent the traditional subject of intensive experimental and theoretical research due to their significant effects on the functional properties of nano- and polycrystalline materials, e.g., [1]. In recent years, triple junctions of GBs have been recognized as structural elements with the structure and properties being different from those of the GBs that they adjoin [2]. From experimental data and theoretical models it follows that triple junctions of GBs play the role as nuclei of the second phase segregation [3,4]; strengthening elements [5-8], carriers of enhanced diffusional creep [9] and sources of lattice dislocations during plastic deformation [10]; and drag centers of GB migration during re-crystallization processes [11]. This allows one to treat triple junctions of GBs as thermodynamically distinct phase, separate from grain interiors and GBs [2].

In general, the specific behavioral peculiarities of triple junctions are not related to only their specific structure and thermodynamics, but also to the specific structure of GBs near them. That is, GBs adjacent to a triple junction are capable of exhibiting the structure and behavior in the vicinity of the triple junction, which, generally speaking, are different from those of GB fragments essentially distant from the GB junction. The fact is that spatial arrangement of GB dislocations near a triple junction is capable of being essentially different from that far from the triple junction, because of the following factors: (i) the elastic interaction between GB dislocations (in particular, between dislocations belonging to different GBs); (ii) the edge effect related to a finite extent of adjacent GBs; (iii) the action of triple junctions as effective obstacles for motion of gliding GB dislocations, carriers of GB sliding.

Isolated aspects concerning the specific structural and behavioral features of GB dislocation struc-

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tures near triple junctions have been theoretically examined earlier. Thus, in paper [12] it has been theoretically revealed that a distribution of GB dislocations deviates from conventional periodic distribution, near a triple junction modeled as a disclinated termination point of GBs. The model [12] has focused, in fact, on finite extent of GBs and the role of triple junctions as termination points of finite GBs, in which case the elastic interaction between adjacent GBs (which is strong near triple junctions) and its dependence on dihedral angles between the GBs have been neglected. In addition, the model [12] has considered the discussed effect in only polycrystalline materials, dealing with continuous distributions of GB dislocations. Also, recently, a theoretical model of local migration of GBs near triple junctions in plastically deformed polycrystals has been suggested [5]. In doing so, Astanin et al [5] treat that the local migration of GBs in vicinities of triple junctions makes GBs to be curved, in which case the interspacings between gliding GB dislocations – carriers of GB sliding – stopped by a triple junction increase. This leads to a release of the elastic energy of these GB dislocations, which serves as the key driving force for the local GB migration. However, the viewpoint [5] does not take into account the effects of intrinsic immobile GB dislocations associated with GB misorientation on the local GB migration. At the same time, such immobile GB dislocations are known to strongly influence the GB behavior and often cause GB structural transformations; see, e.g., [13-16]. The main aim of this paper is to suggest a theoretical model that describes the specific structural and behavioral features of GB dislocation structures near triple junctions, with all the factors (i)-(iii) taken into account. The suggested model will operate with discrete distributions of GB dislocations, in which case its results are effective for a description of GB structures in nano- and polycrystalline materials.

2. GRAIN BOUNDARIES ADJACENT TO TRIPLE JUNCTION. DISLOCATION MODEL. ENERGETIC CHARACTERISTICS

Let us consider a model specimen of the cylindrical shape with radius R, containing the three GBs which form a triple junction at the cylinder center (Fig. 1). The ith GB (i = 1,2,3) contains $N_{(i)}$ GB dislocations with Burgers vectors perpendicular to boundary plane. Following the theory of GB dislocations [13], such immobile dislocations cause GB misorientation in the case of low-angle boundaries, and are responsible for deviations of GB misorientation from that of favourable (low-energy) boundaries in the case of high-angle boundaries. In the initial state of the defect structure under consideration, GB dislocations are assumed to be arranged periodically with period $h_{(i)}$ at the ith boundary (i = 1,2,3). The dislocation of the ith boundary, nearest to the triple junction is distant by $h_{(i)}$ /2 from the junction central point (cylinder center). For definiteness, we consider the situation with the 1st and 2nd GBs containing GB dislocations with Burgers vector magnitude b and the 3rd GBs containing GB dislocations with Burgers vector magnitude -2b (Fig. 1). The ith and jth GB planes make an angle $\alpha_{(i-j)}$ ($i \neq j$, i,j= 1,2,3).

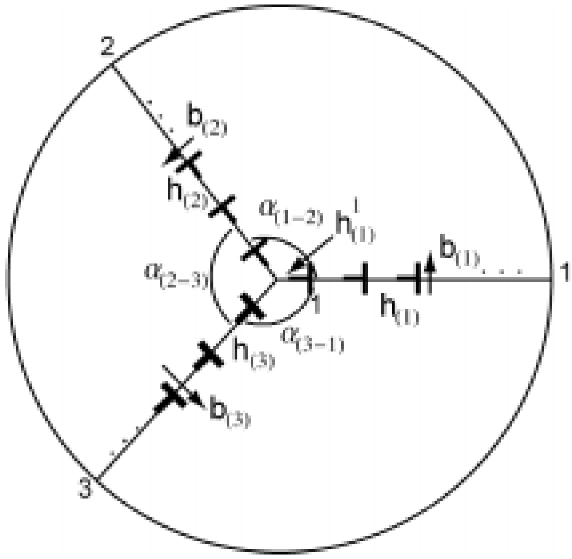

Fig. 1. Grain boundaries that form a triple junction in a cylinder. Immobile intrinsic dislocations are arranged periodically at each boundary.

Let us calculate the elastic energy E_{el} of the GB dislocation ensemble (Fig. 1) under consideration. Following the approach [17], E_{el} can be calculated as:

$$E_{el} = -\frac{1}{2} \int_{S_{cyl}/S_{core}} \beta^*_{kl} \sigma_{kl} dS'. \tag{1}$$

Here β^*_{kl} and σ_{kl} are respectively the sum plastic distortion and the sum stress field of all the GB dislocations shown in Fig. 1b. Integration region S_{cyl}/S_{core} in formula (2) is the cross section of the cylinder with dislocation core regions excluded.

The plastic distortions of isolated dislocations composing the GB dislocation ensemble under consideration is defined in the standard way [17] as follows:

$$\beta_{kl}^{*disl} = -b_l \delta_k (S). \tag{2}$$

Here b_l is the ith component of the dislocation Burgers vector, and $\delta_k(S)$ denotes the three-dimensional delta-function on the imaginary surface S formed behind the dislocation during its transfer from the cylinder free surface to its current position.

The stress field σ_{kl}^{disl} of an edge dislocation in a solid cylinder with central axis OZ can be found using the corresponding stress function χ^{disl} as follows:

$$\sigma_{xx} = \frac{\partial^2 \chi^{disl}}{\partial^2 y}, \quad \sigma_{yy} = \frac{\partial^2 \chi^{disl}}{\partial^2 x}, \quad \sigma_{xy} = -\frac{\partial^2 \chi^{disl}}{\partial y \partial x}. \tag{3}$$

In its turn, the stress function of an edge dislocation in a cylinder is calculated using formula [18] for stress function for a disclination dipole in a cylinder in the corresponding limiting case. In doing so, we find the stress functions of edge dislocations having line core (in the coordinate system shown in Fig. 1b) and having Burgers vectors $\boldsymbol{b} = b\boldsymbol{e}_x$ and $\boldsymbol{b} = b\boldsymbol{e}_y$, respectively, to be as follows:

$$x^{disl}(\boldsymbol{b} = b\boldsymbol{e}_x) = -\frac{Gby}{4\pi(1-\nu)}\left[\frac{x_0^2(R^2 - x_0^2)(R^2 - x^2 - y^2)}{R^2((R^2 - x_0 x)^2 + x_0^2 y^2} + \ln\frac{R^2((x_0^2 - x)^2 + y^2)}{(R^2 - x_0 x)^2 + x_0^2 y^2}\right], \tag{4}$$

$$x^{disl}(\boldsymbol{b} = b\boldsymbol{e}_y) = -\frac{Gby}{4\pi(1-\nu)}\left[\frac{x_0^2(x^2 + y^2)}{R^2} - \frac{(R^2 - x^2 - y^2)((x_0^2 + R^2)x - x_0(R^2 + x^2 + y^2)}{(R^2 - x_0 x)^2 + x_0^2 y^2} + (x_0 - x)\ln\frac{R^2((x_0^2 - x)^2 + y^2)}{(R^2 - x_0 x)^2 + x_0^2 y^2}\right]. \tag{5}$$

Here $\boldsymbol{e}_x$ and $\boldsymbol{e}_y$ are unit vectors along axis OX and OY, respectively, R denotes the cylinder radius, G the shear modulus, and ν the Poisson ratio. Formulae (3)-(5) allow one to calculate stress field of a dislocation with both line core parallel with z-axis and Burgers vector having arbitrary x- and y-components.

3. SPATIAL ARRANGEMENT OF GRAIN BOUNDARY DISLOCATIONS NEAR TRIPLE JUNCTION

Let us consider spatial arrangement of intrinsic GB dislocations (associated with GB misorientation) near a triple junction. A detailed analysis of displacement of all GB dislocations from their positions corresponding to a periodic arrangement (inherent to a GB highly distant from a triple junction) is very complicated. Therefore, in order to identify existence of the triple junction effect (occuring due to finite extent of GBs and the elastic interaction between boundary dislocations belonging to adjoining GBs) on spatial arrangement of GB dislocations, here we examine the only displacement of one dislocation in vicinity of a triple junction, with other GB dislocations assumed to be immobile. Thus, let us consider a spatial position of a GB dislocation of the 1st GB, nearest to the triple junction (Fig. 1). It is unambigiously characterized by distance $h_{(1)}^{1,opt}$ which is found as that corresponding to minimum of the elastic energy E_{el} of the GB dislocation configuration shown in Fig. 1, provided all other dislocations are immobile.

With formulae (1)-(5), we have calculated dependence of $h_{(1)}^{1,opt}$ on dihedral angles, $\alpha_{(1\text{-}2)}$ and $\alpha_{(3\text{-}1)}$, characterizing the triple junction. (Notice that $\alpha_{(2\text{-}3)}$ is dependent on $\alpha_{(1\text{-}2)}$ and $\alpha_{(3\text{-}1)}$: $\alpha_{(2\text{-}3)}=360°-(\alpha_{(1\text{-}2)}+\alpha_{(3\text{-}1)})$). The calculated dependence is shown in Fig. 2. From Fig. 2 it follows that the equilibrium position of the GB dislocation under consideration highly deviates from the position corresponding to a periodic dislocation arrangement when $0° \le \alpha_{(1\text{-}2)} \le ... \le 210°$. That is, the effect of triple junction on $h_{(1)}^{1,opt}$ is strong in the case of triple junctions with highly non-symmetric geometry of adjacent GBs.

4. LOCAL MIGRATION OF GRAIN BOUNDARIES NEAR TRIPLE JUNCTIONS IN PLASTICALLY DEFORMED SOLIDS

Let M gliding GB dislocations under the action of shear stress move along the 1st GB towards the triple junction near which the dislocations are stopped (Fig. 3). Burgers vectors $\boldsymbol{b}_g$ of these gliding dislocations are parallel with the 1st boundary plane.

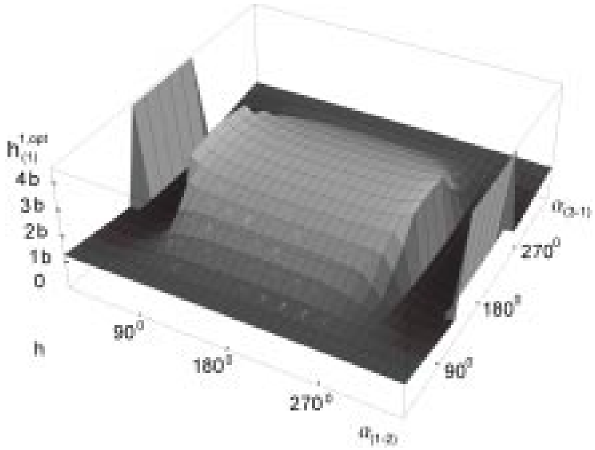

Fig. 2. Dependence of boundary dislocation coordinate $h_{(1)}^{1,opt}$ on dihedral angles, $\alpha_{(1-2)}$ and $\alpha_{(3-1)}$, that characterize triple junction of grain boundaries.

The gliding GB dislocations form a pile-up stopped near the triple junction and create their stress fields. In these circumstances, the GB fragment nearest to the triple junction, containing the GB dislocation pile-up, serves as a source of the stress field being the superposition of the stress fields induced by the gliding and intrinsic GB dislocations. In the first approximation, we assume that $M=N_{(1)}$ gliding dislocations are stopped near the triple junction, in which case the sum stress field of the gliding and intrinsic dislocations can be represented as that created by $N_{(1)}$ GB dislocations with Burgers vector $\tilde{\boldsymbol{b}}_1=\boldsymbol{b}_1+\boldsymbol{b}_g$.

In general, the elastic energy of the ensemble of GB dislocations with Burgers vectors $\tilde{\boldsymbol{b}}_1$ can be released due to its re-arrangement. Here we consider a re-arrangement due to GB migration resulting in rotation of the 1st boundary as a whole relative to the triple junction (Fig. 3). That is, the 1st boundary moves to a new position characterized by angle $\alpha_{(3-1)}^{opt}$ made by its plane and the immobile 3rd boundary plane (Fig. 3). The angle $\alpha_{(3-1)}^{opt}$ corresponds to minimum of the energy E of the GB configuration shown in Fig. 1b. The energy E consists of the two basic terms:

$$E = E_{el} + \Delta E, \tag{6}$$

where E_{el} denotes the elastic energy of GB dislocations, and ΔE the energy change associated with extension of GB due to rotation of its fragment containing both immobile and stopped gliding GB dislocations.

E_{el} is calculated using formulae (1)-(5). Let us consider term ΔE. In reality, local migration of a GB does not result in rotation of the boundary as a whole, but makes it to be curved and, therefore, extended (Fig. 4). The GB extension leads to an increase of its energy by value of $\Delta E \approx \gamma\Delta d$, where γ denotes the GB energy per its unit area, and Δd the GB length extension due to local migration.

With formulae (1)-(6) and estimate $\Delta E \approx \gamma\Delta d$, we have calculated the optimum angle $\alpha_{(3-1)}^{opt}$, for the following values of characteristic parameters for aluminum: $N_{(2)}=N_{(3)}=3$, $h_{(2)}=h_{(3)}=5b$, $b_g=b=0.3$ nm, $\gamma=0.6$ J/m^2 (see experimental data [19]), , and initial angle $\alpha_{(3-1)}^{opt}$. In the first approximation, Δd is taken

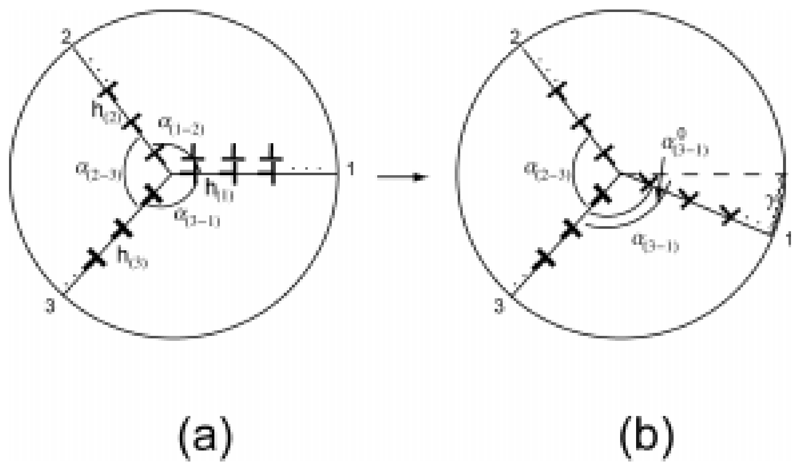

Fig. 3. Triple junction of grain boundaries in a plastically deformed material. (a) Gliding boundary dislocations at the 1st grain boundary are stopped near triple junction. (b) Local migration (rotation) of the 1st grain boundary, induced by a release of elastic energy of grain boundary dislocation ensemble.

Table 1. Characteristic angle $\alpha^{opt}_{(3-1)}$ and its deviation from initial value $\alpha_{(3\text{-}1)}$.

$N_{(1)}$	$\alpha^{opt}_{(3-1)}$	$\alpha_{(3\text{-}1)}$-$\alpha^{opt}_{(3-1)}$
3	120°±1°	±1°
4	104°±1°	16°±1°
5	96°±1°	24°±1°

as the length of a segment of the model cylinder free surface swept by the GB when it moves from initial position characterized by $\alpha^{opt}_{(3-1)}$ to its final position characterized by $\alpha^{opt}_{(3-1)}$ (see Fig. 4c). The results of our calculations are presented in Table 1. With these results, we come to the conclusion that deformation-induced generation of gliding GB dislocations and their accumulation near triple junctions of GBs is capable of causing local migration of GBs.

The GB containing the stopped gliding GB dislocations tends to move to a position where the sum Burgers vector of the stopped gliding dislocations and immobile intrinsic GB dislocations (associated with the initial GB misorientation) is perpendicular to the GB plane. That is, the dislocation ensemble at the GB fragment nearest to a triple junction tends to be transformed into a dislocation wall configuration (characterized by minimum elastic energy, compared to energies characterizing dislocation configurations with other geometries). The difference between the initial ($\alpha_{(3\text{-}1)}$) and final ($\alpha^{opt}_{(3-1)}$) values of the angle that characterizes a triple junction respectively before and after accumulation of gliding GB dislocations near the triple junction can be rather large. Say, according to our calculations, the difference in question reaches 24º in the case of $N_{(1)}$=5 (see Table 1). This is in agreement with experimental data of the work [5] reporting on local rotation of the GB plane by tentatively 20º in vicinity of the triple junction in a plastically dedformed tricrystal of aluminum.

The discussed transformations of GBs in plastically deformed nano- and polycrystalline materials either facilitate or hamper GB sliding, depending on the mutual orientation of the maximum shear stress and Burgers vectors of immobile intrinsic GB dislocations at the boundary where the gliding dislocations are stopped. Actually, in the situations shown in Fig. 4a and b, the GB plane in its final position (after the local migration) is oriented respectively close to and far from the direction of the maximum shear stress τ_{max} action. In these circumstances, intensive GB sliding accompanied by local migration of GBs gives rise to the formation of the so-called “soft” and “hard” triple junctions where the migration-assisted GB sliding occurs or does not, respectively, at given conditions of loading (say, a value of the applied mechanical stress). In this context, the volume fraction F_s of soft triple junctions effectively characterizes the contribution of GB sliding to plastic deformation and, therefore, is an im-

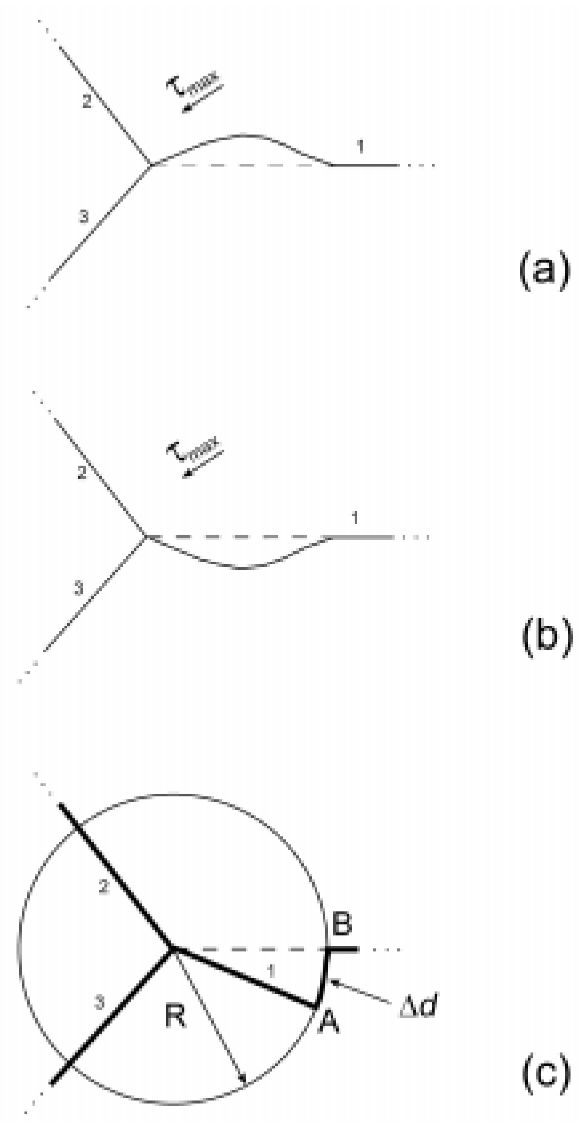

Fig. 4. The combined effects of gliding and intrinsic grain boundary dislocations cause a grain boundary to be curved near a triple junction. In real cases (a) and (b), curvature is distributed along a rather long fragment of grain boundary. In the case (a) ((b), respectively), local migration of grain boundary facilitates (hampers, respectively) grain boundary sliding. (c) Model case. Curvature is distributed along a short fragment AB of grain boundary.

portant structure-sensitive parameter of the behavior of nano- and polycrystalline materials under mechanical loading.

The discussed effects of triple junctions on the deformation behavior and the transformations of hard triple junctions into soft ones account for the plastic flow localization experimentally observed [20-23] in nanocrystalline materials. Actually, with results of our theoretical analysis, the difference between homogeneous and inhomogeneous regimes of plastic deformation in nanocrystalline materials is naturally explained as that associated with the behavior of GBs near triple junctions. If the mean volume fraction $<F_s>$ of soft triple junctions is low, the grain boundary sliding occurs in only some local regions where local value of F_s is comparatively high. In doing so, the grain boundary sliding induces local migration of GBs, accompanied by transformations of hard triple junctions into soft ones in these local regions, thus intensifying localization of plastic flow. In other terms, the GB sliding occurs as a self-supporting percolation process in some local regions, in which case a deformed sample exhibits the inhomogeneous deformation regime with plastic flow being localized in shear bands. If $<F_s>$ is high, the GB sliding effectively occurs within the mechanically loaded sample as a whole, causing homogeneous plastic deformation.

5. CONCLUDING REMARKS

Thus, in this paper we have theoretically examined the effects of triple junctions on GB dislocation structures. In doing so, we have taken into consideration the following factors: (i) the elastic interaction between GB dislocations (in particular, between dislocations belonging to different GBs); (ii) the edge effect related to a finite extent of adjacent GBs; (iii) the action of triple junctions as effective obstacles for motion of gliding GB dislocations, carriers of GB sliding. It has been shown that GB dislocation arrangement in vicinity of a triple junction deviates from a periodic arrangement inherent to GB structures highly distant from triple junctions. This phenomenon gives rise to the specific structural peculiarities of GB dislocation configurations in nanocrystalline materials (where GBs are short and the volume fraction of triple junctions is extremely high), differing defect structure in such materials from that in conventional coarse-grained polycrystals. Also, the deviations of GB dislocation structures near triple junctions from those at conventional GB fragments cause the hampering force for migration of triple junctions, because such migration should be accompanied by specific re-arrangements of GB dislocation structures. This statement is indirectly supported by experimental data [11] indicating on the role of triple junctions as drag centers of GB migration during re-crystallization processes.

Also, we have theoretically described local migration of GBs near triple junctions in plastically deformed nano- and polycrystalline materials. It has been shown that the combined effects of stopped gliding and intrinsic immobile grain boundary dislocations cause the local GB migration which is capable of either enhancing or hampering GB sliding, depending on characteristics of the dislocations.

In our analysis we have focused on the only role of triple junctions as obstacles for plastic flow occurring via GB sliding. In general, triple junctions are also capable of essentially contributing to plastic flow due to enhanced diffusional mass transfer along triple junction tubes [9]. In doing so, as with GB causing Coble creep in nanocrystalline materials [24,25], triple junctions give rise to the softening of plastically deformed nanocrystalline materials [9]. It is contrasted to their strenghtening role as obstacles for GB sliding in the situation where the GB sliding dominates. In this context, the role of triple junctions in plastic deformation processes is crucial, in particular, in selecting the dominant deformation mechanism (lattice dislocation slip, GB sliding, GB diffusional creep, or rotational deformation [26,27]) realized in mechanically loaded nano-crystalline materials where the volume fraction of the GB phase is extremely high.

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REFERENCES

[1] *Science and Technology of Interfaces*, ed. by S. Ankem, C.S. Pande, I.A. Ovid'ko and S. Ranganathan (TMS: Warrendale 2002).
[2] A.H. King // *Interf. Sci.* **7** (1999) 251.
[3] K.-M. Yin, A.H. King, T.E. Hsieh, F.-R. Chen, J.J. Kai and L. Chang // *Micros. Microanal.* **3** (1997) 417.
[4] M.Yu. Gutkin and I.A. Ovid'ko // *Philos. Mag.* A **70** (1994) 561.
[5] V.V. Astanin, A.V. Sisanbaev, A.I. Pshenichnyuk and O.A. Kaibyshev // *Scr. Mater.* **36** (1997) 117.

[6] D.A. Kostantinidis and E.C. Aifantis // *Nanostruct. Mater.* **10** (1998) 1111.

[7] H. Hahn, P. Mondal and K.A. Padmanabhan // *Nanostruct. Mater.* **9** (1997) 603.

[8] O.A. Kaibyshev // *Mater. Sci. Forum* **304-306** (1999) 21.

[9] A.A. Fedorov, M.Yu. Gutkin and I.A. Ovid'ko // *Scr. Mater.* **47** (2002) 51.

[10] K. Owusu-Boahen and A.H. King // Acta Mater. **49** (2001) 237.

[11] G. Gottstein, A.H. King and L.S. Shvindlerman // *Acta Mater.* **48** (2000) 397.

[12] N.A. Enikeev, A.A. Nazarov and R.Z. Valiev // *Fiz. Metal. Metallov.* **77**, No. 5 (1994) 31 (transl. in *Phys. Met. Metallogr.*)

[13] A.P. Sutton and R.W. Balluffi, *Interfaces in Crystalline Materials* (Claredon Press, Oxford, 1995).

[14] B. Vuchik, K.L. Merkle, K. Char, D.B. Buchholz, R.P.H. Chang and L.D. Marks // *J. Mater. Res.* **11** (1996) 2429.

[15] M.Yu. Gutkin and I.A. Ovid'ko // *Phys. Rev.* B **63** (2001) 064515.

[16] S.V. Bobylev, I.A. Ovid'ko and A.G. Sheinerman // *Phys. Rev.* B **64** (2001) 224507.

[17] T. Mura, in: *Advances in Material Research*, vol. 3, ed. by H. Herman (Interscience: New York, 1968) p.1.

[18] A.E. Romanov and V.I. Vladimirov, in: *Dislocations in Solids,* vol.9, ed. by F.R.N. Nabarro (North-Holland: Amsterdam,1992) pp.189-302.

[19] G.C. Hasson and C. Goux // *Scipta Metall.* **5** (1971) 889.

[20] G.W. Niemann, J.R. Weertman and R.W. Siegel // *J. Mater. Res.* **6** (1991) 1012.

[21] A.B. Witney, P.G. Sanders, J.R. Weertman and J.A. Eastman // *Scr. Metall. Mater.* **33** (1995) 2025.

[22] J.E. Carsley, W.W. Milligan, S.A. Hackney and E.C. Aifantis // *Metall. Mater. Trans.* **26A** (1995) 2479.

[23] R.A. Andrievskii, G.V. Kalinnikov, N.P. Kobelev, Ya.M. Soifer and D. Shtansky // *Phys.Sol. State* **39** (1997) 1661.

[24] R.A. Masumura, P.M. Hazzledine and C.S. Pande // *Acta Mater.* **46** (1998) 4527.

[25] H.S. Kim, Y. Estrin and M.B. Bush // *Acta Mater.* **48** (2000) 493.

[26] M.Yu. Gutkin, A.L. Kolesnikova, I.A. Ovid'ko and N.V. Skiba // *J. Metast. Nanocryst. Mater.* **12** (2002) 47.

[27] I.A. Ovid'ko // *Science* **295** (2002) 2386.