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DISLOCATION CLIMB IN NANOCRYSTALLINE MATERIALS UNDER HIGH-STRAIN-RATE SUPERPLASTIC DEFORMATION

I.A. Ovid'ko and A.G. Sheinerman

Institute for Problems of Mechanical Engineering, Russian Academy of Sciences, Bolshoj 61, Vas. Ostrov, St. Petersburg 199178, Russia

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Abstract. A theoretical model is suggested which describes the role of grain boundary dislocation climb in high-strain-rate superplastic deformation of nanocrystalline materials. In the framework of the model, grain boundary sliding causes the dislocation storage at triple junctions of grain boundaries in nanocrystalline materials under superplastic deformation. This effect is responsible for strengthening. The dislocation climb along grain boundaries adjacent to dislocated triple junctions provides relaxation of the dislocation charge accumulated at the triple junctions. As a corollary, the grain boundary dislocation climb hampers the nanocrack generation and gives rise to softening of nanocrystalline materials under superplastic deformation.

1. INTRODUCTION

High-strain-rate superplasticity of nanocrystalline materials (Ni_3Al, Al- and Ti-based alloys) represents the subject of growing interest for fundamental and applied research [1-9]. The specific features of superplasticity in the nanocrystalline matter are very high flow stresses and the essential strengthening at the extensive stage of deformation [1-8]. These specific features and, in general, the outstanding mechanical properties exhibited by nanocrystalline materials are treated to be caused by grain boundaries (GBs) providing the action of the specific deformation mechanisms in such materials; see, e.g.,[10-23]. In particular, following reviews [7,8] of experimental data on high-strain-rate superplasticity in nanocrystalline materials, grain boundary sliding is the dominant mechanism of superplastic deformation. At the same time, the conventional lattice dislocation slip also essentially contributes to superplastic deformation [7,8]. Based on these experimental data, a theoretical model [9, 24] has been suggested describing the unusual strengthening in superplastic nanocrystalline materials as the phenomenon related to storage of GB dislocations at triple junctions of GBs. In its turn, the dislocation storage is capable of causing the stress concentration and consequent generation of nanocracks in vicinities of triple junctions [25]. Such triple junction nanocracks have been experimentally observed by Kumar *et al.* [17] in nanocrystalline Ni showing a good ductility. In the context discussed, it is highly interesting to identify the processes that affect the GB storage at triple junctions and generation of triple junction nanocracks in deformed nanocrystalline materials. The main aim of this paper is to suggest a theoretical model describing the GB dislocation climb and its effects on both the GB dislocation storage and generation of nanocracks at triple junctions of GBs in nanocrystalline materials during high-strain-rate superplastic deformation.

Corresponding author: I.A. Ovid'ko, e-mail: ovidko@def.ipme.ru

2. GRAIN BOUNDARY DISLOCATION CLIMB IN NANOCRYSTALLINE MATERIALS UNDER SUPERPLASTIC DEFORMATION. MODEL

Let us consider a nanocrystalline solid under superplastic deformation occurring via both GB sliding (dominant mode) and conventional lattice dislocation slip. In the framework of our model, the combined action of these deformation mechanisms is realized as follows. In a mechanically loaded material, dislocation sources emit lattice dislocations that move towards GBs (Fig. 1a). The lattice dislocations are absorbed by GBs where they split into GB dislocations. For definiteness, we assume that the splitting results in the formation of GB dislocations of two types: gliding and climbing GB dislocations with the Burgers vectors being parallel and perpendicular to the GB plane, respectively. The gliding dislocations move under the action of the external stress along GB planes towards triple junctions (Fig. 1b). At a certain level of the stress, these gliding dislocations reach triple junctions where they converge (Fig. 1c). As a result of this dislocation reaction, sessile dislocations are formed at triple junctions (Fig. 1c). With rising the plastic strain ε, the discussed process repeatedly occurs, which results in the formation of superdislocations in the triple junctions O and C (Fig. 1d). They hamper movement of new gliding dislocations towards triple junctions (Fig. 1d) and thereby cause the strengthening effect in nanocrystalline materials [9,24]. These superdislocations split into gliding dislocations, that eventually annihilate, and sessile superdislocations in triple junctions O and C (Fig. 1e). These sessile dislocations create tensile stresses that are capable of inducing the formation of nanocracks at triple junctions [25] (Fig. 1f). In this case, evolution of sessile dislocations at triple junctions can crucially affect the deformation behavior of nanocrystalline materials. In particular, this evolution is influenced by the climb of GB dislocations towards triple junctions where the climbing dislocations come into reactions with the sessile dislocations (Fig. 1e) and thereby decrease the stress concentration at triple junctions. We think the climb to be the process hampering the nano-crack generation and, as a corollary, enhancing ductility of nanocrystalline materials.

First, let us consider evolution of sessile dislocations at triple junctions of GBs in the situation where the shear stress level is sufficient to provide movement of gliding GB dislocations towards triple junctions and their convergence. In the situation discussed, evolution of sessile dislocations at triple junctions is caused by the following two processes:

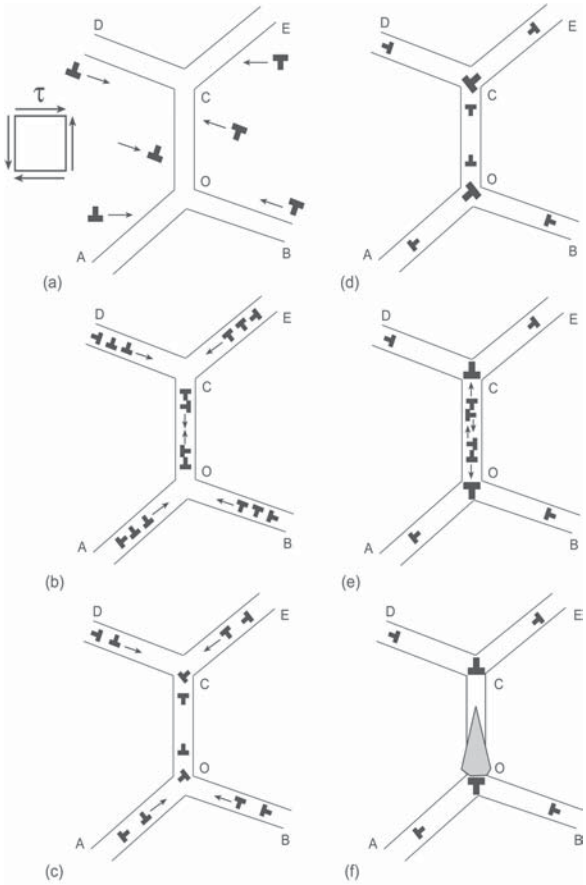

Fig. 1. Formation of superdislocations at triple junctions of grain boundaries. (a) Lattice dislocations move under the external stress action towards grain boundaries where they split into gliding and climbing GB dislocations. (b) Grain boundary dislocations in boundaries OA, OB, CD and CE glide towards triple junctions O and C. (c) As a result of dislocation reactions, sessile dislocations are formed at these triple junctions. (d) Glide of new GB dislocations along boundaries OA, OB, CD and CE leads to the formation of triple junction superdislocations. (e) Triple junction superdislocations split into dislocations that glide along boundary OC and sessile superdislocations that stay at triple junctions O and C. Climb of grain boundary dislocations along boundary OC towards triple junctions O and C tends to decrease Burgers vectors of sessile superdislocations at these triple junctions. (f) Nanocrack is generated at superdislocation at triple junction O.

(i) convergence of gliding GB dislocations and pre-existent sessile dislocations (Figs. 1c and 1d);
(ii) convergence of sessile dislocations with GB dislocations climbing towards triple junctions (Fig. 1e).

The process (i) gives rise to accumulation of the sessile dislocation charge at triple junctions, enhancing the nucleation of triple junction nanocracks. The process (ii) leads to a decrease of the sessile dislocation charge (Burgers vector) at triple junctions, hampering the nucleation of triple junction nanocracks.

Let us consider the process (ii) in the exemplary case shown in Fig. 1. In doing so, for the sake of simplicity, we assume that the sessile dislocation comes into reaction with only those GB dislocations that climb along the boundary OC. (This assumption simplifies our mathematical analysis of the problem but does not affect essentially the basic results of this analysis.) Commonly, the velocity of conservative glide of GB and lattice dislocations is much larger than the velocity of non-conservative climb of GB dislocations; see, e.g.,[26-28]. In these circumstances, the rate of the process (i) - convergence of the sessile dislocation with gliding GB dislocations - is determined by the frequency of generation of gliding GB dislocations (due to the splitting of lattice dislocations trapped at GBs) and the probability of their annihilation (in the case of meeting of two dislocations with opposite Burgers vectors). The rate of the process (ii) - convergence of climbing GB dislocations and the sessile dislocation at triple junction (Fig. 1e) - is controlled by frequency of generation of the climbing GB dislocations and their climb velocity.

Let b_l and b be Burgers vector magnitudes of respectively lattice and GB dislocations. The sessile dislocations at triple junctions O and C result from the two processes: (i) convergence of n GB dislocations gliding along boundary OA and n GB dislocations gliding along boundary OB (n GB dislocations gliding along boundary CD and n GB dislocations gliding along boundary CE, respectively); see Fig. 1b, c, and d; and (ii) consequent glide of dislocations – elements of the triple junction sessile dislocation – along boundary OC (Fig. 1e). Let the Burgers vector magnitude of such dislocations be designated as $B=\beta nb$, where β is the geometric factor depending on the angles made by GB planes adjacent to the triple junctions O and C ($0 \leq \beta < 2$).

For simplicity, we assume that all GBs have the same length d, and the number $u(t)$ of lattice dislocations (emitted by dislocation sources) that reach a GB per unit time t is the same for all GBs. Also, we suppose the number $2K$ of gliding GB dislocations formed in every GB per unit time to be equal to the number of climbing GB dislocations. Since triple junctions serve as effective geometric obstacles for movement of GB dislocations, transfer of such dislocations from one boundary to another is hampered and the processes of this transfer very weakly influence evolution of the GB dislocations density. (The increase in the GB dislocation density due to movement of GB dislocations through triple junctions is tentatively equal to the corresponding decrease). In these circumstances, GB dislocations are generated mostly due to splitting of lattice dislocations trapped by GBs. As a corollary, the following approximate equation is valid: $2K \approx (1/2)u\, b_l/b$. For simplicity, we assume the rates of formation of GB dislocations having opposite Burgers vectors to be the same and thereby equal to K. Let N be the number of GB dislocations that have the same Burgers vector direction (dislocation sign) and climb along one GB. Also, in the first approximation, the velocity v_c of GB dislocation climb is independent on both time and dislocation location.

3. DISLOCATION KINETICS IN NANOCRYSTALLINE MATERIALS UNDER SUPERPLASTIC DEFORMATION

Let us calculate the dependence of the Burgers vector magnitude B (that characterizes sessile superdislocations at triple junctions) on time t. To do so, we will write equation which describes frequency ν of dislocation annihilation reactions between climbing GB dislocations. With the climb velocity v_c being constant, frequency ν is equal to frequency of reactions between the triple junction superdislocation and GB dislocations climbing towards the triple junction (Fig. 1e). More precisely, the frequency ν is given as: $\nu = N\, v_c/d$, where ratio d/N is the mean interspacing between neighbouring dislocations that climb in the boundary. Then the sum number νN of climbing GB dislocations of one sign (Burgers vector), which annihilate with climbing GB dislocations of opposite sign per unit time, is equal to $(v_c/d)\, N^2$. In calculation of the dependence of B on time t, it is convenient to replace discrete spectra of values of n and N by continuous ones. In these circumstances, evolution of n and N in time is described by the following system of kinetic equations:

$$\beta\dot{n} = \alpha\beta K - \frac{v_c}{d}N,$$
$$\dot{N} = K - \frac{v_c}{d}N - \frac{v_c}{d}N^2. \quad (1)$$

The quantity K on right-hand-sides of equations (1) characterizes the rate of generation of gliding or climbing GB dislocations (resulted from splitting of lattice dislocations trapped at GBs), the coefficient α ($0< \alpha \leq 1$) takes into account both annihilation of gliding GB dislocations (of opposite signs) and 'absorption' of gliding GB dislocations of opposite sign by sessile triple junction superdislocations. The second term on the right-hand-sides of equations (1) describes a decrease in n and N due to the 'absorption' of climbing GB dislocations by triple junction superdislocations. The third term on the right-hand-side of the second equation in formula (1) characterizes a decrease in the number of climbing GB dislocations owing to their annihilation.

In order to solve kinetic equations (1), let us find the relationship between K and plastic strain rate $\dot{\varepsilon}$. In the considered case of intermediate temperature and comparatively large nanograins (with size d>30 nm), the basic deformation mechanism is the dislocation movement [7,8,17]. In the general situation, movement of various lattice and GB dislocations causes plastic flow characterized by various components of the plastic strain tensor. Here, for simplicity, in spirit of classic dislocation models of plastic flow [26], we will focus our analysis to the case with all the dislocations carrying only one component of the plastic strain tensor. In this partial case (which, nevertheless, takes into account the key tendencies of the phenomenon of superplastic deformation in nanocrystalline materials), the plastic strain rate $\dot{\varepsilon}$ can be represented as the sum $\dot{\varepsilon}=\dot{\varepsilon}_g+\dot{\varepsilon}_c$, of terms $\dot{\varepsilon}_g$ and $\dot{\varepsilon}_c$ describing contributions of the dislocation slip and GB dislocation climb, respectively.

Since GBs and triple junctions serve as sinks for gliding lattice dislocations and GB dislocations, respectively, the distance moved by the gliding lattice or GB dislocation towards its sink is tentatively equal to the grain size d. In the situation with one lattice dislocation gliding to each GB, the density $\rho^{(1)}$ of lattice dislocations is about $1/d^2$. As a corollary, the plastic strain $\varepsilon^{(1)}$ related to the glide of one lattice dislocation towards a GB and consequent glide of GB dislocations resulted from the splitting of the lattice dislocation is given as $\varepsilon^{(1)} \approx \rho^{(1)} b_l d \approx b_l/d$. Then the plastic strain rate that characterizes the dislocation glide is as follows:

$$\dot{\varepsilon}_g = \varepsilon^{(1)}u = \frac{b_l u}{d}. \quad (2)$$

The plastic strain rate that characterizes the dislocation climb is given as:

$$\dot{\varepsilon}_c \approx \frac{Nbv_c}{d^2}. \quad (3)$$

The sum of expressions (2) and (3) yields the total plastic strain rate:

$$\dot{\varepsilon} = \dot{\varepsilon}_g + \dot{\varepsilon}_c = \frac{b_l u}{d} + \frac{Nbv_c}{d^2}. \quad (4)$$

With formula (4) and the approximate relationship $2K \approx (1/2)\,ub_l/b$, we find:

$$K = \frac{\dot{\varepsilon}d}{4b} - \frac{v_c}{4d}N. \quad (5)$$

Substitution of (5) to formula (1) and the condition $t = \varepsilon/\dot{\varepsilon}$ (where ε is the plastic strain) gives:

$$\beta\frac{dn}{d\varepsilon} = \alpha\beta\frac{d}{4b} - (\alpha\beta+4)\frac{v_c}{4\dot{\varepsilon}d}N,$$
$$\frac{dN}{d\varepsilon} = \frac{d}{4b} - \frac{5v_c}{4\dot{\varepsilon}d}N - \frac{v_c}{\dot{\varepsilon}d}N^2. \quad (6)$$

For definiteness, we consider the situation where GBs do not contain gliding and climbing GB dislocations at ε=0, when the lattice dislocation sources start to emit dislocations. In this situation, the following initial conditions for equations (6) are realized: $n(\varepsilon=0)=N(\varepsilon=0)=0$. Solution of system (6) under the conditions in question is as follows:

$$N(\varepsilon) = \frac{5}{4}\left[\kappa - \frac{1}{2} - \frac{2\kappa}{L_0\exp(2\kappa\tilde{v}_c\varepsilon)+1}\right], \quad (7)$$

$$\beta n(\varepsilon) = \frac{5}{4}\left(1+\frac{\alpha\beta}{4}\right)\left\{\left(\kappa+\frac{1}{2}\right)\left[s\left(\kappa-\frac{1}{2}\right)+1\right]\tilde{v}_c\varepsilon - \ln\frac{L_0\exp(2\kappa\tilde{v}_c\varepsilon)+1}{L_0+1}\right\}, \quad (8)$$

where $\tilde{v}_c=5v_c/(4\dot{\varepsilon}d)$, $s=4\alpha\beta/(\alpha\beta+4)$, $\kappa=\sqrt{\eta+1/4}$, $\eta=d/(5b\tilde{v}_c)$, and $L_0=(2\kappa+1)/(2\kappa-1)$. In the limit of $\varepsilon\to\infty$, we find: $\beta n(\varepsilon\to\infty)\approx[5(\alpha\beta+4)/16](\kappa-1/2)\,[s(\kappa+1/2)-1]\tilde{v}_c\varepsilon$. From the definition of κ it follows that $\kappa > 1/2$. Therefore, $n(\varepsilon\to\infty)\to+\infty$, if $s(\kappa+1/2)-1>0$ (or, in other terms, for $\tilde{v}_c < (s^2d)/[5(1\text{-}s)b])$, and $n(\varepsilon\to\infty)\to-\infty$, if $s<1$ and $\tilde{v}_c > (s^2d)/[5(1\text{-}s)b]$.

It is evident that the solution is meaningful from a physical viewpoint only in the case of $n>0$, because climb of GB dislocations does not result in a decrease of the superdislocation Burgers vector in the case of $n<0$. In these circumstances, the negative values of n in formula (8) correspond, in fact, to the situation with $n=0$.

4. CONDITIONS FOR NUCLEATION OF SUPERDISLOCATIONS AND NANOCRACKS AT TRIPLE JUNCTIONS OF GRAIN BOUNDARIES

The dependences of parameter βn (which characterizes the Burgers vector magnitude for triple junction superdislocations) on plastic strain ε are presented in Fig. 2, for $\alpha\beta$ = 0.7, d/b = 500 and different values of $\tilde{v}_c$. As follows from Fig. 2, at small $\tilde{v}_c$ ($\tilde{v}_c < (s^2d)/[5(1\text{-}s)b]$), n indefinitely grows with plastic strain ε. At $\tilde{v}_c = (s^2d)/[5(1\text{-}s)b]$, n tends to a constant value at large ε. At large $\tilde{v}_c$ ($\tilde{v}_c > (s^2d)/[5(1\text{-}s)b]$), n first grows and then decreases down to 0 with rising ε. In this case, the maximum value of βn can be found from the condition $dn/d\varepsilon$ = 0. This maximum value βn_{max} is given as:

$$\beta n_{max} = \frac{5(\alpha\beta+4)}{32\kappa}\{(\kappa-1/2)[1-s(\kappa+1/2)]\ln[1-s(\kappa+1/2)]+(\kappa+1/2)[1+s(\kappa-1/2)]\ln[1+s(\kappa-1/2)]\},\quad s(\kappa+1/2)<1. \tag{9}$$

An analysis of formula (9) shows that the upper limit for the values of βn_{max} can be found from the condition $s(\kappa+1/2)=1$; it is equal to (5/4)ln2 ($\approx$ 0.87). Since the largest value of βn_{max} does not exceed 1, in the case $s(\kappa+1/2)<1$ (or, in other terms, $\tilde{v}_c > (s^2d)/[5(1\text{-}s)b]$), the superdislocations do not nucleate.

With relationship $\tilde{v}_c=5v_c/(4d\dot{\varepsilon})$, the condition $\tilde{v}_c < (s^2d)/[5(1\text{-}s)b]$ of potential nucleation of superdislocations can be re-written in the following form: $\dot{\varepsilon} > \dot{\varepsilon}_0$, were

$$\dot{\varepsilon}_0 = \frac{25(1-s)}{4s^2}\frac{bv_c}{d^2}. \tag{10}$$

As follows from formula (10), the critical plastic strain rate $\dot{\varepsilon}_0$ grows when the dislocation climb velocity v_c increases and/or the grain size d decreases. At sufficiently large values of the plastic strain rate ($\dot{\varepsilon} > \dot{\varepsilon}_0$) the triple junction superdislocations are capable of inducing the formation of nanocracks in the vicinity of triple junctions. Such experimentally observed [17] nanocracks grow, converge with nanocracks growing at neighbouring GBs and, thus, initiate macroscale fracture of a mechanically loaded nanocrystalline sample.

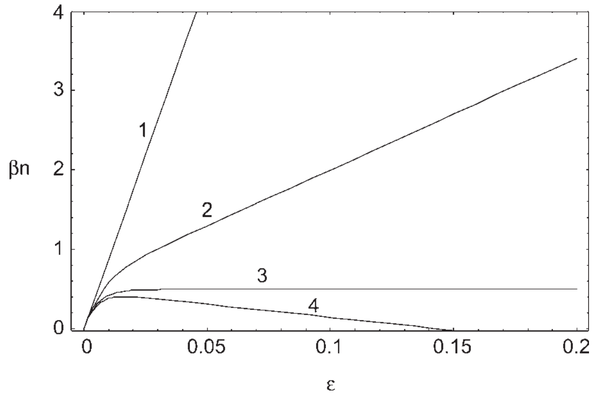

Fig. 2. Dependences of parameter βn on plastic strain ε for $\alpha\beta$ = 0.7, d/b = 500, and $\tilde{v}_c$=0 (curve 1), $\tilde{v}_c$=50 (curve 2), $\tilde{v}_c=(s^2d)/[5(1\text{-}s)b]\approx87.8$ (curve 3), and $\tilde{v}_c$=100 (curve 4).

The probability of an energetically favourable nucleation of a triple junction nanocrack and its equilibrium length strongly depend on the Burgers vector magnitude that characterize the triple junction superdislocation [25]. Therefore, conditions of the nanocrack generation are sensitive to the GB dislocation climb which, as shown above, influences the Burgers vector magnitude. In the next section, we will reveal the conditions at which nanocracks are generated along GBs in the stress fields of triple junction superdislocations with Burgers vectors whose evolution is caused by both the GB dislocation climb and GB sliding.

5. EFFECT OF GRAIN BOUNDARY DISLOCATION CLIMB ON GENERATION AND GROWTH OF TRIPLE JUNCTION NANOCRACKS

Consider a nanocrack generated at the superdislocation (with the Burgers vector $n\mathbf{b}$) located at the triple junction O (Fig. 1f). This nanocrack is characterized by an equilibrium length l_e. The value of the equilibrium nanocrack length l_e is mainly influenced by the stress field of its parent superdislocation, while the effect of the stress fields of other dislocations may be neglected. Then, in the considered case of an elastically isotropic solid, the equilibrium length of the triple junction nanocrack is calculated using the following general formula [29]:

$$l_e = \frac{n^2 G b^2}{8\pi(1-\nu_p)\gamma_e}. \quad (11)$$

Here G is the shear modulus, ν_p is the Poisson ratio, $\gamma_e = \gamma_s - \gamma_b/2$, where γ_s is the specific surface energy and γ_b is the specific energy of the GB per unit area of its plane. The growth of the nanocrack (Fig. 1f) is energetically favorable, if $l< l_e$, and unfavorable, if $l>l_e$.

For illustration of the effect of the GB dislocation climb on the nanocrack growth, with formula (11), we have calculated dependences of the non-dimensional equilibrium length l_e of a triple junction nanocrack on plastic strain ε, for various values of the velocity $\tilde{v}_c$ of GB dislocation climb. These dependences are presented in Fig. 3, for the following characteristic values of parameters of the defect system and material parameters of nanocrystalline Ni: b=0.1 nm, α = 0.7, β = 1, γ_s = 1.725 J/m^2 [27], γ_b = 0.69 J/m^2 [27], $G = 0.79\cdot10^{11}$ Pa [30], and ν_p =0.31 [30]. The dependences under consideration have been calculated and shown in Fig. 3 in the case $\tilde{v}_c>(s^2d)/[5(1-s)b]$, in which the nanocrack formation (Fig. 1f) is energetically favorable. As follows from Fig. 3, the equilibrium length l_e of the triple junction nanocrack grows with rising plastic strain ε.

In order to characterize the effect of the GB dislocation climb on the nanocrack growth, let us consider the equilibrium length l_e at a constant value of ε, but different values of the velocity v_c of GB dislocation climb. As follows from Fig. 3, for the same value of ε, the equilibrium length l_e decreases with rising the velocity v_c of GB dislocation climb. This is indicative of the role of the GB dislocation climb as a factor hampering the nanocrack growth in deformed nanocrystalline materials. Also, notice that v_c increases with rising temperature T. Since, for a specified plastic strain ε, the equilibrium nanocrack length l_e decreases with rising v_c, l_e also decreases with rising temperature T. At the same time, l_e decreases with reducing the plastic strain rate $\dot{\varepsilon}$. In these circumstances, the triple junction nanocrack growth is hampered with rising T and/or decreasing $\dot{\varepsilon}$.

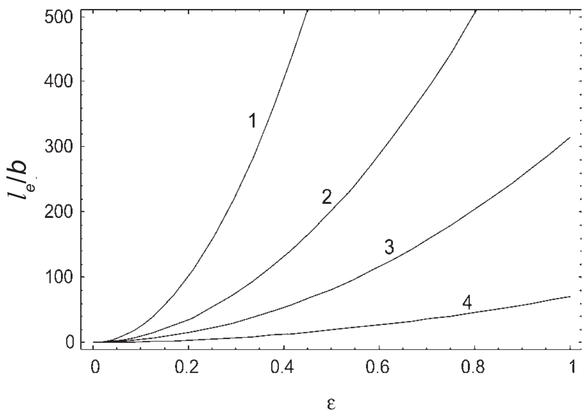

Fig. 3. Dependences of equilibrium nanocrack length l_e/b on plastic strain ε, for α = 0.7 , β = 1, d/b = 500, and $\tilde{v}_c$ = 0, 10, 25 and 50 (curves 1, 2, 3 and 4, respectively).

6. CONCLUDING REMARKS

In this paper, it has been shown theoretically that the characteristics of high-strain-rate superplastic deformation in nanocrystalline materials are influenced by the GB dislocation climb. Superplastic deformation occurring by GB sliding in nanocrystalline materials gives rise to the storage of GB dislocations at triple junctions, which provides the strengthening effect (for details, see theoretical model [9,24].) The strengthening effect is controlled by the rate of the GB dislocation accumulation at triple junctions. The dislocation climb along GBs adjacent to the dislocated triple junctions provides relaxation of the dislocation charge accumulated at triple junctions. In doing so, the GB dislocation climb causes a decrease of the rate of the dislocation accumulation and thus leads to softening of a deformed nanocrystalline material. Also, the GB dislocation climb hampers the nanocrack generation and growth in the vicinities of triple junctions (see Fig. 3). These effects of the GB dislocation climb should be definitely taken into account in further experimental and theoretical studies of high-strain-rate superplasticity in nanocrystalline materials.

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