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RAPID COMMUNICATION

Strengthening mechanism for high-strain-rate superplasticity in nanocrystalline materials

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Abstract
A theoretical model is suggested that describes the strengthening of nanocrystalline materials under superplastic deformation due to the effects of triple junctions of grain boundaries (GBs) as obstacles for GB sliding. In the framework of the model, dependences of the yield stress for the GB sliding on parameters of defects and triple junctions are revealed. The results of the model account for experimental data from nanocrystalline materials exhibiting superplasticity, reported in the literature.

1. Introduction

Unique mechanical properties of nanocrystalline materials represent the subject of intensive studies in applied physics and materials science (see, e.g. [1–5]). Of particular interest is superplasticity exhibited by some nanocrystalline solids at relatively high strain rates and low temperatures [5–9]. It is characterized by very high flow stresses and strengthening [5–9] which are the specific features of superplastic nanocrystalline materials, differing their deformation behaviour from that of conventional microcrystalline materials exhibiting superplasticity. These features are the subject of growing fundamental interest [5–9] motivated by a range of new applications based on the use of superplasticity of nanocrystalline materials. In general, the outstanding mechanical properties of nanocrystalline materials are caused by deformation modes conducted by grain boundaries (GBs), which are often suppressed in conventional coarse-grained polycrystals (see, e.g. [10–17]). The dominant mode of superplasticity in nanocrystalline materials is viewed to be GB sliding [5–9], in which case the unusual strengthening should be related to the specific features of the GB sliding in nanocrystalline materials. The main aim of this paper is to suggest a theoretical model describing the strengthening in nanocrystalline materials exhibiting superplasticity as the phenomenon caused by transformations of GB dislocations—carriers of GB sliding—at triple junctions of GBs.

2. Model

Let us consider evolution of GB defects in a nanocrystalline solid under mechanical load. GBs with excess density of GB dislocations—carriers of GB sliding—often exist in as-fabricated nanocrystalline materials (see, e.g. [3, 7–9]). When a mechanical load is applied to the specimen, mobile GB dislocations (with Burgers vector being parallel to GB planes) move causing GB sliding (figure 1(*a*)). They are hampered at triple junctions of GBs that represent effective obstacles for dislocation movement. In nanocrystalline materials with their high-density ensembles of triple junctions, the critical shear stress needed for GB dislocations to overcome triple junctions specifies the contribution of GB sliding to the yield stress. Following [5–9], GB sliding is the dominant mode of superplasticity. In this context, the effects of triple junctions cause the critical shear stress and, therefore, the flow stress of superplastic deformation in nanocrystalline materials.

In this paper we will calculate the critical shear stress in the framework of the following first approximation model. We consider a model configuration of GB dislocations in a nanocrystalline material, which is formed near a triple junction under the action of shear stress τ (figure 1(*a*)). The configuration consists of two GB dislocations with the Burgers vectors $\boldsymbol{b}_1$ and $-\boldsymbol{b}_2$ (the $\boldsymbol{b}_1$- and $-\boldsymbol{b}_2$-dislocations, respectively) which are parallel to the corresponding GB planes adjacent to the triple junction. The GB dislocations are stopped in vicinity

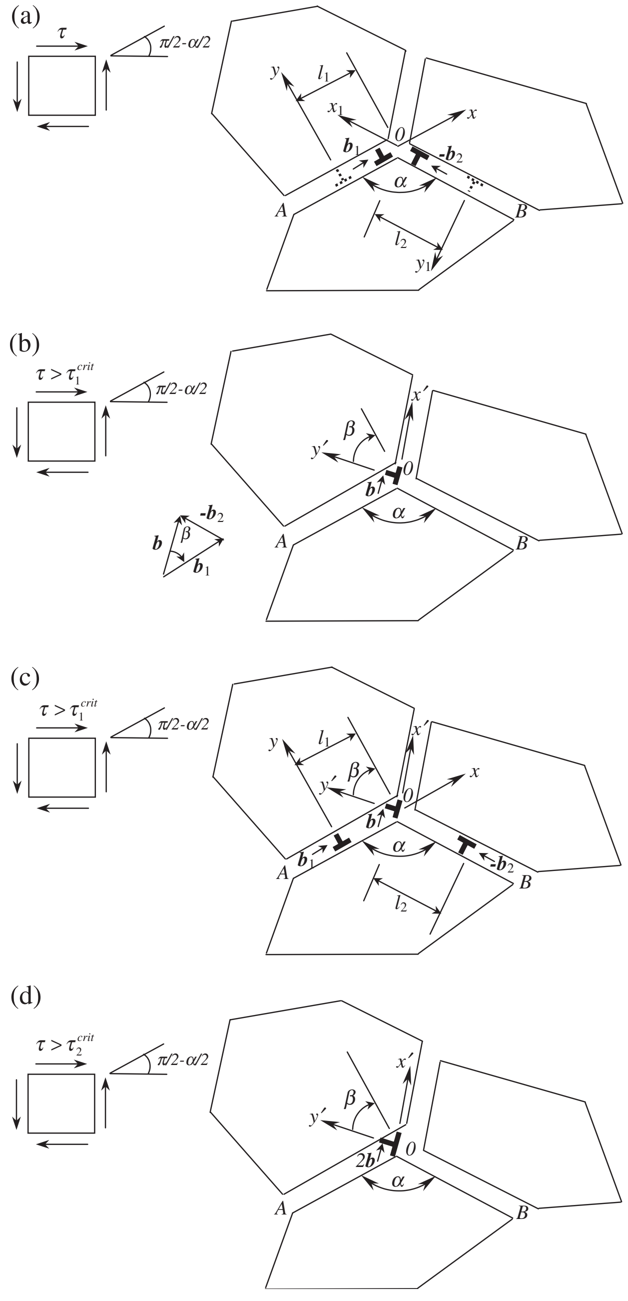

Figure 1. Transformations of GB dislocations near a triple junction. (*a*) Initial (0th) state of defect configuration. Two gliding GB dislocations move towards triple junction O. (*b*) Sessile dislocation with the Burgers vector $\boldsymbol{b}$ is formed. (*c*) Generation of two new gliding GB dislocations with the Burgers vectors $\boldsymbol{b}_1$ and $-\boldsymbol{b}_2$, that move towards the triple junction. (*d*) Sessile dislocation with the Burgers vector $2\boldsymbol{b}$ is formed.

of the triple junction when $\tau < \tau_1^{\rm crit}$. When the shear stress reaches its critical value $\tau_1^{\rm crit}$, the $\boldsymbol{b}_1$- and $-\boldsymbol{b}_2$-dislocations move over short distances l_1 and l_2, respectively, and 'meet' at the triple junction (figure 1(*b*)). It is accompanied by a dislocation reaction at the triple junction, which involves the $\boldsymbol{b}_1$- and $-\boldsymbol{b}_2$-dislocations and results in the formation of a sessile GB dislocation with the Burgers vector $\boldsymbol{b} = \boldsymbol{b}_1 - \boldsymbol{b}_2$ (the $\boldsymbol{b}$-dislocation) (see figure 1(*b*)). In the framework of our model, the process discussed is an elementary relaxation process of superplastic deformation of a nanocrystalline specimen under mechanical load.

After the dislocation reaction (figures 1(*a*) and (*b*)) at the triple junction has occurred, two new GB dislocations are generated and move under the shear stress action towards the triple junction (figure 1(*c*)). (For simplicity, hereinafter, we assume that all moving GB dislocations at boundary *AO* (*OB*, respectively) are characterized by the Burgers vector $\boldsymbol{b}_1$ ($-\boldsymbol{b}_2$, respectively).) These moving $\boldsymbol{b}_1$- and $-\boldsymbol{b}_2$-dislocations elastically interact with the sessile GB dislocation which hampers the movement of the new dislocations. At the stress level $\tau_2^{\rm crit} > \tau_1^{\rm crit}$, a new elementary act of GB sliding at the triple junction occurs. With the Burgers vector conservation law, the elementary act results in the formation of a new sessile dislocation with the Burgers vector $\boldsymbol{b} = \boldsymbol{b}_1 - \boldsymbol{b}_2$ (figure 1(*d*)). The new and pre-existent sessile dislocations converge resulting in the formation of a new sessile dislocation with the Burgers vector $2\boldsymbol{b} = 2(\boldsymbol{b}_1 - \boldsymbol{b}_2)$ (figure 1(*d*)).

The process under consideration repeatedly occurs which is accompanied by increase of the Burgers vector of the sessile dislocation by the vector $\boldsymbol{b} = \boldsymbol{b}_1 - \boldsymbol{b}_2$ at each step. Since the sessile dislocation hampers the moving GB dislocations, the critical shear stress increases with evolution of the defect structure. We think that this evolution namely is responsible for the experimentally detected strengthening [5–9] in nanocrystalline materials at the first long stage of superplastic deformation.

3. Results and discussion

Let us examine the energy characteristics of the reaction between GB dislocations at the *n*th step of the transformation process, that is, the transformation at a triple junction containing a sessile dislocation with the Burgers vector $(n-1)\boldsymbol{b}$ (the $(n-1)\boldsymbol{b}$-dislocation, see figures 1(*c*) and (*d*) in the exemplary case with $n = 2$). The transformation in question is characterized by the difference $\Delta W_n = W_n - W_{n-1}$ in the energy between the *n*th (W_n) and $(n-1)$th (W_{n-1}) states of the defect system; see figures 1(*c*) and (*d*), respectively. The transformation is energetically favourable, if $\Delta W_n < 0$. The set of critical parameters, including the critical shear stress for the GB sliding across the triple junction with the sessile $(n-1)\boldsymbol{b}$-dislocation, is derived from equation $\Delta W_n = 0$.

The energy W_{n-1} (per unit length of a GB dislocation) consists of six terms:

$$W_{n-1} = E_{\rm self}^{b_1} + E_{\rm self}^{b_2} + E_{\rm self}^{(n-1)b} + E_{\rm int}^{b_1-b_2} + E_{\rm int}^{b_1-(n-1)b} + E_{\rm int}^{b_2-(n-1)b}, \quad (1)$$

where $E_{\rm self}^{b_1}$, $E_{\rm self}^{b_2}$ and $E_{\rm self}^{(n-1)b}$ are the self-strain energies of the $\boldsymbol{b}_1$-, $-\boldsymbol{b}_2$- and $(n-1)\boldsymbol{b}$-dislocations, respectively, $E_{\rm int}^{b_1-b_2}$ is the energy of interaction between the mobile $\boldsymbol{b}_1$- and $-\boldsymbol{b}_2$-dislocations, and $E_{\rm int}^{b_1-(n-1)b}$ ($E_{\rm int}^{b_2-(n-1)b}$, respectively) is the energy of interaction of the $\boldsymbol{b}_1$-dislocation (the $-\boldsymbol{b}_2$-dislocation, respectively) with the $(n-1)\boldsymbol{b}$-dislocation.

The self-strain energies $E_{\rm self}^{b_1}$, $E_{\rm self}^{b_2}$ and $E_{\rm self}^{(n-1)b}$ are given by the standard formulae (e.g. [18]) as follows:

$$E_{\rm self}^{b_i} = \frac{Db_i^2}{2}\left(\ln\frac{R}{r_{{\rm c}_i}} + 1\right),$$
$$E_{\rm self}^{(n-1)b} = \frac{D((n-1)b)^2}{2}\left(\ln\frac{R}{(n-1)r_{\rm c}} + 1\right). \quad (2)$$

Here $D = G/[2\pi(1-\nu)]$, G denotes the shear modulus, ν the Poisson ratio, $r_{c_i} \approx r_c$ the cut-off radius of the stress fields of the $\boldsymbol{b}_1$- and $-\boldsymbol{b}_2$-dislocations, for $i = 1$ and 2, respectively, and R the screening length of the dislocation stress field.

The energy of elastic interaction between two defects can be calculated as the work spent to transfer one defect from a free surface of a solid to its current position in the stress field created by another defect [19]. In the framework of this approach, in our case with two GB dislocations (figure 1(c)), their interaction energy $E_{\rm int}^{b_1-b_2}$ can be calculated by using the formula:

$$E_{\rm int}^{b_1-b_2} = -b_1 \int_{-R}^{0} \tau_{xy}^{b_2}(x, y=0)\,{\rm d}x, \qquad (3)$$

where $\tau_{xy}^{b_2}$ is the shear stress which is induced by the $-\boldsymbol{b}_2$-dislocation and acts on the $\boldsymbol{b}_1$-dislocation. This stress is written as follows:

$$\tau_{xy}^{b_2}(x, y) = \tfrac{1}{2}(\sigma_{x_1x_1}^{b_2} - \sigma_{y_1y_1}^{b_2})\sin 2\alpha + \sigma_{x_1y_1}^{b_2}\cos 2\alpha, \qquad (4)$$

where the dislocation stress field components $\sigma_{x_1x_1}^{b_2}$, $\sigma_{y_1y_1}^{b_2}$ and $\sigma_{x_1y_1}^{b_2}$ are written in the coordinate system Ox_1y_1 associated with the Burgers vector $-\boldsymbol{b}_2$ and rotated by α relative to the coordinate system Oxy associated with the Burgers vector $\boldsymbol{b}_1$ (figure 1(a)). These components are given by the formulae [18] as:

$$\begin{aligned}
\sigma_{x_1x_1}^{b_2} &= -Db_2\frac{y_1(y_1^2+3x_1^2)}{(x_1^2+y_1^2)^2},\\
\sigma_{y_1y_1}^{b_2} &= Db_2\frac{y_1(x_1^2-y_1^2)}{(x_1^2+y_1^2)^2}, \qquad (5)\\
\sigma_{x_1y_1}^{b_2} &= Db_2\frac{x_1(x_1^2-y_1^2)}{(x_1^2+y_1^2)^2}.
\end{aligned}$$

In formulae (5), the coordinates (x_1, y_1) are in the following relationships with the coordinates (x, y):

$$\begin{aligned}
x_1 &= -(x-x_0)\cos\alpha + (y+y_0)\sin\alpha,\\
y_1 &= (x-x_0)\sin\alpha + (y+y_0)\cos\alpha,
\end{aligned} \qquad (6)$$

where $x_0 = l_1 - l_2\cos\alpha$, $y_0 = l_2\sin\alpha$, and α is the triple junction angle (figure 1).

With formulae (5) and (6), substitution of (4) to formula (3) yields:

$$\begin{aligned}
E_{\rm int}^{b_1-b_2} = Db_1b_2\Bigg(&\frac{1}{2}\cos\alpha\ln\left[1+\frac{R^2+2R(l_1-l_2\cos\alpha)}{l_1^2+l_2^2-2l_1l_2\cos\alpha}\right]\\
&-\frac{l_1l_2\sin^2\alpha}{l_1^2+l_2^2-2l_1l_2\cos\alpha}\\
&+\frac{2l_2(R+l_1)\sin^2\alpha}{R^2+2R(l_1-l_2\cos\alpha)+l_1^2+l_2^2-2l_1l_2\cos\alpha}\Bigg). \qquad (7)
\end{aligned}$$

The interaction energies $E_{\rm int}^{b_1-(n-1)b}$ and $E_{\rm int}^{b_2-(n-1)b}$ are calculated in the same way as the energy $E_{\rm int}^{b_1-b_2}$ (see formulae (3)–(7)). In doing so, we get:

$$E_{\rm int}^{b_1-(n-1)b} = D(n-1)bb_1\cos\beta\ln\frac{R+l_1}{l_1}, \qquad (8)$$

$$E_{\rm int}^{b_2-(n-1)b} = D(n-1)bb_2\cos(\beta-\alpha)\ln\frac{R+l_2}{l_2}. \qquad (9)$$

The energy of the defect configuration in its nth state (figure 1(b)) consists of three terms:

$$W_n = W_{\rm b} + A_\tau + E_{\rm self}^{nb}. \qquad (10)$$

Here $W_{\rm b}$ is the energetic barrier for movement of the $\boldsymbol{b}_1$- and $-\boldsymbol{b}_2$-dislocations in the triple junction area, A_τ is the work of the shear stress τ, spent to transfer the $\boldsymbol{b}_1$-dislocation over the distance l_1 and $-\boldsymbol{b}_2$-dislocation over the distance l_2, and $E_{\rm self}^{nb}$ denotes the self-strain energy of the sessile $n\boldsymbol{b}$-dislocation.

The atomic arrangement in the triple junction area is different from that in GB regions [20]. This causes the existence of the energetic barrier for GB dislocation movement within the triple junction area, which is assumed to be $W_{\rm b} = 0.5G\kappa(b_1^2 + b_2^2)$; this gives $W_{\rm b} = Gb_1^2\kappa$ in our case when $b_1 = b_2$ is also supposed. Here κ is the adjusting parameter being in the order of unity.

The work of the shear stress, spent to transfer GB dislocations is written in the standard way as:

$$A_\tau = \tau(b_1l_1 + b_2l_2)\cos\alpha. \qquad (11)$$

The self-strain energy of the sessile dislocation is given by the standard formula [18] (similar to formula (2)):

$$E_{\rm self}^{nb} = \frac{D(nb)^2}{2}\left(\ln\frac{R}{nr_c}+1\right). \qquad (12)$$

From figures 1(a) and (b), after some algebra, one finds the following relationships between the Burgers vector magnitudes b, b_1 and b_2, characterizing the sessile and the moving GB dislocations as well as geometric parameters of the triple junction:

$$\begin{aligned}
b^2 &= b_1^2 + b_2^2 + 2b_1b_2\cos\alpha,\\
\beta &= \operatorname{arcctg}(\operatorname{cosec}\alpha - \operatorname{ctg}\alpha).
\end{aligned} \qquad (13)$$

Here β is the angle by which the coordinate system (x', y') is rotated relative to the coordinate system (x, y) (figure 1(b)).

With formulae (1), (2), (7)–(13), we find the expression for the characteristic energy difference $\Delta W_n (= W_n - W_{n-1})$:

$$\begin{aligned}
\Delta W_n = {}& Gb_1^2\kappa + \tau(b_1l_1 + b_2l_2)\cos\alpha\\
&+ D\Bigg\{((b_1^2+b_2^2)(n-1)\\
&+ b_1b_2(2n-1)\cos\alpha)\left(\ln\frac{R}{r_c}+1\right)\\
&+ \frac{b^2}{2}[(n-1)^2\ln(n-1) - n^2\ln n] - b(n-1)\\
&\times\left(b_1\cos\beta\ln\frac{R+l_1}{l_1} + b_2\cos(\beta-\alpha)\ln\frac{R+l_2}{l_2}\right)\\
&+ b_1b_2\Bigg[-\frac{1}{2}\cos\alpha\ln\left(1+\frac{R^2+2R(l_1-l_2\cos\alpha)}{l_1^2+l_2^2-2l_1l_2\cos\alpha}\right)\\
&+ \frac{l_1l_2\sin^2\alpha}{l_1^2+l_2^2-2l_1l_2\cos\alpha}\\
&- \frac{2l_2(R+l_1)\sin^2\alpha}{R^2+2R(l_1-l_2\cos\alpha)+l_1^2+l_2^2-2l_1l_2\cos\alpha}\Bigg]\Bigg\}.
\end{aligned} \qquad (14)$$

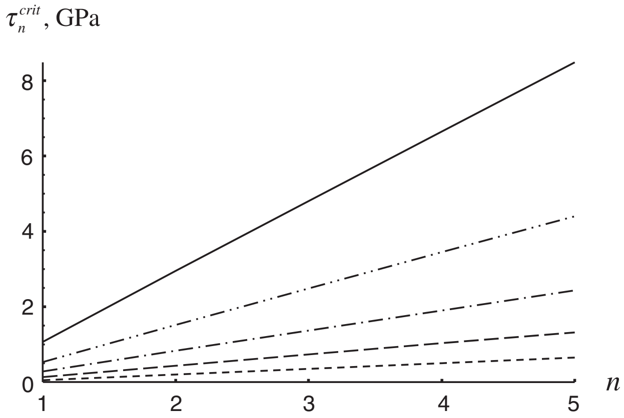

Figure 2. Dependence of critical shear stress $\tau_n^{\rm crit}$ on n, the number of the transformation step, for different values of the triple junction angle: $\alpha = 110°$, 120°, 130°, 140° and 150° (from top to bottom).

Now let us calculate the shear stress $\tau_n^{\rm crit}$ needed for the deformation act (figures 1(*c*) and (*d*)) to occur at a triple junction containing a sessile $(n-1)\boldsymbol{b}$-dislocation. This stress can be found from the condition that $\Delta W_n = 0$. In doing so, we have:

$$\tau_n^{\rm crit} = -\frac{1}{(b_1 l_1 + b_2 l_2)\cos\alpha} \times (E_{\rm self}^{nb} - E_{\rm self}^{(n-1)b} - E_{\rm int}^{b_1-(n-1)b} - E_{\rm int}^{b_2-(n-1)b} - E_{\rm self}^{b_1} - E_{\rm self}^{b_2} - E_{\rm int}^{b_1-b_2} + W_{\rm b}). \quad (15)$$

With formulae (7)–(13) and (15), we have numerically calculated the dependences $\tau_n^{\rm crit}$ on n, for different values of the angle α that characterizes geometry of the triple junction. The following values for the system parameters have been used in calculations: $G = 70$ GPa, $\nu = 0.314$, $b_1 = b_2 = 0.1$ nm, $l_1 = l_2 = l = 10$ nm, $R = 10^7$ nm, $r_{\rm c} = 0.05$ nm, and κ figuring in $W_{\rm b}$ has been assumed to be 1. These dependences are presented in figure 2, showing that $\tau_n^{\rm crit}$ increases with rising n (and, therefore, plastic strain ε). It is indicative of the strengthening.

4. Conclusions

Thus, in this paper, it has been theoretically revealed that superplastic deformation occurring through the GB sliding in nanocrystalline materials is characterized by strengthening due to transformations of gliding GB dislocations at triple junctions. Our theoretical analysis of the energy characteristics of the transformations has indicated that the transformations of GB dislocations at triple junctions (figure 1) are energetically favourable in certain ranges of parameters of the defect configuration. The corresponding flow stress is caused by $\tau_n^{\rm crit}$ which is highly sensitive to triple junction geometry characterized by angle α and plastic strain degree characterized by n (see figure 2). In particular, in the case of nearly equi-axed grains with α being close to 120°, the critical stress $\tau_n^{\rm crit}$ shows a substantial increase just for several deformation acts (just for $n < 10$) at triple junctions (see figure 2). This is in agreement with the experimentally detected [5–9] fact that nanocrystalline materials exhibit strengthening at the first extended stage of high-strain-rate superplastic deformation. The strengthening mechanism considered in this paper is specific for namely nanocrystalline materials where the volume fraction of triple junctions is extremely high, causing their crucial role in superplastic deformation processes.

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