Rotational Deformation Mechanism in Fine-Grained Materials Prepared by Severe Plastic Deformation

Mikhail Yu. Gutkin, Anna L. Kolesnikova, Ilya A. Ovid'ko and Nikolai V. Skiba

Institute of Problems of Mechanical Engineering
Russian Academy of Sciences
Bolshoj 61, Vas.Ostrov, St.Petersburg 199178, Russia
E-mail: ovidko@def.ipme.ru

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Abstract. A theoretical model is suggested which describes the rotational deformation mechanism in fine-grained materials prepared by severe plastic deformation. In the framework of the model, the rotational deformation occurs via the motion of grain boundary disclination dipoles, associated with emission of dislocation pairs from grain boundaries into the adjacent grain interiors. Energetic characteristics of the disclination dipole motion are calculated. Ranges of parameters of the defect system are revealed at which the disclination motion is energetically favourable. It is shown that the rotational deformation mechanism associated with the emission of dislocation pairs is capable of essentially contributing to plastic flow in fine-grained materials prepared by severe plastic deformation.

1 Introduction

Grain boundaries (GBs) in nano- and polycrystalline materials often undergo the transformations strongly influencing both the structure and the properties of such materials, e. g., [1–17]. Thus, the processes of plastic deformation in fine-grained polycrystals are associated with GB sliding, GB migration, GB diffusion, re-arrangements of GB ensemble, grain rotations, etc. [1–12]. In particular, the changes of misorientation parameters of GBs, that are capable of resulting in the grain rotations, have been experimentally detected in fine-grained materials under (super)plastic deformation (see, e. g., [1–4]). Recently, grain rotations have also been observed experimentally in thin polycrystalline films of gold under thermal treatment [18]. According to the theoretical representations on GBs, changes of their misorientation parameters occur via the motion of GB disclinations, defects of the rotational type [5, 19, 20]. Such disclinations are intensively formed in nano- and polycrystalline materials during their fabrication at highly non-equilibrium conditions [21]. In particular, the GB disclinations are inherent to the structure of the fine-grained materials prepared by severe plastic deformation [22–24]. In these circumstances, the motion of disclination dipoles is capable of causing the rotational mode of plastic deformation essentially contributing to the plastic flow in such fine-grained materials.

Motion of GB disclinations in plastically deformed solids is commonly treated as that associated with absorption of lattice dislocations (that are generated and move in grains under the action of mechanical load) by GBs [4, 5]. This micromechanism, according to paper [4], is responsible for the grain rotations observed experimentally in fine-grained materials during (super)plastic deformation. However, the consequent motion of a GB disclination requires the processes of dislocation absorption by the GB to be well ordered in space and time. In particular, lattice dislocations with certain Burgers vectors have to reach a GB in only vicinity of the disclination that moves along the boundary plane due to the acts of absorption of these dislocations. This is in an evident contradiction with the fact that the sources of lattice dis-

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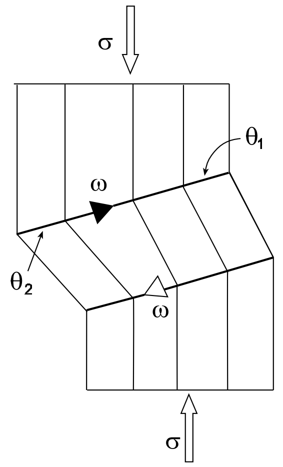

Fig. 1. Motion of a disclination dipole may be considered as similar to the motion of a (super)dislocation.

locations in plastically deformed materials are commonly distributed in a rather irregular way within a grain and, therefore, are not capable to provide a regular flow of the dislocations to the disclination moving along a GB. Also, in the situation with the grain rotations in thin films of gold under thermal treatment [18], the absorption of lattice dislocations by GBs hardly plays an important role in the changes of boundary misorientation parameters, because the dislocation density in grain interiors is too low to cause the grain rotations. With the aforesaid taken into account, we think that the evolution of boundary misorientation parameters and the rotational deformation occur mostly via the motion of the GB disclinations and their dipoles, associated with the emission of dislocation pairs from the GBs into the adjacent grain interiors. The evidence of disclination motion through issuing dislocations follows from the general geometric theory of disclinations (see, e. g., [25, 26]) as well as from simple dislocation models of partial disclinations in crystals [5, 26]. The main aim of this paper is to suggest a theoretical model which describes the rotational mode of plastic flow in the fine-grained materials prepared by severe plastic deformation as that occurring via the motion of GB disclination dipoles, associated with the emission of pairs of lattice dislocations.

2 Motion of dipoles of grain boundary disclinations, associated with emission of dislocation pairs. Key aspects

Following the theory of GBs, the two fragments of a GB that are characterized by different values of misorientation parameter are divided by a disclination, a line defect of the rotational type; see, e.g., [5, 19, 20]. More precisely, the line that separates the two tilt boundary fragments with the different misorientation parameters θ_1 and θ_2, respectively, is described as the line of a GB wedge disclination with the strength $\omega = \theta_1 - \theta_2$ (Fig. 1). In the framework of the discussed representations, the evolution (in time) of misorientation along the GBs is treated as that related to the motion of GB disclinations [5, 19]. Motion of dipoles of the GB disclinations may be considered as similar to the motion of (super)dislocations and essentially contributes to high-strain deformation (Fig. 1) [5].

Let us consider a model which describes the rotational deformation in a fine-grained material, occurring via the stress-induced motion of a dipole of GB disclinations. In the framework of the model, the dipole consists of two GB disclinations with the strengths $+\omega$ and $-\omega$, respectively, and has the arm L. The disclination of the strength $+\omega$ ($+\omega$-disclination) transfers by the

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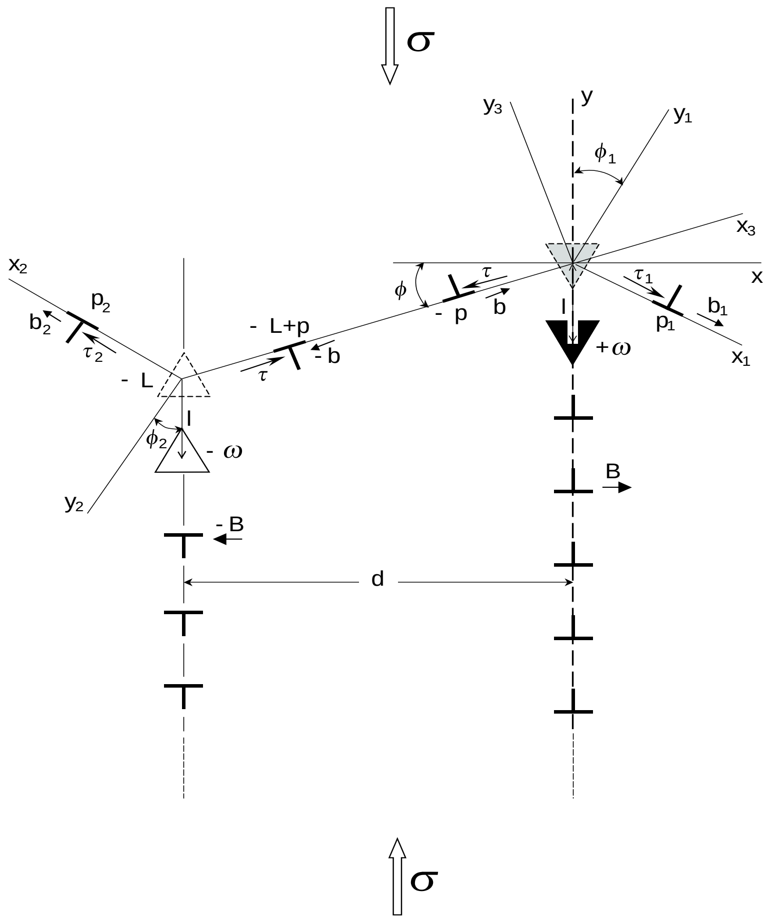

Fig. 2. Motion of a dipole of grain boundary disclinations is accompanied by emission of lattice dislocations from the grain boundaries into the adjacent grains. The dislocation slip planes are inclined at the angles ϕ, ϕ_1 and ϕ_2 to the x-axis.

distance l due to the emission of two lattice dislocations with the Burgers vectors $\boldsymbol{b}$ and $\boldsymbol{b}_1$ into the adjacent grains (Fig. 2). The dislocation with the Burgers vector $\boldsymbol{b}$ moves along its gliding plane towards the disclination of the strength $-\omega$ ($-\omega$-disclination). This disclination moves by the distance l in the same direction as the $+\omega$-disclination due to the emission of two lattice dislocations with the Burgers vectors $-\boldsymbol{b}$ and $\boldsymbol{b}_2$ into the abutting grains (Fig. 2). The dislocations with the Burgers vector $\boldsymbol{b}$ and $-\boldsymbol{b}$, emitted by respectively the $+\omega$- and $-\omega$-disclinations, annihilate.

The model under consideration (Fig. 2) describes in the first approximation the real situation where disclinations with various values of strength are distributed in a rather disordered manner along non-equilibrium grain boundaries formed during severe plastic deformation. In a real fine-grained material fabricated by severe deformation method, a lattice dislocation emitted by a $+\omega$-disclination may recombine with the disclination of strength $-\omega'$ ($\neq -\omega$) located on the same slip plane in the facing GB. It is not reflected in our model (Fig. 2). In addition, grain interiors of a fine-grained material contain many lattice dislocations generated during severe plastic deformation. These dislocations are capable of interacting and annihilating with the dislocations emitted by GB disclinations. Thus, real processes occurring during motion of GB disclinations can be very complicated and different from those described by a first approximation model suggested here. However, the model discussed (Fig. 2) is convenient for

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a strict mathematical analysis and effective for understanding the key peculiarities of the GB disclination motion accompanied by emission of lattice dislocations. Also, the model can serve as a basis for further detailed consideration of evolution of GB defects in plastically deformed fine-grained materials.

The cooperative motion of the GB disclinations composing the dipole causes the plastic deformation of a fine-grained material. Following [5], the plastic deformation associated with transfer of a disclination dipole is equivalent to that associated with the motion of a (super)dislocation characterized by the Burgers vector magnitude $B = 2d\tan(\omega/2)$ ($\approx \omega d$ at small ω), where d is the distance between the planes along which the disclinations move (Fig. 2).

3 Energetic characteristics of disclination dipole motion associated with emission of dislocation pairs

Let us examine the energetic characteristics of the disclination motion under consideration. The disclination motion is energetically favourable, if the difference, $\Delta W = W_2 - W_1$, between the system energy densities (per unit disclination length) after (W_2) and before (W_1) the dipole elementary transfer is negative ($\Delta W < 0$).

The energy of the disclination dipole in its initial state (before the transfer) is its proper strain energy given as [5]:

$$W_1 = E_d = \frac{D\omega^2 L^2}{2}\left(\ln\frac{R}{L} + \frac{1}{2}\right), \tag{1}$$

Here $D = G/2\pi(1-\nu)$, G denotes the shear modulus, ν the Poisson ratio, and R the screening length of stress fields of the disclination dipole.

After the external stress has applied, the disclination dipole has moved in accordance to the scenario discussed above (see Fig. 2). The disclination dipole motion is accompanied by the emission of the lattice dislocations, in which case the energy density W_2 of the defect system consists of the five following terms:

$$W_2 = E_d + E_{b_1} + E_{b_2} + E_{bb} + E_{int}\ , \tag{2}$$

Here E_{b_1} and E_{b_2} are the proper energies of the emitted dislocations with the Burgers vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$, respectively; E_{bb} is the proper energy of the dislocation dipole consisting of the emitted dislocations with Burgers vectors $\boldsymbol{b}$ and $-\boldsymbol{b}$; and E_{int} is the sum energy that characterizes all the interactions between the defects composing the system (Fig. 2) (except between both the disclinations whose interaction energy is included in E_d), and between the defects and the applied stress σ.

The energy E_{int} can be decomposed into nine terms as follows:

$$E_{int} = E_d^{b_1} + E_d^{b_2} + E_d^{bb} + E_{b_2}^{b_1} + E_{bb}^{b_1} + E_{bb}^{b_2} + E_\sigma^{b_1} + E_\sigma^{b_2} + E_\sigma^{bb}\ , \tag{3}$$

Here $E_d^{b_1}$, $E_d^{b_2}$ and E_d^{bb} denote the energies that characterize the interaction of the disclination dipole with respectively the dislocations with the Burgers vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$, and the dislocation dipole; $E_{b_1}^{b_2}$ is the energy of the interaction between the emitted dislocations with the Burgers vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$; $E_{bb}^{b_1}$ and $E_{bb}^{b_2}$ denote the energies that characterize the interaction of the dislocation dipole with the dislocations having the Burgers vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$, respectively; $E_\sigma^{b_1}$, $E_\sigma^{b_2}$ and E_σ^{bb} are the energies that characterize the interaction of the applied stress σ with respectively the emitted dislocations having the Burgers vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$, and the dislocation dipole.

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Let us consider the energies figuring on the r.h.s. of formula (2). The proper energies of the dislocations are given by the following well-known [27] formula:

$$E_{b_i} = \frac{Db_i^2}{2}\left(\ln\frac{R}{r_c}+1\right), \tag{4}$$

where $i = 1, 2$ and r_c is the dislocation core radius (assumed to be the same for all the dislocations shown in Fig. 2).

Let us examine the proper energy E_{bb} of the dislocation dipole in the coordinate system $(x_3y_3z_3)$ associated with it (see Fig. 2). In accordance to the general approach [28], the energy E_{bb} can be written via the dipole stress tensor σ_{ik}^{bb} components as follows:

$$E_{bb} = -\frac{b}{2}\int_{-L+p+r_c}^{-p-r_c} \sigma_{x_3y_3}^{bb}(x_3, y_3=0)\,dx_3\,. \tag{5}$$

The formula for the $\sigma_{x_3y_3}^{bb}$-component of the dislocation dipole stress tensor, figuring on the r.h.s. of (5), is given by [27]:

$$\sigma_{x_3y_3}^{bb} = Db\left\{\frac{(x_3+L-p)[y_3^2-(x_3+L-p)^2]}{[y_3^2+(x_3+L-p)^2]^2} - \frac{(x_3+p)[y_3^2-(x_3+p)^2]}{[y_3^2+(x_3+p)^2]^2}\right\}. \tag{6}$$

From (5) and (6) we have:

$$E_{bb} = Db^2\left(\ln\frac{|L-2p-r_c|}{r_c}+1\right), \tag{7}$$

where the last term "1" in the brackets is introduced to take the dislocation core energies into account.

The energy that characterizes the interaction between the disclination dipole and the dislocation with the Burgers vector $\boldsymbol{b}_1$ can be written as follows:

$$E_d^{b_1} = b_1\int_{p_1}^{R} \tau_d^{b_1}(x_1, y_1=0)\,dx_1\,. \tag{8}$$

Here $\tau_d^{b_1}$ is the disclination-dipole-induced shear stress acting in the gliding plane of the dislocation under consideration. In the (xyz) coordinate system shown in Fig. 2 (with the z-axis being parallel with the disclination lines), the non-vanishing components of the disclination dipole stress tensor may be adapted from [5] as

$$\begin{aligned}
\sigma_{xx}^d &= D\omega\left\{\frac{(y+l)^2}{x^2+(y+l)^2} - \frac{(y+L\sin\phi+l)^2}{(x+L\cos\phi)^2+(y+L\sin\phi+l)^2}\right.\\
&\qquad\left.+\frac{1}{2}\ln\frac{x^2+(y+l)^2}{(x+L\cos\phi)^2+(y+L\sin\phi+l)^2}\right\},\\
\sigma_{yy}^d &= D\omega\left\{\frac{x^2}{x^2+(y+l)^2} - \frac{(x+L\cos\phi)^2}{(x+L\cos\phi)^2+(y+L\sin\phi+l)^2}\right.\\
&\qquad\left.+\frac{1}{2}\ln\frac{x^2+(y+l)^2}{(x+L\cos\phi)^2+(y+L\sin\phi+l)^2}\right\},\\
\sigma_{zz}^d &= \nu\left(\sigma_{xx}^d+\sigma_{yy}^d\right),\\
\sigma_{xy}^d &= D\omega\left\{\frac{(x+L\cos\phi)(y+L\sin\phi+l)}{(x+L\cos\phi)^2+(y+L\sin\phi+l)^2} - \frac{x(y+l)}{x^2+(y+l)^2}\right\}.
\end{aligned} \tag{9}$$

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These components cause the shear stress $\tau_d^{b_1}$ acting in the gliding plane of the emitted dislocation with the Burgers vector $\boldsymbol{b}_1$ along the x_1-axis of the $(x_1y_1z_1)$ coordinate system (Fig. 2). From the geometry of the (xyz) and $(x_1y_1z_1)$ coordinate systems shown in Fig. 2, we find:

$$\tau_d^{b_1} = \sigma_{xx}^d \alpha_1\alpha_2 + \sigma_{yy}^d \beta_1\beta_2 + \sigma_{xy}^d(\alpha_1\beta_2 + \alpha_2\beta_1) \; , \tag{10}$$

where α_1, α_2, β_1 and β_2 are defined as follows:

$$\begin{aligned} \alpha_1 &= \cos(x_1, x) = \cos\phi_1 \; , \quad \beta_1 = \cos(x_1, y) = -\sin\phi_1 \; , \\ \alpha_2 &= \cos(x_2, x) = \sin\phi_1 \; , \quad \beta_2 = \cos(x_2, y) = \cos\phi_1 \; . \end{aligned} \tag{11}$$

With formulae (9), (10) and (11), the disclination shear stress $\tau_d^{b_1}$ reads:

$$\begin{aligned} \tau_d^{b_1} = D\omega \Bigg\{ & \frac{\sin 2\phi_1}{2} \left(\frac{(y+l)^2 - x^2}{x^2 + (y+l)^2} + \frac{(x + L\cos\phi)^2 - (y + L\sin\phi + l)^2}{(x + L\cos\phi)^2 + (y + L\sin\phi + l)^2} \right) \\ & + \cos 2\phi_1 \left(\frac{(x + L\cos\phi)(y + L\sin\phi + l)}{(x + L\cos\phi)^2 + (y + L\sin\phi + l)^2} - \frac{x(y+l)}{x^2 + (y+l)^2} \right) \Bigg\} , \end{aligned} \tag{12}$$

where l is the distance between the GB dislocations composing a ragged dislocation wall terminated by a disclination. This distance is expressed through the Burgers vector $\boldsymbol{B}$ of the GB dislocations and the disclination Frank vector magnitude ω as follows:

$$l \approx |\boldsymbol{B}|/\omega \; , \tag{13}$$

where $\boldsymbol{B}$ and other geometric characteristics of the defect configuration under consideration satisfy the following relationships: $|\boldsymbol{B}| = |\boldsymbol{b}_1|\cos\phi_1 + |\boldsymbol{b}|\cos\phi$ and $|\boldsymbol{b}_1|/|\boldsymbol{b}| = \sin\phi/\sin\phi_1$. As a result, we have

$$l \approx \frac{|\boldsymbol{b}|\sin(\phi + \phi_1)}{\omega\sin\phi_1} \; . \tag{14}$$

Integration in formula (8) is made along the x_1-axis of the $(x_1y_1z_1)$ coordinate system, in which case we need the shear stress to be written in this coordinate system. Since the integration in formula (8) is made at $y_1 = 0$, the coordinate transformation is as follows:

$$x = x_1\cos\phi_1, \qquad y = -x_1\sin\phi_1 \; . \tag{15}$$

With (15), from formula (12) we have:

$$\tau_d^{b_1} = D\omega L \frac{[l\cos\phi - x_1\sin(\phi_1 + \phi)]\{l[L\cos(\phi_1 + 2\phi) + l\cos 2\phi_1] - x_1[L\cos(\phi_1 + \phi) - 2l\sin\phi_1] - x_1^2\}}{(l^2 - 2lx_1\sin\phi_1 + x_1^2)\{L^2 + l^2 + 2Ll\sin\phi + 2x_1[L\cos(\phi_1 + \phi) - l\sin\phi_1] + x_1^2\}} . \tag{16}$$

With (16) substituted into Eq.(8), after integration, we find the energy $E_d^{b_1}$ to be given as:

$$E_d^{b_1} = \frac{D\omega b_1}{2} \Psi(p_1, \phi, \phi_1) \; , \tag{17}$$

where the denotation

$$\begin{aligned} \Psi(p_1, \phi, \phi_1) = & -l\cos\phi_1 \ln\frac{R^2 + l^2 - 2Rl\sin\phi_1}{p_1^2 + l^2 - 2p_1 l\sin\phi_1} \\ & + [l\cos\phi_1 + L\sin(\phi + \phi_1)] \ln\frac{L^2 + R^2 + l^2 + 2LR\cos(\phi + \phi_1) + 2Ll\sin\phi - 2Rl\sin\phi_1}{L^2 + p_1^2 + l^2 + 2Lp_1\cos(\phi + \phi_1) + 2Ll\sin\phi - 2xl\sin\phi_1} \end{aligned} \tag{18}$$

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is used.

The energies $E_d^{b_2}$ and E_d^{bb} that characterize respectively the interaction between the disclination dipole and the dislocation with the Burgers vector $\boldsymbol{b}_2$, and the interaction between the disclination dipole and the dislocation dipole can be found in the same way as with $E_d^{b_1}$. In doing so, we have:

$$E_d^{b_2} = \frac{D\omega b_2}{2}\,\Psi(p_2, -\phi, -\phi_2) \tag{19}$$

and

$$E_d^{bb} = -\frac{D\omega bl}{2}\cos\phi \ln\frac{(L-p)^4 + l^4 + 2(L-p)^2 l^2 \cos 2\phi}{p^4 + l^4 + 2p^2 l^2 \cos 2\phi}\,. \tag{20}$$

Now let us calculate the energy $E_{b_2}^{b_1}$ characterizing the interaction between the dislocations with the Burgers vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$. This energy can be written in an integral form as follows:

$$E_{b_2}^{b_1} = b_2 \int_{p_2}^{R} \tau_{b_1}^{b_2}(x_2, y_2 = 0)\, dx_2\,, \tag{21}$$

where $\tau_{b_1}^{b_2}$ is the shear stress induced by the dislocation with the Burgers vector $\boldsymbol{b}_1$ and acting on the dislocation with the Burgers vector $\boldsymbol{b}_2$ during the motion of the latter along its slip plane. The stress components in the $(x_1 y_1 z_1)$ coordinate system, which contribute to the shear stress $\tau_{b_1}^{b_2}$, read [27]

$$\begin{aligned}
\sigma_{x_1x_1}^{b_1} &= -Db_1 \frac{y_1[y_1^2 + 3(x_1-p_1)^2]}{[(x_1-p_1)^2 + y_1^2]^2}\,,\\
\sigma_{y_1y_1}^{b_1} &= Db_1 \frac{y_1[(x_1-p_1)^2 - y_1^2]}{[(x_1-p_1)^2 + y_1^2]^2}\,,\\
\sigma_{x_1y_1}^{b_1} &= Db_1 \frac{(x_1-p_1)[(x_1-p_1)^2 - y_1^2]}{[(x_1-p_1)^2 + y_1^2]^2}\,.
\end{aligned} \tag{22}$$

Owing to geometry of the defect system (Fig. 2), the following substitutions of the coordinates in formula (22) are valid:

$$\begin{aligned}
x_1 &= -L\cos(\phi_1 + \phi) - x_2\cos(\phi_2 - \phi_1)\,,\\
y_1 &= -L\sin(\phi_1 + \phi) + x_2\sin(\phi_2 - \phi_1)\,.
\end{aligned} \tag{23}$$

The shear stress $\tau_{b_1}^{b_2}(x_2, y_2 = 0)$ is now calculated in analogy to the procedure described by equations (10)-(12), with using the stress components (22) and the coordinate transformations (23). The corresponding expression for $\tau_{b_1}^{b_2}(x_2, y_2 = 0)$ is then inserted to Eq. (21) and integrated to obtain $E_{b_2}^{b_1}$. Thus, after some algebra, we find:

$$E_{b_2}^{b_1} = -Db_1 b_2 \left(\frac{S_1 S_2}{P^2} + \cos(\phi_1 - \phi_2)\ln\frac{R}{|P|}\right), \tag{24}$$

where the following denotations

$$\begin{aligned}
S_1 &= p_1\sin(\phi_1 - \phi_2) - L\sin(\phi + \phi_2)\,,\\
S_2 &= p_2\sin(\phi_1 - \phi_2) + L\sin(\phi + \phi_1)\,,\\
P^2 &= L^2 + p_1^2 + p_2^2 + 2p_1p_2\cos(\phi_1 - \phi_2) + 2Lp_1\cos(\phi + \phi_1) + 2Lp_2\cos(\phi + \phi_2)
\end{aligned} \tag{25}$$

are used.

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The energies $E_{bb}^{b_1}$ and $E_{bb}^{b_2}$ that characterize the interactions between the dislocation dipole and the dislocations with the Burgers vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$, respectively, can be written in an integral form as follows:

$$E_{bb}^{b_i} = b_i \int_{p_i}^{R} \tau_{bb}^{b_i}(x_i, y_i = 0)\, dx_i \,, \tag{26}$$

with $i = 1, 2$. The calculation of the integral figuring on the r.h.s. of Eq. (26) is made in the same way as with the other integrals considered in this section. The shear stress induced by the dislocation dipole and acting on the dislocation with the Burgers vector $\boldsymbol{b}_i$, is calculated in accordance to formulae (10) and (11). After the expression for the shear stress have been re-written in the coordinates (x_i, y_i) and substituted into the integral (26), we find the following formula for $E_{bb}^{b_i}$:

$$E_{bb}^{b_i} = \frac{Dbb_i}{2}\, \Phi(p_i, \phi, \phi_i) \tag{27}$$

with

$$\Phi(p_i, \phi, \phi_i) = \cos(\phi + \phi_i) \ln \frac{(L-p)^2 + p_i^2 + 2(L-p)p_i \cos(\phi + \phi_i)}{p^2 + p_i^2 + 2pp_i \cos(\phi + \phi_i)} - \frac{2p_i(L-2p)(p^2 + p_i^2 - Lp)\sin^2(\phi + \phi_i)}{[(L-p)^2 + p_i^2 + 2(L-p)p_i \cos(\phi+\phi_i)][p^2 + p_i^2 + 2pp_i\cos(\phi+\phi_i)]} \,. \tag{28}$$

The work spent to transfer (under the action of an external stress σ) the dislocation with the Burgers vector $\boldsymbol{b}_i$ over the distance p_i along the dislocation slip plane is

$$E_\sigma^{b_i} = -\tau_i b_i p_i \,. \tag{29}$$

Here τ_i is the shear stress acting on the dislocation with the Burgers vector $\boldsymbol{b}_i$ along its slip plane. From geometry of the defect system under consideration (Fig. 2) we have:

$$\tau_i = \frac{\sigma}{2} \sin 2\phi_1 \,. \tag{30}$$

With Eqs. (29) and (30), the energy $E_\sigma^{b_i}$ reads:

$$E_\sigma^{b_i} = -\frac{\sigma}{2}\, b_i p_i \sin 2\phi_i \,. \tag{31}$$

The work E_σ^{b} consumed on transferring the dislocations composing the dipole configuration (Fig. 2), is calculated in the same way as $E_\sigma^{b_i}$, in which case we find:

$$E_\sigma^{b} = -\frac{\sigma}{2}\, bp \, \sin 2\phi \,. \tag{32}$$

With all the formulae for the constituents of the total energies W_1 and W_2, we find $\Delta W = W_2 - W_1$ to be as follows:

$$\Delta W = \frac{D}{2} \left\{ (b_1^2 + b_2^2)\left(\ln \frac{R}{r_c} + 1\right) + 2b^2 \left(\ln \frac{|L - 2p - r_c|}{r_c} + 1\right) - 2b_1 b_2 \left(\frac{S_1 S_2}{P^2} + \cos(\phi_1 - \phi_2) \ln \frac{R}{|P|}\right) - \frac{\sigma}{D}\,(2bp \sin 2\phi + b_1 p_1 \sin 2\phi_1 + b_2 p_2 \sin 2\phi_2) + b\,[b_1 \Phi(p_1, \phi, \phi_1) + b_2 \Phi(p_2, \phi, \phi_2)] + \omega\,[b_1 \Psi(p_1, \phi, \phi_1) + b_2 \Psi(p_2, -\phi, -\phi_2)] - \omega bl \, \cos\phi \, \ln \frac{(L-p)^4 + l^4 + 2(L-p)^2 l^2 \cos 2\phi}{p^4 + l^4 + 2p^2 l^2 \cos 2\phi} \right\} . \tag{33}$$

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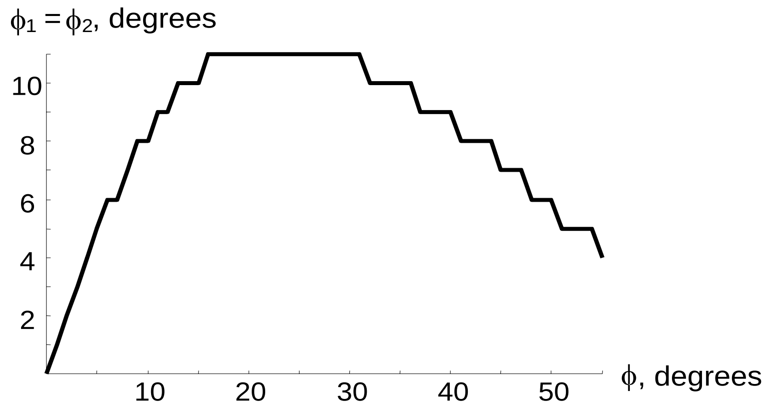

Fig. 3. ϕ-dependence of the angles ϕ_1 and $\phi_2(=\phi_1)$ corresponding to the minimum of the energy difference ΔW, for the following parameters of the model: $\omega = 0.1$, $p_1 = p_2 = p = b$, $\sigma = 5 \cdot 10^{-3}\, G$, $R = 10^7\, b$ and $L = 1000\, b$.

4 Results

Let us present the results of our model as numerically calculated relationships (given by Eq. (33)) between the parameters of the system under consideration. Thus, the dependences of the characteristic angles ϕ_1 and ϕ_2 on the angle ϕ are shown in Fig. 3, in the case with $\phi_1 = \phi_2$. These dependences, for the given values of ϕ, indicate the angles ϕ_1 and ϕ_2 at which the disclination dipole motion (Fig. 2) is characterized by the lowest value ΔW_{min} (where $\Delta W < 0$) of the energy difference (33) that corresponds to the start of the disclination dipole motion (or, in other words, by the largest energy gain due to the start of motion of emitted lattice dislocations, associated with the process in question). In doing so, for simplicity, we restrict ourselves to consideration of the characteristic range of ϕ from $0°$ to $55°$. As it follows from Fig. 3, the angles ϕ_1 and $\phi_2(=\phi_1)$ (corresponding to the minimum of ΔW) increase with rising ϕ from $0°$ to $\approx 15°$, have the constant value of $\approx 11°$ in the range of ϕ from $\approx 15°$ to $\approx 30°$, and decrease from $\approx 11°$ to $\approx 4°$ with rising ϕ from $\approx 30°$ to $\approx 55°$.

The angles ϕ_1 and $\phi_2(=\phi_1)$ that correspond to the minimum of the energy difference ΔW, weakly depend on the other parameters (L, σ, ω) of the system. At the same time, the minimum value ΔW_{min} of this characteristic energy difference is sensitive to the parameters discussed. In Fig. 4, the dependences of ΔW_{min} on the disclination dipole arm L are presented for various values of the angle ϕ. It follows from Fig. 4 that the disclination dipole motion is energetically favourable ($\Delta W_{min} < 0$), if the dipole arm L exceeds a critical value L_c which is ϕ-dependent and close to $\approx 150b \approx 50$ nm. In the range of ϕ from $1°$ to tentatively $30°$, the dependences $\Delta W_{min}(L)$ coincide; they are presented as curve 1 in Fig. 4. The dependences $\Delta W_{min}(L)$ at $\phi = 40°$ and $50°$ (see curves 2 and 3, respectively, in Fig. 4) are different from those at $\phi \leq 30°$. They indicate that $\Delta W_{min}(L)$ slightly decreases with rising ϕ from $30°$ to $50°$. To summarize, $\Delta W_{min} < 0$, i.e. the disclination dipole motion (Fig. 2) is an energetically favourable process in certain ranges of parameters that characterize the defect configuration under consideration.

We have considered the ranges of parameters at which the disclination dipole motion and the associated plastic deformation are energetically favourable. In general, the lattice dislocations emitted into the adjacent grain interiors during the motion of the grain boundary disclinations (Fig. 2) exhibit the correlated behavior, if the influence of other dislocations in grain interiors is neglected. However, it is not the case with the fine-grained materials fabricated by severe

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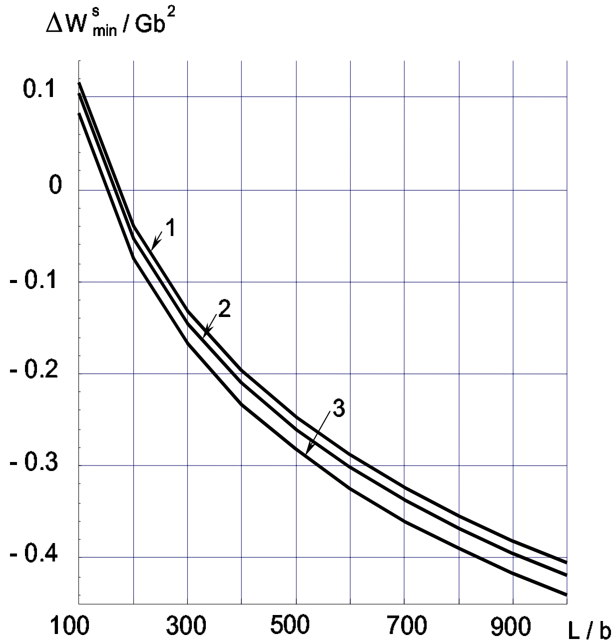

Fig. 4. Dependence of the energy difference ΔW on the disclination dipole arm L, for the following parameters of the model: $\omega = 0.1$, $p_1 = p_2 = p = b$, $\sigma = 5 \cdot 10^{-3}\, G$, $R = 10^7\, b$ and $\phi = 30°$ (curve 1), $40°$ (2) and $50°$ (3).

plastic deformation which produces high-density ensembles of lattice dislocations in the grain interiors. Such deformation-produced dislocations are also capable of affecting the energetic characteristics of the disclination dipole motion (Fig. 2). Due to this effect, the disclination dipole motion is either facilitated or hampered in local regions of a deformed specimen, depending on spatial arrangement of deformation-produced dislocations near the moving grain boundary disclinations. A detailed analysis of these processes (which needs detailed information on dislocation ensembles in the grain interiors as input) is beyond the scope of this paper.

5 Concluding remarks

In this paper, it has been theoretically revealed that the rotational mode of plastic flow in the fine-grained materials produced by severe plastic deformation can effectively occur via the grain boundary disclination dipole motion associated with the emission of dislocation pairs into the adjacent grains (Fig. 2). Our theoretical analysis of energetic characteristics of the grain boundary disclinations which move emitting the dislocation pairs, has indicated that the disclination dipole motion in question is energetically favourable in certain ranges of parameters of the system. In contrast to the previously considered [3, 4] situation with the disclination motion associated with the absorption (ordered in space and time) of dislocations by grain boundaries, the disclination dipole motion associated with the emission of dislocation pairs does not require any correlated flux of dislocations from grain interiors to grain boundaries. The suggested micromechanism for the disclination motion (Fig. 2) can be responsible for the rotations of grains experimentally observed [1–4, 18] in the fine-grained materials under (super)plastic deformation and thermal treatment. The disclination dipole motion associated with the emission of dislocation pairs is capable of effectively contributing to the plastic deformation in the fine-grained materials fabricated by severe plastic deformation, where the density of grain boundary disclinations is expected to be very high. With results of this paper, the role of the rotational mode

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of plastic flow should be taken into account in future experimental and theoretical studies of the outstanding mechanical properties of the fine-grained materials fabricated by severe plastic deformation.

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