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Analysis of the conditions of crack nucleation during lattice dislocations transition through grain boundary

V.N. Perevesentsev[1], S.V. Kirikov[1]✉, N.Yu. Zolotorevsky[1,2]

[1]Mechanical Engineering Research Institute of the Russian Academy of Sciences, 603024, Nizhny Novgorod, Russia

[2]Peter the Great St. Petersburg Polytechnic University, Polytekhnicheskaya 29, 195251, St. Petersburg, Russia

✉ ksv.kirikov@yandex.ru

Abstract. The formation of deformation facets at high-angle grain boundaries during their interaction with lattice dislocation pile-ups is accompanied by the appearance of wedge disclination dipoles disposed on the plane of the facets. Their elastic energy increases as the dislocations of pile-up penetrate the grain boundary and the deformation facet lengthens. A possibility was considered for the relaxation of elastic energy of the disclination dipole and the pile-up stored in the vicinity of the facet. A concept of the least possible length of the crack in a crystalline solid was introduced, and an energetic criterion of its nucleation was suggested. An analysis of conditions for the crack nucleation in configuration space of considered system parameters – the total Burgers vector of pile-up, the strength of disclination dipoles, and the value of external load – has been carried out.
Keywords: disclination, dislocation, dislocation pile-up, grain boundary, microcrack

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1. Introduction

It is generally accepted that high local stresses, which are assumed to initiate fracture, relate to inhomogeneous plastic deformation [1]. Indeed, the strain inhomogeneity occurring within a grain ensemble leads to the appearance of plastic incompatibility at grain boundaries in the form of orientation misfit dislocations (OMDs) [2]. Under conditions of their sufficiently uniform distribution over the facets of grain boundaries, the OMDs can be conveniently described in terms of "mesodefects". The latter are planar defects of shear and rotational type – the uniform continual distributions of tangential and normal components of OMD Burgers vector, respectively [3,4]. Linear rotational defects and junction disclinations are formed at junctions and ledges of grain boundaries [5]. The strength of mesodefects and the intensity of elastic stresses generated by them increase during plastic deformation. If their relaxation owing to plastic accommodation is hampered, the only possible way of relaxation is the appearance of a crack. Conditions of the nucleation and characteristics of stable cracks formed under stresses generated by the mesodefects, such as a wedge disclination, a dipole of

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wedge disclinations, combined shear-rotational mesodefects, and more complex systems of mesodefects, have been considered in many studies [6-12].

Under low homological temperature conditions, plastic deformation is characterized by its strong localization within separate slip planes of lattice dislocations. This, in its turn, leads to the appearance of planar dislocation pile-ups near grain boundaries. Conditions for the crack nucleation in the head of the pile-up hampered by an impenetrable barrier were considered in the classical Stroh model [13,14]. At that, grain boundaries were usually assumed to be such barriers. In this framework, a pile-up composed of a few hundred of dislocations is needed for the crack nucleation, however, so great pile-ups were not observed by electron microscopy. Moreover, generally, the grain boundaries are not impenetrable barriers. So, relaxation of the hampered pile-up can occur by way of lattice shear passing across the grain boundary. Various aspects of the process were considered earlier [15-20]. It has been shown [20] that the process depends on the lattice shear geometry, grain boundary misorientation, and the distance between a dislocation source and the boundary. The dislocations passing across the grain boundary can create extended grain boundary facets containing the planar mesodefects of rotational type in the form of biaxial dipoles of wedge disclinations. In its turn, these defects can generate cracks.

The aim of the present research is an analysis of conditions for the crack nucleation in the vertex of the deformation facet; the latter being formed by the lattice shear passing across a high-angle grain boundary.

2. Model description

Consider a pile-up of dislocations with Burgers vector $\mathbf{b_1}$, located in the first grain and pressed by the external load $\mathbf{P} = P\mathbf{n}$ ($\mathbf{n}$ is the unit vector along an axis of loading) to the high-angle tilt boundary with the misorientation $\boldsymbol{\theta} = \theta\mathbf{e_z}$, ($\mathbf{e_z}$ is directed at the right angle to the drawing plane, Fig. 1). Suppose that slip planes of these dislocations are oriented so that the resolved shear stress is maximal, that is $\angle(\mathbf{b_1},\mathbf{n}) = \pi/4$. For crossing the boundary, the dislocation of the first grain must dissociate into the dislocation of the second grains with Burgers vector $\mathbf{b_2}$ and orientation misfit dislocations (OMD) with the residual Burgers vector $\Delta\mathbf{b}$: $\mathbf{b_1} = \mathbf{b_2} + \Delta\mathbf{b}$. Because of these reactions and subsequent runaway of the dislocation $\mathbf{b_2}$ into the second grain, the OMD appear, which are associated with a ledge of height $\Delta l = b\cos\theta$ directed along the slip plane of dislocations of the first grain.

As dislocations $\mathbf{b_2}$ run away into the second grain, the pile-up is pressed by external stress to the grain boundary, and then the next dislocation crosses the boundary. Multiple repetitions of the process leads to the formation of the facet with the length of $l_f = n\Delta l$ (*n* is a number of dislocations gone away into the second grain) oriented along the slip plane of the first-grain dislocations. Resolving Burgers vector of OMDs $\Delta\mathbf{b}$ into the normal and tangential components relative to the facet plane, its defect content can be described as a superposition of two planar distributions of virtual dislocations.

The first distribution can be represented as a continual uniform distribution of sessile dislocations. It will be considered next as a biaxial dipole of wedge disclinations with an arm coinciding with the facet length l_f and strength $\mathbf{w_{dp}}$ equal to Burgers vector density of the sessile dislocations. Frank vector $\mathbf{w_d}$ of the disclinations constituting the dipole relates to $\mathbf{w_{dp}}$ as:

$$\mathbf{w_d}(\mathbf{r_1}) = \frac{\mathbf{w_{dp}} \times (\mathbf{r_1} - \mathbf{r_2})}{\|\mathbf{r_1} - \mathbf{r_2}\|}, \quad \mathbf{w_d}(\mathbf{r}_2) = \frac{\mathbf{w_{dp}} \times (\mathbf{r}_2 - \mathbf{r}_1)}{\|\mathbf{r_1} - \mathbf{r_2}\|}, \tag{1}$$

where $\mathbf{w_d}(\mathbf{r_1})$ and $\mathbf{w_d}(\mathbf{r_2})$ are the Frank vectors of the disclinations located in the points with radius-vectors $\mathbf{r_1}$ and $\mathbf{r_2}$, respectively. Taking into account that $\mathbf{w_{dp}} = w_{dp}\mathbf{e_y}$, one can obtain $w_{dp} = -\tan\theta$.

It is worth noting that the sign of the disclination located in the head of the pile-up depends on the orientation of the dislocation slip plane in the second grain. We consider the most preferred for crack nucleation case, when a negative disclination generating tensile stress field is located in the head of the pile-up, which corresponds to values $\theta < 0$ (Fig. 1).

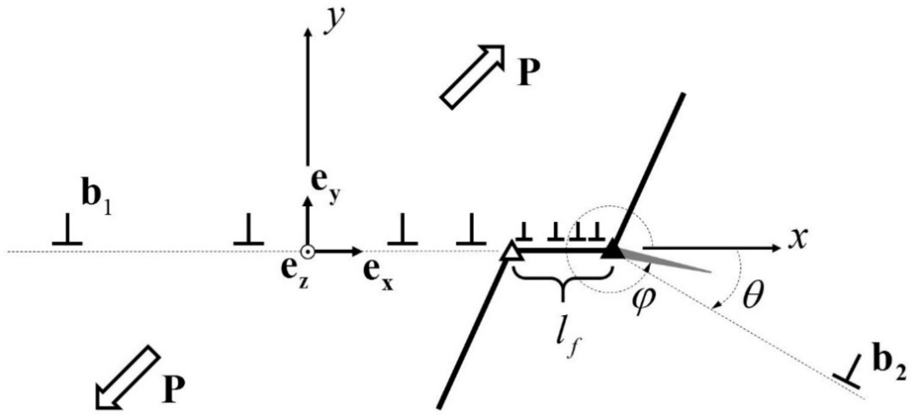

Fig.1. Schematic representation of dislocation pile-up crossing grain boundary

It is convenient for subsequent calculations to set parameters characterizing the system on every stage of the facet formation, namely, the total Burgers vector of dislocations in the pile-up $\mathbf{B} = (B, 0)$ and the facet length l_f. Let us choose Cartesian coordinate system *Oxyz* and the corresponding orthonormal basis associated with the facet as shown in Fig. 1; the origin of coordinates is set in the center of the pile-up. Since the disclination dipole is located in the facet plane oriented along the dislocation slip plane of the first grain and, hence, does not interact with the dislocations of the pile-up, the length of the pile-up *L* and the Burgers-vector-density distribution $\rho(x)$ are determined by the expressions [21]:

$$L = \frac{GB}{\pi(1-\nu)\tau_1}, \quad \rho(x) = \frac{2(1-\nu)\tau_1}{G}\sqrt{\frac{L/2 + x}{L/2 - x}}, \tag{2}$$

where $\tau_1 = \mathbf{e_y} \cdot (P\mathbf{n} \otimes \mathbf{n}) \cdot \mathbf{e_x}$ is the shear stress in the slip plane of dislocations $\mathbf{b_1}$, G and ν are the shear modulus and Poisson coefficient, respectively. A drag force $f^{(dp)}$ acts from the disclination dipole on the dislocation going into the second grain. A value of the force increases as the dislocations cross the grain boundary and the facet lengthens. When the facet length reaches a certain value $l_f^{(dp)}$, this force balances the total force acting on the dislocation going into the second grain from the external stress $f^{(ext)}$ and the dislocation pile-up $f^{(p)}$. As a result, the process of a grain boundary crossing by the dislocations stops. A criterion for the stop of the facet lengthening can be written in the form:

$$\min_{x,y}\left(f^{(p)}(x,y) + f^{(ext)} + f^{(dp)}(x,y)\right) = 0. \tag{3}$$

Let $\mathbf{n_2}$ be the unit vector of the normal to the dislocation slip plane in the second grain. Thus, the forces acting on the going off dislocation:

$$f^{(p)}(x,y) = \mathbf{n_2} \cdot \left(\int_{-L/2}^{L/2} \rho(x')\mathbf{G}(x-x',y)dx' \right) \cdot \mathbf{b_2},$$
$$f^{(dp)}(x,y) = \mathbf{n_2} \cdot \left(\boldsymbol{\sigma}_\mathbf{d}(x - L/2 + l_f^{(dp)}, 0) \right) \cdot \mathbf{b_2}, \quad f^{(ext)} = \mathbf{n_2} \cdot \left(P\mathbf{n} \otimes \mathbf{n} \right) \cdot \mathbf{b_2}, \tag{4}$$

where $\mathbf{G}(x-x',y)$ is the function of stress produced by the dislocation located in point (x', 0) with unit Burgers vector [21] oriented along axis Ox, $\boldsymbol{\sigma}_\mathrm{d}$ is a function of stress tensor from the positive disclination of the dipole (negative disclination does not produce shear stresses in the slip plane of dislocation $\mathbf{b_2}$ located in point $(L/2 - l_f^{(dp)}, 0)$ [22]).

The action of the tensile stresses from the dislocation pile-up, the stresses from the negative disclination, and the external stress in the vicinity of the facet can lead to the formation of a crack. Usually, the crack nucleation is considered in the micromechanics of fracture in terms of an energetic approach. According to the approach, the crack nucleates if the interval of its length $(0, l_0]$ exists, in which the following condition is fulfilled:

$$\frac{\partial E}{\partial l} \le 0, \ \forall l \in (0, l_0], \tag{5}$$

where E is the energy of the system, and l_0 is the limit point, where condition (5) ceases to fulfil. At that, if $l_0 < \infty$, then an equilibrium stable crack is generated. Otherwise, if $l_0 = \infty$, then the main crack is produced. However, the application of this criterion for the model considered seems to be not quite justified. Actually, based on the earlier results [1] it can be shown that the relaxation of disclination elastic energy $\left(E_{el}^{\Delta}\right)'_l$ near point $l = 0$ is infinitesimal. Consequently, the presence of the disclination dipole has no effect on the fulfillment of criterion (5). Nevertheless, it is quite apparent that a powerful tensile stress field from the negative disclination can facilitate significantly the crack nucleation in its vicinity. The disclination effect can be accounted for, if to suppose that the propagating crack does not pass through all intermediate states near point $l = 0$, but rather opens up spasmodically to a certain finite length l_{nucl}. Based on physical consideration, the length equal to two periods of the crystal lattice, $l_{nucl} = 2b$, can be taken as a minimal length of the crack. Thus the criterion of crack nucleation can be expressed using a finite increment of energy:

$$\Delta E = E(2b) - E_0 \le 0, \tag{6}$$

where $E(2b)$ is the energy of the system with a crack of length $2b$, E_0 is the energy of the system without a crack. Assuming a negligible contribution of dissipative processes to the energy changing during crack nucleation, as well as the independence of the free surface of a crack tip from the crack length, one can obtain ΔE as:

$$\Delta E = \Delta E_{el} + \Delta E_{\gamma} = \Delta E_{el} + 4\gamma b, \tag{7}$$

where γ is the specific energy of the free surface. At the same time, the change of potential energy E_{el} can be calculated as:

$$\Delta E_{el} = -\int_0^{2b} F(l,\varphi)dl. \tag{8}$$

Here $F(l,\varphi)$ is the configurational force defined as the elastic energy released during crack propagation per unit length:

$$F(l,\varphi)=\frac{l}{8D}\left(\bar{\sigma}_{\varphi\varphi}{}^{2}+\bar{\sigma}_{r\varphi}{}^{2}\right), \tag{9}$$

where $D=G/[2\pi(1-\nu)]$, φ is the angle determining the crack orientation, $\bar{\sigma}_{\varphi\varphi},\bar{\sigma}_{r\varphi}$ are the averaged total stresses:

$$\bar{\sigma}_{\varphi\varphi}=\frac{2}{\pi l}\int_{0}^{l}\sigma_{\varphi\varphi}(r,\varphi)\sqrt{\frac{r}{l-r}}dr,\quad \bar{\sigma}_{r\varphi}=\frac{2}{\pi l}\int_{0}^{l}\sigma_{r\varphi}(r,\varphi)\sqrt{\frac{r}{l-r}}dr, \tag{10}$$

where $\sigma_{\varphi\varphi}$, $\sigma_{r\varphi}$ are the components of total stress produced by the biaxial dipole of wedge disclinations, the hampered pile-up, and the external load in the vicinity of the microcrack. We have used the polar system of coordinates, where the pole coincides with the location of the negative disclination of the dipole. Taking equation (8) into account, criterion (6) for the nucleation of the crack oriented along angle φ becomes (for given values of parameters l_f, B, P, w_{dp}):

$$\Delta E=4\gamma b-\int_{0}^{2b}F(l,\varphi)dl\le 0. \tag{11}$$

The most energetically preferred orientation of the nucleating crack is such direction $\varphi_{\max}$ that provides the maximal relaxation of the stress field:

$$\Delta E_{el}(\varphi_{\max})=\max_{\varphi}\int_{0}^{2b}F(l,\varphi)dl. \tag{12}$$

Naturally, the values of $\varphi_{\max}$ will differ for different sets of parameters l_f, B, P, w_{dp}. For given values of *B*, *P*, w_{dp}, the minimal facet length $l_f^{(cr)}$, for which the crack nucleation becomes possible, can be found in the equation:

$$4\gamma b-\int_{0}^{2b}F\left(l,\varphi_{\max}(l_f^{(cr)}),l_f^{(cr)}\right)\Big|_{B,P,w_{dp}}dl=0. \tag{13}$$

It is evident that, for $l_f>l_f^{(cr)}$, a direction always exists, in which the nucleation of the crack of length $l_0=2b$ becomes energetically preferable; but for $l_f<l_f^{(cr)}$, the crack does not nucleate according to this criterion. Hence, crack nucleation at a faceted boundary is possible only in the case when $l_f^{(cr)}\le l_f^{(dp)}$. Then, the functions $l_f^{(cr)}(B,w_{dp},P)$ and $l_f^{(dp)}(B,w_{dp},P)$ can be obtained by numerical calculations varying parameters B, P, w_{dp}.

3. Results of numerical calculations and discussion

The calculations were carried out for the following values of parameters: $G=45000$ MPa, $\nu=0.3$, $b=3\cdot 10^{-4}$ μm, $B\in[20b,50b]$, $\theta\in[-15^{\circ},-30^{\circ}]$, $P=\{0.005G,0.0075G\}$, $\gamma=Gb/8$. Figure 2 shows a typical view of the configurational force dependence on the crack length, calculated with $\varphi=300^{\circ}$, $B=40b$, $l_f=388.7b$, $w_{dp}=0.3$, $P=0.005G$.

Figure 3a and 3b show the dependencies of $l_f^{(dp)}/b$ and $l_f^{(cr)}/b$ on the total Burgers vector of the pile-up B normalized to b, calculated for fixed values of the disclination dipole strength w_{dp} and external load P. Intersection points of the curves $l_f^{(dp)}/b$ and $l_f^{(cr)}/b$

correspond to the threshold values of the total Burgers vector of pile-up B^*, at exceeding which the crack nucleates.

Figure 4 shows the dependencies of the threshold value of the total Burgers vector of pile-up B^* / b on the disclination dipole strength w_{dp} for the values of external load $P = 0.005G$ and $P = 0.0075G$.

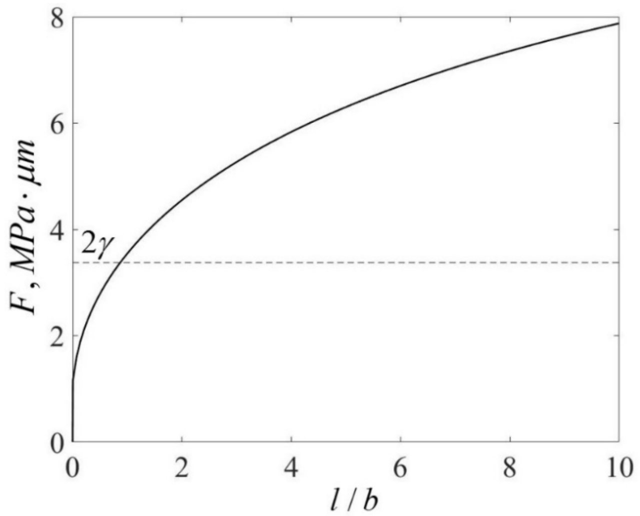

Fig. 2. Typical dependence of configurational force on a crack length

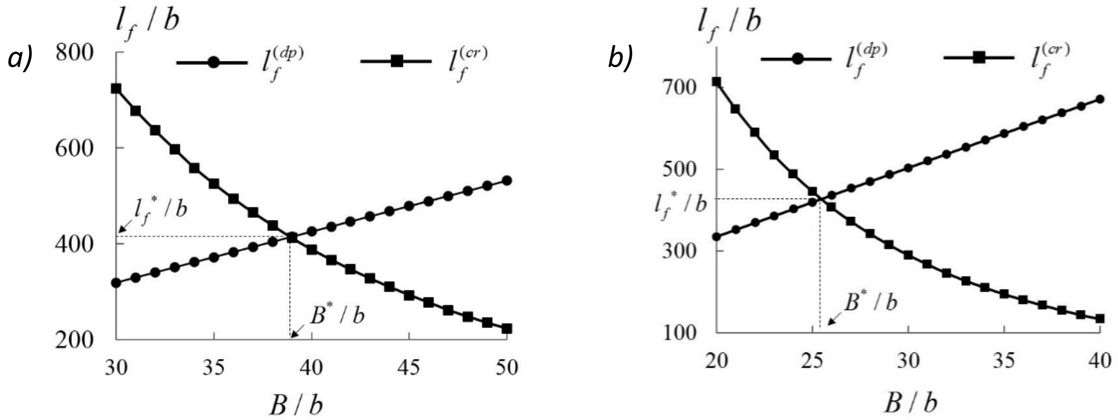

Fig. 3. Dependencies of $l_f^{(dp)} / b$ and $l_f^{(cr)} / b$ on the total Burgers vector of the pile-up B normalized to Burgers vector of a lattice dislocation b

One can see that the dependence of B^* / b on the disclination dipole strength is nonmonotonic. With increasing w_{dp}, that is, with increasing the misorientation of the original grain boundary, the value of B^* / b at first decreases and then grows. Such behaviour can be explained based on the following reasons. The fulfilment of the crack nucleation criterion with fixed external stress is provided owing to the growth of the stresses generated by the pile-up and the disclination dipole in the crack vicinity. At that, the disclination dipole has a dual role. Increasing the strength of the negative disclination leads to the growth of tensile stresses that it produces. Thus, all other things being equal, the less dislocations in pile-up is needed for the fulfilment of criterion (6). On the other hand, the greater the strength of the disclination dipole, i.e. the greater the misorientation angle of the original grain boundary, the smaller the arm of the dipole, i.e. the smaller the length of the facet, which is needed to stop boundary crossing by dislocations. Decreasing the length of the deformation facet and, hence, the arm of the dipole, enlarges, in its turn, the screening effect of the positive disclination on the elastic field of the negative one. Correspondently, more dislocations in pile-up are needed to fulfil criterion (6). The influence of those factors predetermines the occurrence of the minimum on the curves shown in Fig. 4. Taking into account the relation $w_{dp} = -\tan\theta$, from Fig. 4 it follows that the minimal number of dislocations in the pile-up, are needed for the crack nucleation, occurs when the dislocations cross grain boundaries with misorientation angles about 22°.

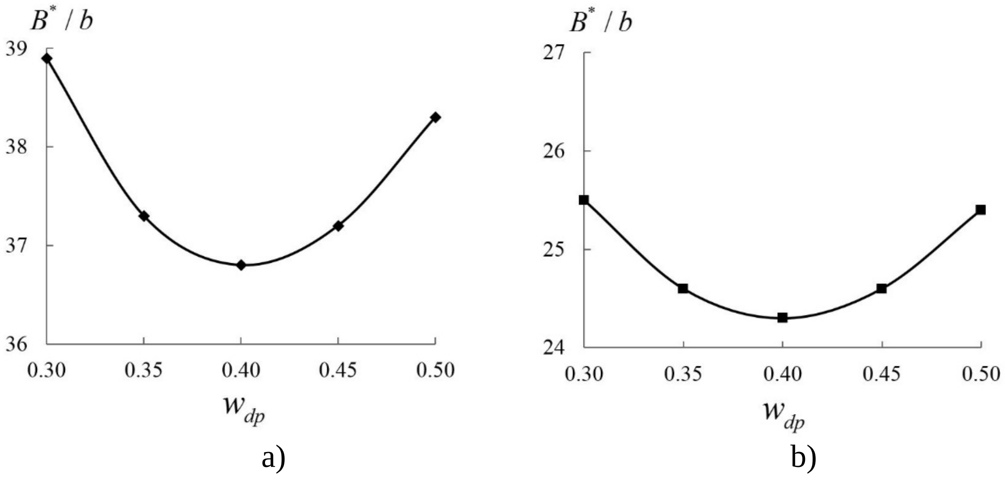

Fig. 4. Dependencies of the threshold value of the total Burgers vector of the pile-up B^* / b on the disclination dipole strength w_{dp} (crack orientation is within the interval $\varphi_{\max} = [298°, 313°]$)

The dependence of the threshold length of deformation facet l_f^* / b on the disclination-dipole strength is illustrated in Fig. 5. One can see that the value of l_f^* / b decreases monotonically with increasing strength of disclination dipole, and depends weakly on an external load.

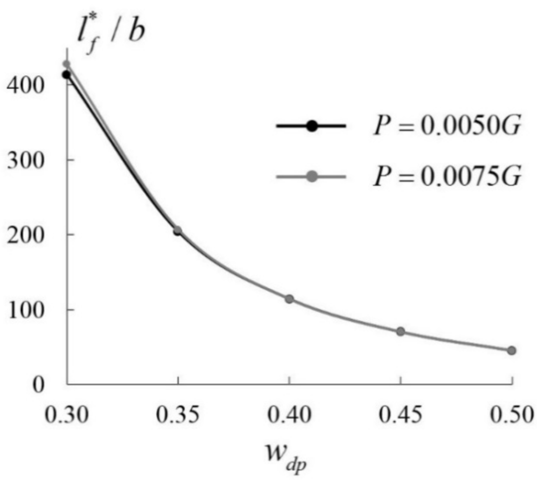

Fig. 5. Dependence of the normalized threshold length l_f^* / b of deformation facet on the strength of disclination dipole at external load $P = 0.005G$ and $P = 0.0075G$

4. Conclusion

We have shown that the formation of the disclination dipole due to grain boundary crossing by dislocations enables initiating fracture with less number of dislocations in pile-up (within the range from 25 to 40 dislocations) than in the framework of Stroh model. In the latter for coalescence of dislocations in the head of pile-up, it is needed ~150-200 dislocations (under external stresses considered in the present study). It should be emphasized that, in the framework of our study, the conditions for the nucleation of a crack and for its subsequent growth are fulfilled simultaneously. At that, the microcrack can transform into a stable one or open to the main crack, depending on particular parameters of the system considered and on the value of external stresses. For analysis of possible ways of its evolution, it is necessary to take into account dumping dislocations into the growing crack. This problem will be analyzed separately.

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THE AUTHORS

V.N. Perevesentsev
e-mail: v.n.perevezentsev@gmail.com
ORCID: 0000-0002-0437-8540

S.V. Kirikov
e-mail: ksv.kirikov@yandex.ru
ORCID: 0000-0002-5039-2271

N.Yu. Zolotorevsky
e-mail: zolotorevskii@mail.ru
ORCID: 0000-0002-0185-5452