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CRACK ARREST BY THE ELASTIC FIELD OF WEDGE DISCLINATION AND PLANAR SHEAR MESODEFECT

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Abstract. The arrest conditions due to the action of the elastic fields of a dipole of wedge disclinations and a planar shear mesodefect are considered for dislocation cracks propagating under external loading. The regions of stable cracks existence are determined using the method of configurational force in the configuration space of the system parameters (the mesodefect strength vs the Burgers vector of the crack) and the maps of the cracks lengths distribution were plotted at various values of the external stress. The length of the cracks turns out to be comparable with the mean size of fragments and lies in the range of 0.1-0.3 μm at the parameters of the fragmented structure and values of the external stress typical for the stage of material pre-fracture. It is shown, that both in the case of the disclination dipole and in the case of the planar shear mesodefect the regions of instability of cracks shift towards lower dislocation charge of the crack and higher values of the mesodefects strength with an increase in the external stress. It is concluded, that the considered mesodefects can effectively arrest the propagation of cracks in the fragmented structure, thereby providing their accumulation in certain areas of the material and creating the "fracture nuclei".
Keywords: dislocation crack, disclination dipole, shear mesodefect, crack arrest, configuration force method

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1. Introduction

It is known that ductile fracture of metals and alloys occurs through the accumulation of microcracks in local areas of the material ("fracture nuclei") and the subsequent stage of quasi-brittle fracture associated with a weakening of the specimen cross-section. It was shown that in these areas of the material a specific fragmented structure is formed [1]. This structure appears during plastic deformation of the material by dividing the original grains of polycrystal into mutually misoriented regions (fragments), separated by strain-induced grain boundaries. At sufficiently large plastic deformations preceding the stage of ductile fracture, the size of fragments in the cross-section of the specimens is usually 0.2-0.3 μm. An important feature of the fragmented structure is the presence of plastic incompatibilities at the boundaries and junctions of grains (fragments) associated with the inhomogeneity of plastic

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deformation on the ensemble of grains (fragments) of the polycrystal. It is generally accepted to describe them in terms of mesodefects in the physics of large plastic deformations. With a homogeneous plastic deformation in the volume of grains (fragments), the mismatch of plastic rotations along the grain boundaries leads to the appearance of rotational-type mesodefects at the grain junctions and ledges of grain boundaries – junction disclinations [2,3], and the mismatch of plastic shear across the grain boundary leads to the appearance of planar shear-type mesodefects [4.5]. Mesodefects generate powerful elastic stress fields in neighboring regions of grains. Up to the stage of material fracture, the relaxation of these fields is provided by accommodative plastic deformation in the vicinity of mesodefects. However, with continuing plastic deformation this process becomes exhausted in some "critical" areas of the fragmented structure. Under these conditions, the only channel for the relaxation of the elastic fields of mesodefects is the appearance of cracks. The conditions for the Zener-Griffith crack initiation in the field of disclination dipole were considered in [6]. Models of crack nucleation in materials with a fine-grained structure based on the concept of the stress concentrators formation near the grains triple junctions due to grain boundary sliding were considered in [7-9]. The conditions for crack initiation at the grain junction during athermal pure grain-boundary sliding according to the Stroh mechanism and as a result of the accumulation of orientational misfit dislocations at the junction were analyzed in [7, 8]. The role of the shear-type planar mesodefect located at the grain boundary on crack nucleation during threshold athermal grain boundary sliding was considered in [9]. It should be noted that rotational-shear mesodefects play a double role in the process of ductile fracture. On the one hand, they provide the cracks nucleation, and on the other hand, they can arrest their further propagation, creating conditions for the cracks accumulation and limiting their lengths to the sizes comparable to the average size of the fragments. The conditions for the existence of the stable crack in elastic fields of wedge disclinations, disclinations dipoles, and a combined rotational-shear mesodefect were analyzed in [5,10]. In this paper, we consider the conditions for the arrest of dislocation cracks by elastic fields of rotational-shear mesodefects (a dipole of wedge disclinations and a planar shear mesodefect).

2. Description of the model

To investigate the influence of the dipole of wedge disclinations on the crack arrest let us consider a grain structure element, consisting of two triple junctions of grains, with unlike wedge disclinations located along the lines of triple junctions. These disclinations form a biaxial dipole of wedge disclinations situated along the grain boundary as is shown in Fig. 1a.

A disclination dipole is modeled by a wall of virtual edge dislocations uniformly distributed at the boundary. In this case, the strength of the disclination dipole $\mathbf{w_N}$ is determined as a value equal to the density of the Burgers vector of dislocation wall. The strength of the disclination dipole $\mathbf{w_N}$ and Frank vectors $\mathbf{w_d}$ of disclinations are related by the expressions:

$$\mathbf{w_d}(\mathbf{r}_1) = \frac{\mathbf{w_N} \times (\mathbf{r}_1 - \mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|}; \quad \mathbf{w_d}(\mathbf{r}_2) = \frac{\mathbf{w_N} \times (\mathbf{r}_2 - \mathbf{r}_1)}{|\mathbf{r}_2 - \mathbf{r}_1|}., \tag{1}$$

where $\mathbf{w_d}(\mathbf{r_1})$ is the Frank vector of disclination located at the point with the radius vector $\mathbf{r_1}$, $\mathbf{w_d}(\mathbf{r_2})$ is the Frank vector of disclination located at the point with the radius vector $\mathbf{r_2}$. In the case of 2D geometry, the Frank vector is directed perpendicular to the plane of the figure, therefore we will characterize it by the value of the projection w_d of the vector $\mathbf{w_d}$ on the Oz axis. The strength of the disclination dipole will be characterized by the value of the projection w_N of the vector $\mathbf{w_N}$ on the Ox axis. If the value of projection $w_N > 0$, the crack propagates from the triple grain junction with positive disclination creating compressive stresses near the crack. If $w_N < 0$ the crack propagates from the junction with negative disclination creating tensile stresses.

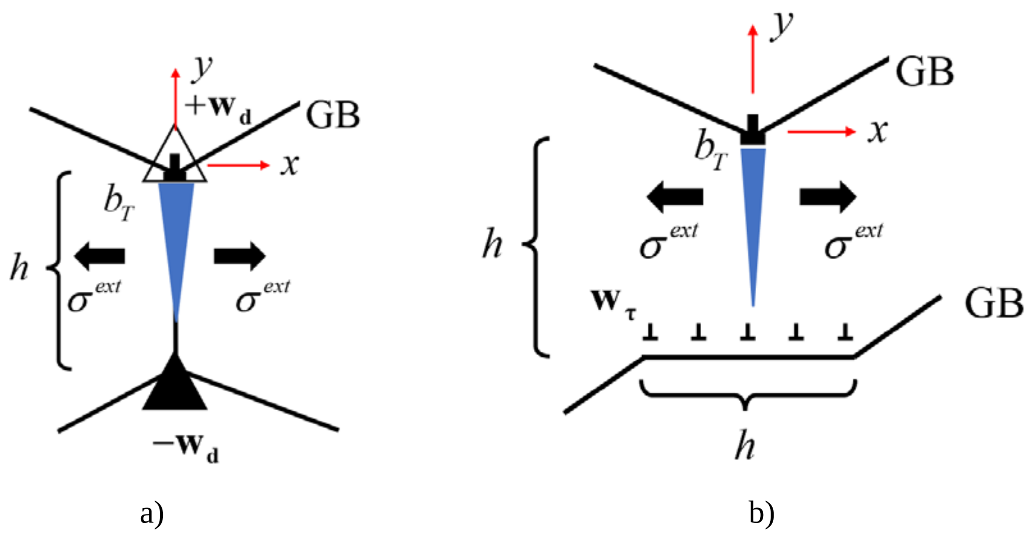

Fig. 1. Schematic plot of the dislocation crack, in the case of (a) the dipole of wedge disclinations (b) planar shear mesodefect

To investigate the influence of the elastic field of the planar shear mesodefect on the crack arrest we consider a dislocation crack propagating from the grain junction along the normal to the plane of the mesodefect located at a distance h from the grain junction (see Fig. 1b). In Figure 1 the shear mesodefect being by nature of plastic shear uniformly distributed in the plane of the grain boundary is schematically represented in the form of a uniform distribution of virtual glissile edge dislocations. The density of the Burgers vector of dislocations distributed along the boundary $\mathbf{w}_\tau$ will be defined below as the strength of the mesodefect. We will assume that the strength of this mesodefect is positive if the projection w_τ of the vector $\mathbf{w}_\tau$ on the Ox axis is positive ($w_\tau > 0$), and negative otherwise ($w_\tau < 0$). Note that in the region $-h < y \le 0$ a shear mesodefect with $w_\tau > 0$ creates compressive stresses, and a mesodefect with $w_\tau < 0$ creates tensile stresses.

Crack stability analysis is carried out using the configurational force method [11,12]. Note that for both of the considered cases, the shear stress from mesodefects σ_{xy}^{mes} is equal to zero in the plane of crack propagation. For plane strain of an isotropic material, the expression for the configurational force F, defined as the value of the elastic energy released during the propagation of a plane opening mode crack per unit length, has the form

$$F(l) = \frac{l}{8D}\bar{\sigma}_{xx}^{\,2}, \tag{2}$$

where: $D = G/[2(1-\nu)]$, G – shear modulus, ν – Poisson's ratio, l – crack length, $\bar{\sigma}_{xx}$ – weighted average total stresses.

$$\bar{\sigma}_{xx} = \frac{2}{\pi l}\int_{-l}^{0}\left(\sigma^{ext} + \sigma_{xx}^{d}(y, x=0) + \sigma_{xx}^{mes}(y, x=0)\right)\sqrt{\frac{-y}{l+y}}dy\,, \tag{3}$$

where σ^{ext}, $\sigma_{xx}{}^{dis}$, $\sigma_{xx}{}^{mes}$ are the tensile stress components along the Ox axis from external stress, from a dislocation in the crack head, and mesodefect, respectively. The components $\sigma_{xx}{}^{dis}$ and $\sigma_{xx}{}^{mes}$ for a disclination dipole ($\sigma_{xx}{}^{N}$) and a shear mesodefect ($\sigma_{xx}{}^{\tau}$) have the form [13,14,5]:

$$\sigma_{xx}^{dis}(x=0, y) = -D\frac{b_T}{y}, \tag{4}$$

$$\sigma_{xx}^{N}(x=0, y) = Dw_N \ln\left|\frac{y}{y+h}\right|, \tag{5}$$

$$\sigma_{xx}^{\tau}(x=0,y)=Dw_{\tau}\left[\frac{h(y+h)}{(h/2)^2+(y+h)^2}-4\operatorname{arctg}\frac{h}{2(y+h)}\right]. \quad (6)$$

The equilibrium crack lengths satisfy the relation $F(l = l_{eq}) = 2\gamma$, where γ is the specific energy of the free surface. Here and below we neglect the contribution of the surface energy of the grain boundary to the effective fracture work. In this case, the crack with length l_{st} is stable if further crack growth is energetically unfavorable.

The numerical algorithm for stable crack length l_{st} calculation was as follows. Initially, a certain rather small crack length l_0, at which the configurational force F was certainly greater than 2γ was fixed. It is easy to show that such a length always exists since in the case of a dislocation crack $F\rightarrow+\infty$ at $l\rightarrow 0$. Then, a small increment of the crack length $\Delta l = b$ was set, and the configurational force $F(l_0 + \Delta l)$ was calculated again. This procedure was repeated until at some i-th step of the iteration the inequality $F(l_0 + i\Delta l)<2\gamma$ was satisfied. The value of l_{st} should lie in the interval $[l_0 + (i - 1)\Delta l \;\; l_0 + i\Delta l]$ due to the continuity of the function $F(l)$. Its length was found by the dichotomy method. After that, the iterative procedure was terminated.

If, in the course of the iterative procedure, the inequality $F(l)<2\gamma$ was not fulfilled for a given sufficiently large interval of crack lengths, the upper boundary of which was taken to be $4h$, such cracks were classified as unstable and the calculation was terminated. Numerical calculations of improper integrals arising in the determination of the configurational force and crack opening profile were calculated by the method of quasi-uniform meshes [15].

3. Results of calculations and discussion

The calculations were carried out for the following parameter values: $G = 45000$ MPa, $\nu = 0.3$, $\gamma = Gb/8$, $b = 3\cdot10^{-4}$ μm, the strength of the disclination dipole and planar shear mesodefect varied in the interval [-0.08, 0.08], and the external stress value σ^{ext}/G varied in the range [0, 0.03]. The value of the Burgers vector of a dislocation crack b_T depends on the specific mechanism of its initiation and was further considered as a parameter varying in the range of values $b_T \in [2, 30]b$. The value h = 0.2 μm was chosen taking into account its correlation with the average grain (fragment) size at the later stage of fragmentation. The dependences of the configurational force on the crack length at $\sigma^{ext}/G = 0.02$ and $b_T = 15b$, calculated at different strengths and signs of the disclination dipole and planar shear mesodefects, are shown in Fig. 2.

In the absence of mesodefects (when w_N and w_τ are equal to zero), the external stress destabilizes cracks with Burgers vectors $b_T > b_0 = 2\gamma/\sigma^{ext}$. When the external stress is $\sigma^{ext}/G = 0.02$, a crack with Burgers vector $b_T = 15b$ is unstable and can spontaneously open into the main crack. The presence of a disclination dipole or a shear mesodefect with a sufficiently large (in absolute value) strength stabilizes the crack. Results of calculations of the stability regions of cracks in the configuration space of parameters (b_T, w_N) and (b_T, w_τ) and maps of distribution in this space of the stable cracks lengths at the external stresses: $\sigma^{ext}/G = 0.01$; $\sigma^{ext}/G = 0.02$ and $\sigma^{ext}/G = 0.03$ are shown in Figs. 3 and 4. Areas in which stable cracks do not exist are colored in white.

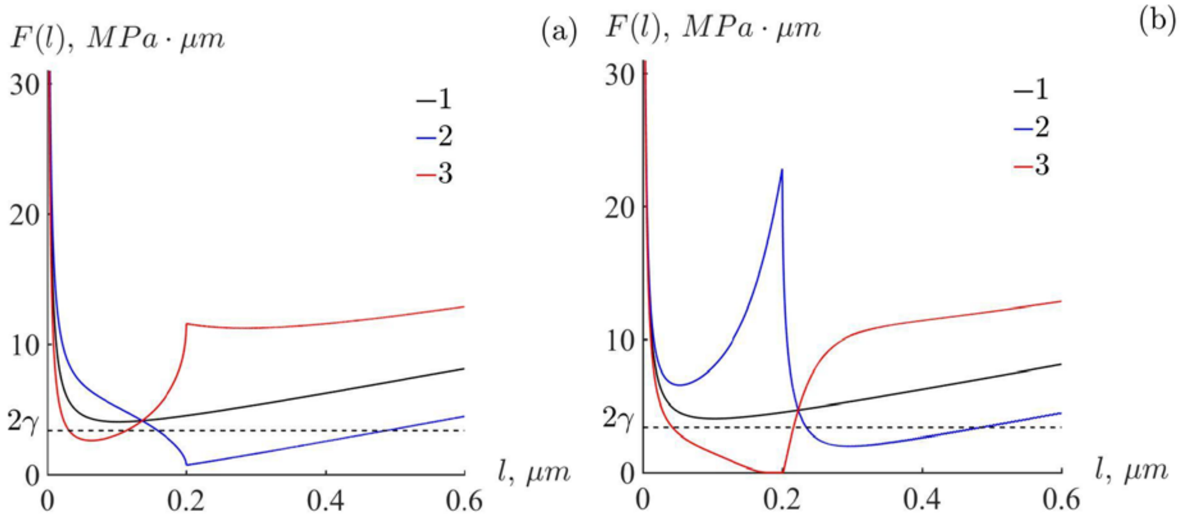

Fig. 2. Dependences of the configurational force on the crack length at $\sigma^{ext}/G = 0.02$ and $b_T = 15b$ (a) – at different values and signs of strengths of the disclination dipole with a length $h = 0.2$ μm (1 – $w_N = 0$; 2 – $w_N = -0.04$; 3 – $w_N = 0.04$); (b) – at different values and signs of strengths of the shear mesodefect with a length $h = 0.2$ μm (1 – $w_\tau = 0$; 2 – $w_\tau = -0.04$; 3 – $w_\tau = 0.04$)

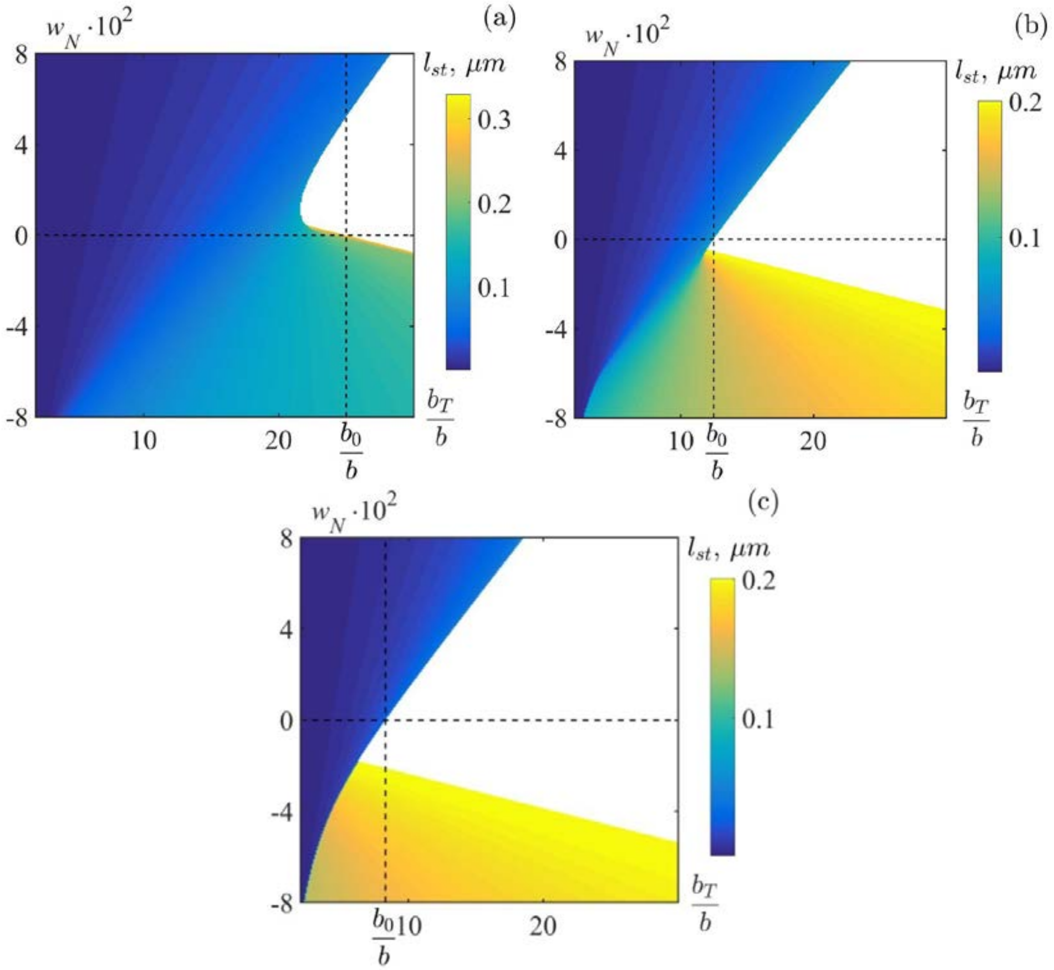

Fig. 3. Maps of the distribution of the stable cracks lengths in the case of their arrest by a disclination dipole at various values of external stresses:
a) $\sigma^{ext}/G = 0.01$, b) $\sigma^{ext}/G = 0.02$, c) $\sigma^{ext}/G = 0.03$

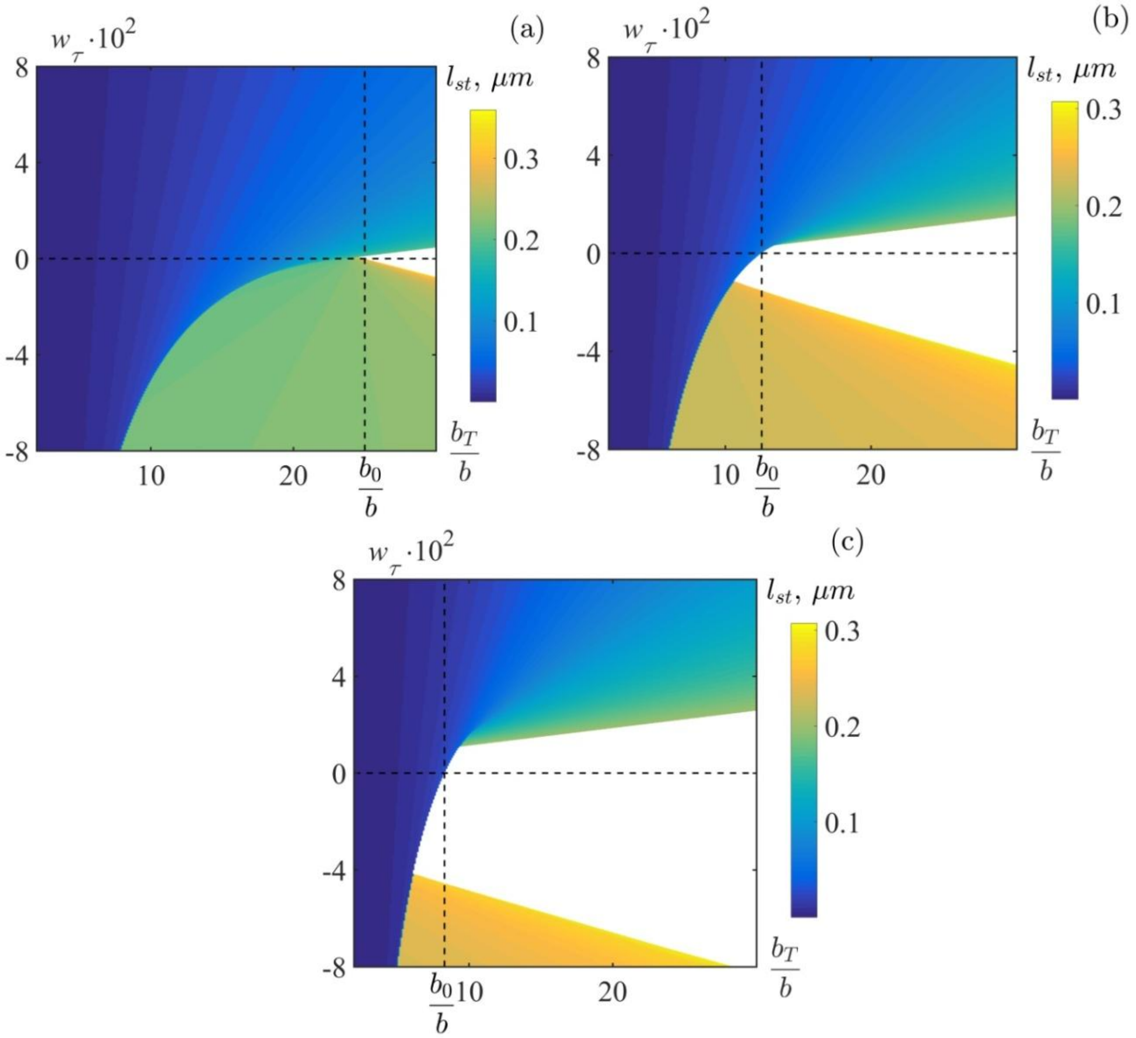

Fig. 4. Maps of the distribution of the stable cracks lengths in the case of their arrest by a planar shear mesodefect at external stresses:
a) $\sigma^{ext}/G = 0.01$; b) $\sigma^{ext}/G = 0.02$; c) $\sigma^{ext}/G = 0.03$

It can be seen that, both in the case of the disclination dipole and in the case of the shear mesodefect, the regions of cracks instability shift towards lower values of b_T (due to the decrease in b_0) and expand towards higher values of the mesodefects strength with the external stress increase. At fixed values of b_T and σ^{ext}, the lengths of stable cracks turn out to be larger at negative values of the mesodefects strengths than at their positive values.

The profile of one of such stable cracks, obtained for the values of the parameters $b_T = 20b$, $w_\tau = -0.04$, $\sigma^{ext}/G = 0.02$, is shown in Fig. 5. The function of normal displacements of the crack edges $u_x(y)$ was found by integrating the expression for the displacement function $u_x(y,t)$ [16] obtained for the case of a force $dP = \sigma_{xx}(t)dt$, normal to the edge, acting in a point $y = t$:

$$u_x(y) = \frac{2(1-\nu)}{\pi G} \int_{-2c}^{0} \sigma_{xx}(t) \ln \frac{c^2 - (t+c)(y+c) + \sqrt{\left(c^2 - (t+c)^2\right)\left(c^2 - (y+c)^2\right)}}{c\,|\,y-t\,|} dt\,, \tag{7}$$

where $c = l/2$.

A visible reduction of the crack width as it passes through the grain boundary containing a shear mesodefect with negative strength is due to the fact that crack propagates from the zone of tensile stresses from the mesodefect to the zone of compressive stresses.

Note that such a characteristic change in the profile of the crack when it passes through the boundary was observed *in situ* during copper deformation [17].

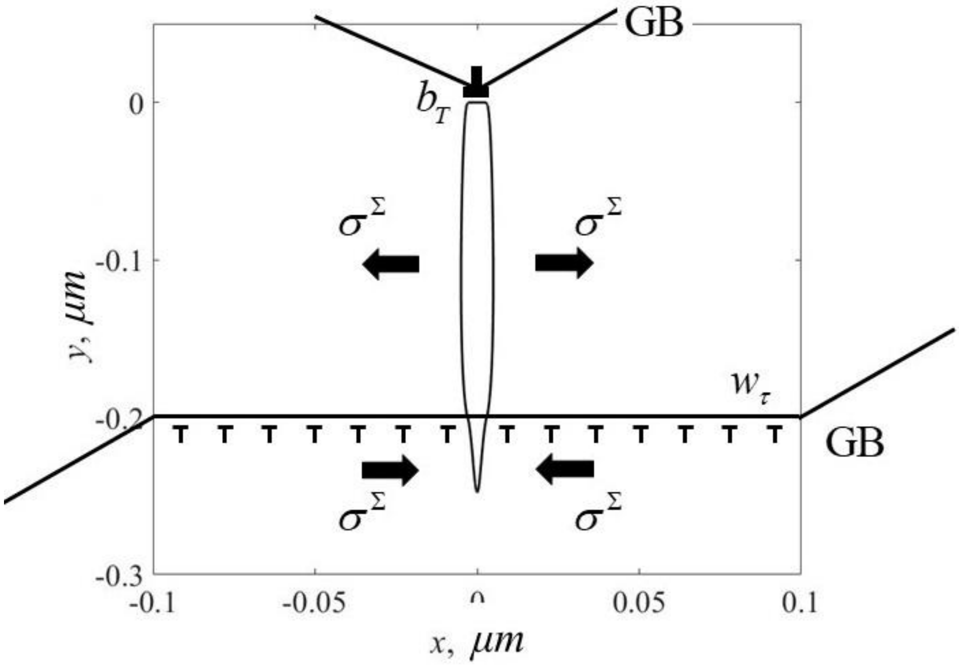

Fig. 5. Profile of the stable dislocation crack obtained for the following parameter values $b_T = 20b$, $w_\tau = -0.04$, $\sigma^{ext}/G = 0.02$, ($l_{st} = 0.25$ μm)

4. Conclusions

As the analysis shows, wedge disclinations dipoles and planar shear mesodefects can arrest the propagation of cracks in the fragmented structure, thereby providing their accumulation and the creation of fracture nuclei in certain areas of the material. In this case, the most effective are those mesodefects that create compressive stresses in the region of the triple junction, in which a dislocation crack nucleates. The length of such cracks turns out to be comparable to the size of fragments and lies in the range of 0.1-0.3 μm.

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