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INVESTIGATION OF THE INFLUENCE OF STRAIN INDUCED JUNCTION DISCLINATIONS ON HARDENING AND NUCLEATION OF CRACKS DURING PLASTIC DEFORMATION OF POLYCRYSTALS

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Abstract. An influence of elastic field of strain induced junction disclinations on hardening and nucleation of a micro-crack in a head of edge lattice dislocations pile-up is considered. Computer simulation method is used to calculate critical external stress for plastic shear propagation throw a force barrier induced by junction disclination. A qualitative explanation is given for the experimentally observed essential growth of the flow stress at sufficiently large plastic deformations. It is shown that the appearance of junction disclinations suppress nucleation of micro-cracks according to the mechanism of pile-up head dislocations confluence proposed by Stroh [1].

Keywords: strain induced junction disclination, plastic deformation, hardening, crack nucleation

1. Introduction

The difference in crystallographic orientations of polycrystal grains leads to their unequal plastic strains under loading. As a consequence it leads to the appearance of rotational type linear mesodefects in triple junctions and on the ledges of grain boundaries [2,3]. These mesodefects, called strain induced junction disclinations, generate powerful field of elastic stresses that essentially influences on plastic flow and fracture of polycrystals. However, up to now the main attention of researchers has been focused on the study of the role of strain induced junction disclinations in fragmentation phenomenon (i. e. subdivision of uniformly oriented initial grains of polycrystal into strongly misoriented regions, viz., fragments during large plastic deformation) [3,4]. The influence of strain induced junction disclinations on strain hardening and fracture of polycrystals remains less investigated [5,6].

In the framework of classical physics of dislocations, an increase of flow stress during plastic deformation is usually associated with an increase of a density of lattice dislocations distributed over the volume of grains, as well as with the interaction of dislocations with high angle grain boundaries and dislocation subboundaries [7]. However, physical models of hardening based on these assumptions do not explain the essential growth of plastic flow stresses up to values of $\sim 10^{-3} \div 10^{-2} G$ (G is the shear modulus) at the true strain values $\varepsilon > 0.2$. In our opinion, it is possible to explain this experimental fact taking into account that the elastic fields of junction disclinations retard the motion of lattice dislocations providing plastic deformation of the body of grains. In present paper computer simulation method is used to investigate the conditions for the propagation of plastic shear carried out by both individual dislocations and pile-up of edge dislocations motion through a force barrier of junction disclination.

Besides, experimental studies show that at large plastic strains the change of fracture mechanisms take place. The nucleation of microcracks occurs according to the disclination mechanism [8], while classical Stroh's mechanism [1] of microcrack initiation in the head of a retarded pile-up of edge dislocations take no place. In this work the limitation of Stroh's model for large plastic deformations is explained by the influence of strain induced junction disclination.

2. Description of the model

Let us consider a junction of three grains plastically deformed up to a strain $\boldsymbol{\varepsilon}_i$ (i = *1, 2, 3*) (See Fig. 1.). The difference of plastic strains of adjacent grains leads to the appearance of additional misorientations on the grain boundaries $\Delta\boldsymbol{\Theta}_j = \boldsymbol{N}_j \times \Delta\boldsymbol{\varepsilon}_j \cdot \boldsymbol{N}_j$ (j = *1, 2, 3*). Their values are determined by the values of plastic deformation jumps $\Delta\boldsymbol{\varepsilon}_i$ at the j-th grain boundary and the orientation of the unit vector of the normal to the boundary $\boldsymbol{N}_j$.

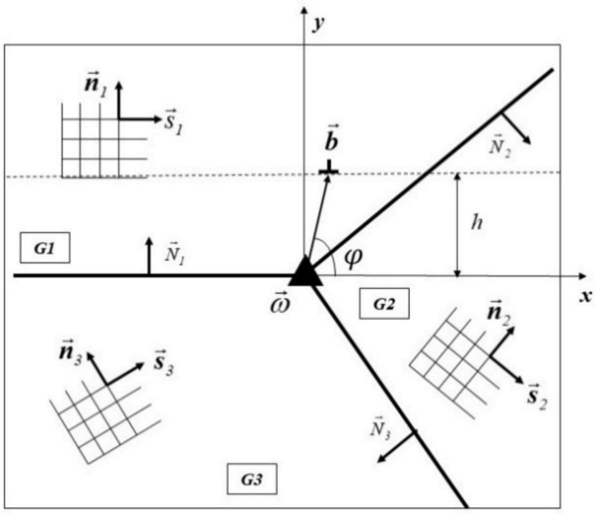

Fig. 1. Schematic plot of grain boundary triple junction.

The difference of additional misorientations on different grain boundaries leads to the appearance of a linear defect of the rotational type, i.e. junction disclination with a strength $\boldsymbol{\omega} = \sum_j \Delta\boldsymbol{\Theta}_j$, in the triple junction. Strain induced junction disclination generate field of elastic stresses that influences on the motion of lattice dislocations providing plastic deformation of the grains body. Further consideration of the model will be performed for two dimentional (2D) case for simplification.

Let edge dislocation with the Burgers vector $\boldsymbol{b} = b\boldsymbol{s_1} = b\boldsymbol{i}$ move in a slip plane placed at some distance $y=h$ from the wedge junction disclination in the grain *G1*.

The disclination act on a probe dislocation in a given slip plane $\boldsymbol{n_1}$ with a force $\boldsymbol{f}_{\boldsymbol{x}}^{\Delta} = \boldsymbol{\sigma}_{xy}^{\Delta}\boldsymbol{b}$, where

$$\sigma_{xy}^{\Delta} = -D\omega\frac{xy}{\left(x^2+y^2\right)} = -\frac{D\omega\sin(2\varphi)}{2}, \tag{1}$$

$D = G/2\pi(1-\nu)$, ν is a Poisson ratio, φ is an angle in polar coordinate system [9].

As seen from (1), this force is positive to the left of the disclination ($x<0$) and negative to the right of it ($x>0$). Thus, in the region $x<0$ the external stress force $f_x^{ext} = \sigma_{xy}^{ext} b$ and disclination force acting on the dislocation are co-directed, and in the region x> 0 these forces are directed oppositely. Therefore in the region $x > 0$ the moving dislocation is retarded by the elastic field of disclination. It is easy to note that a stable equilibrium takes place only if $\sigma^{ext} < \sigma_c^*$, where $\sigma_c^* = D\omega/2$ is equal to maximum shear stress of the disclination (on the ray $\varphi=45^0$ in polar coordinates). Thus, the condition for plastic shear propagation carried out by the motion of a single dislocation takes a form $\sigma^{ext} \geq \sigma_c^*$. Basing on this result, for typical values of the disclination strength $\omega \approx 0.017 \div 0.034$ rad, the flow stress should be of the order of $(2 \div 4)\cdot 10^{-2} G$. However, this value can be smaller if plastic shear is carried out by a motion of group of dislocations.

In the case $\sigma^{ext} < \sigma_c^*$ a single dislocation is stopped by the force barrier of junction disclination, but the emission of new dislocations by a source located in the slip plane leads to the formation of the dislocation pile-up, which creates an additional force acting on the head dislocation facilitating the shear propagation. Let us analyze the conditions for the plastic shear propagation through the disclination force barrier using computer simulation method [10].

The motion of dislocations was considered in a quasi-viscous approximation. The equation of motion for k-th dislocation of the pile-up in the slip plane $y = h$ was written in the form:

$$\boldsymbol{V^{(k)}} = \boldsymbol{Mb^{(k)}\sigma}_{xy}^{\Sigma} \tag{2}$$

Here: $\boldsymbol{V^{(k)}}$ is the dislocation velocity, $\boldsymbol{\sigma}_{xy}^{\Sigma} = \boldsymbol{\sigma}_{xy}^{ext} + \boldsymbol{\sigma}_{xy}^{\Delta} + \boldsymbol{\sigma}_{xy}^{disl}$ is a total field of elastic stress including external stress $\boldsymbol{\sigma}_{xy}^{ext}$, internal stresses caused by disclination $\boldsymbol{\sigma}_{xy}^{\Delta} = -D\omega\left(xh/x^2+h^2\right)$ and dislocations pile-up $\boldsymbol{\sigma}_{xy}^{disl} = Db\sum_{i \neq k}\left(x_k - x_i\right)^{-1}$ $(1 \leq i \leq N_p - 1)$, N_p is a number of dislocations in the pile-up, M is a dislocation mobility.

The formation of the pile-up were performed by sequential emission of positive dislocations by a source located on the left side of the grain *G1*. Each subsequent m + 1 dislocation was emitted when other previously emitted m dislocations of the pile-up reach equilibrium state in order to avoid the influence of the dynamic effects [11] on the motion of dislocations and the configuration of the pile-up.

After emitting of the m + 1 dislocation a new equilibrium pile-up configuration was calculated. Calculation of each configuration (the coordinates of the dislocations) was carried out by the method of sequential time iteration providing sufficiently small dislocation displacements for a given mobility M. The equilibrium configuration of the pile-up was determined from the condition that the forces acting on each dislocation of the pile-up were equal to zero. The condition for the plastic shear propagation were determined as the conditions under which the pile-up loss stability and its head dislocation leaves the pile-up and moves to a sink on the right side of the grain.

3. Results and discussion

Let us consider the influence of the external stress on the equilibrium configuration of the pile-up containing a given number of dislocations. The results of numerical calculation of the pile-up configuration for ten dislocations in the slip plane located at a distance h = 1 μm from the junction dislocation for different values of the external stress are shown in Fig. 2. The axial symmetry of the elastic stresses field of wedge disclination leads to the fact that in the absence of the external stresses ($\sigma^{ext} = 0$) the dislocation pile-up is located symmetrically with respect to the plane passing through the disclination line perpendicular to the slip plane of the dislocations (Fig. 2a). As the external stress σ^{ext} increases, the dislocation pile-up displaces as a whole and its shape becomes more asymmetric (Fig. 2b). Finally, when the external stress

σ^{ext} becomes greater than a certain critical one $\sigma_c = 0.0145D$, the pile-up becomes unstable, its head dislocation leaves the crystal.

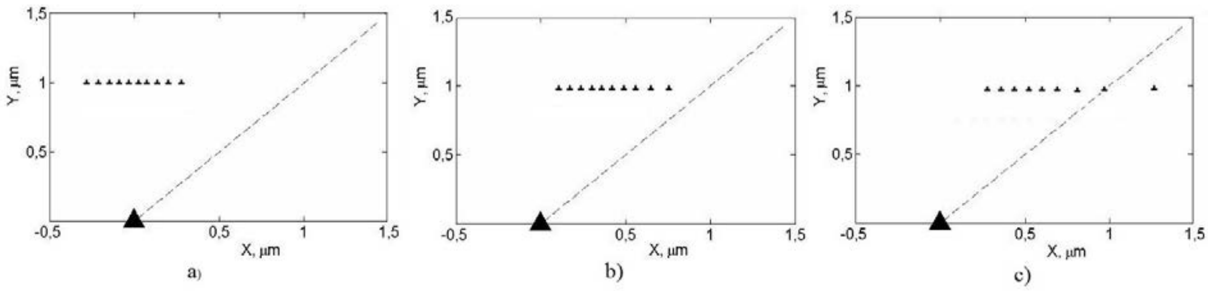

Fig. 2. Equilibrium configuration of the edge dislocations pile-up near disclination $\omega = 0.04\ rad$: (a) $\sigma^{ext} = 0$; (b) $\sigma_c = 0.01D$; (c) remaining part of the pile-up when the head dislocation left the crystal at $\sigma^{ext} = 0.015D$.

At the same time, the remaining dislocations of the pile-up rearrange into a new equilibrium configuration (Fig. 2c). It is obvious that an emission of a new dislocation by dislocation source will lead to the repeating of this process.

The results of calculations for the dependence of the critical shear stress on the number of dislocations in the pile-up for various values of h are shown in Fig. 3.

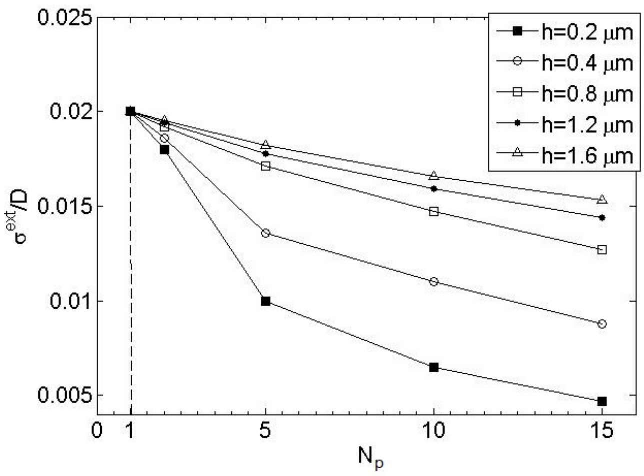

Fig. 3. The dependence of the critical external shear stress on the number of dislocations in the pile-up.

It is seen that for a fixed number of dislocations in the pile-up the value σ_c increases with the increase of the distance between the slip plane and disclination. Thus, when the plastic deformation is localized in certain slip planes, the greatest hardening effect from the elastic fields of disclination is achieved not near the grain boundary, but far from it.

It follows from the analysis that this type of dislocation pile-ups caused by junction disclinations accumulating during plastic deformation may exist in the body of grains in the absence of any visible physical barriers located in the slip plane.

One of the distinguishing features of this type of pile-ups is that they do not disappear under unloading.

Let us consider now the influence of junction disclinations on the nucleation of cracks at the head of the pile-up of edge dislocations stopped by the grain boundary oriented at an angle of 30^0 to the x axis (Fig.4). In the absence of disclinations ($\omega = 0$) the classical scheme for crack initiation according to the Stroh's model takes place. In this model the crack nucleation occurs at $\sigma > \sigma_c$ where σ_c is the value of stress at which two head dislocations of the pile-up come to a distance $d < 2r_c$, where $r_c \sim b$ is the radius of the dislocation core.

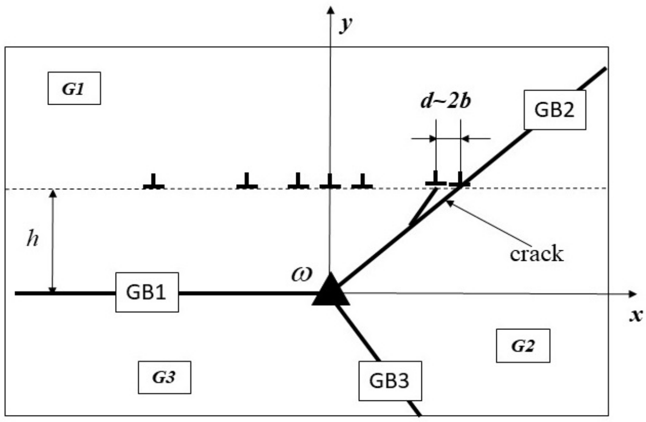

Fig. 4. Schematic plot of the crack nucleation at the head of edge dislocations pile-up.

For a given external stress, the crack nucleation is possible only when the number of dislocations in the pile-up is greater than a certain critical one (curve 2 in Figure 5.) Note that, as Stroh showed, at $\sigma > \sigma_c$ the action of the external stress is sufficient to move the largest part of the remaining dislocations of pile-up into a crack that makes possible the initiation of a Griffith's crack.

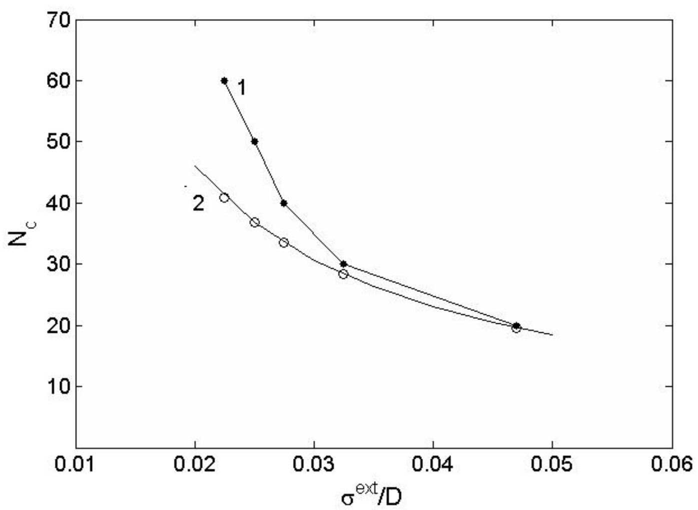

Fig. 5. The dependence of critical number of dislocations in the pile-up on the external stress at junction disclination strength $\omega = 0.01$ (curve 1) and at $\omega = 0$ (curve 2), h=1μm.

The results of computer simulation show that junction disclination supress the crack nucleation. The confluence of the head dislocations of pile-up occurs at a greater number of dislocations than in the Stroh model. The dependence of the critical number of dislocations at the typical disclination strength $\omega = 0.01$ rad is shown in curve 1 in Fig. 5 for h=1μm. Obviously, this effect can be neglected only for very large external stress values $\sigma^{ext} >> D\omega/2$.

4. Conclusion

Basing on the results of the analysis the following conclusion can be summarized:

- A physical mechanism of hardening associated with the accumulation of disclination in triple junctions of high angle grain boundaries at large plastic deformation is developed.
- An existence of special type dislocation pile-ups forming at large plastic deformation in the absence of any visible physical barriers in the body of grains is predicted.
- Strain induced junction disclinations suppress cracks nucleation in the head of dislocations pile-up.

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References

[1] A.N. Stroh // *Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences* **223(1154)** (1954) 404.
[2] V.V. Rybin, A.A. Zisman, N.Yu. Zolotorevsky // *Acta Metallurgica et Materialia* **41(7)** (1993) 2211.
[3] V.V. Rybin // *Problems of materials science* **1(33)** (2003) 9.
[4] A.E. Romanov, A.L. Kolesnikova // *Progress in Materials Science* **54** (2009) 740.
[5] M. Seefeldt // *Reviews on advanced materials science* **2** (2001) 44.
[6] A.E. Romanov // *European Journal of Mechanics A/Solids* **22** (2003) 727.
[7] J. Friedel, *Dislocations* (Pergamon, London 1964) p. 391.
[8] V.N. Perevezentsev, G.F. Sarafanov // *Technical Physics Letters* **41(10)** (2015) 968.
[9] A.E. Romanov, V.I. Vladimirov, In: *Dislocations in Solids*, ed. by F.R.N. Nabarro (North Holland, Amsterdam, 1992), Vol. 9, p. 191.
[10] E. Van der Giessen and A. Needleman // *Modelling and Simulation in Materials Science and Engineering* **3(5)** (1995) 689.
[11] E.A. Rzhavtsev, M.Y. Gutkin // *Scripta Materialia* **100** (2015) 102.