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Theoretical analysis of features of dipole and quadrupole configurations of partial disclinations in nanocrystals of metals

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Abstract. The results of theoretical analysis of fields of local internal stresses and their gradients of nonequilibrium substructures in metal materials during the formation of nanostructural states in conditions of intensive deformation are presented. Possibility of use of disclinational approach within the continual theory of defects for description of the above mentioned states at nanoscale structural level is shown. Dipole and quadrupole configurations of wedge partial disclinations are considered. It's shown that the size of local internal stresses and their gradients can reach $P \approx E/50$ and $\partial P/\partial x \approx 0.02$ nm^{-1} respectively. The calculating experiment demonstrates that high values of local internal stresses and their gradients in the field of elastic distortions can be described by multipole configurations of partial disclinations like dipole/quadrupole. The problem of the nanodipole configuration of partial disclinations and its disintegration on quadrupoles system is considered.

1. Introduction

One of the intensively developing directions of physics of strength and plasticity is creation and study of nanostructural metal materials. By now the experimental results show that the main factor in charge of the formation of unique physical and mechanical properties in such materials is features of their nonequilibrium structure [1 - 4]. Such structure is characterized by existence of the high-defect states differing in elastic fields with the considerable values of local internal stresses [5, 6], and in some cases essential increase of the specific atomic volume [7].

Unfortunately, practically there are no works on the theoretical description and modeling of such non-equilibrium states, which have a direct influence on the evolution of the microstructure, as well as the level of physical and mechanical properties of nanostructured metal materials under different conditions of external impact. The above mentioned problem, in our opinion, is the result of insufficient study of representations of the relationship between the nanograin's sizes and the processes of evolution of defective substructures. Moreover, the development of the most complete model of evolution in metal crystal grains within multilevel approach assumes consideration of

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mechanisms of deformation at the different scale levels [8]. It's important that in contrast to the macro-, meso- and submicrocrystalline scale levels to describe the processes of the transformation of the microstructure on the nanoscale level classical (dislocation) approaches often can't be applied. So in the papers [9 - 10] it's shown that in some materials grains practically don't contain a dislocations after decrease of their sizes to several tens nanometers. At the same time it's established that in conditions of intensive plastic deformation the rotational mode appears in the metal nanocrystals. Such mode leads to the formation of a substructure with high curvature of a crystal lattice, zones of the braked shifts and turns, nanostrips of the reorientation [5, 6]. The existence of this rotational mode indicates the possibility of using disclination models and representations which were applied only to the description of structural conditions of metal materials on meso- and submicrocrystalline scale levels.

In this paper the simulation of the dipole and quadrupole disclination configurations in the field of elastic distortions and the subsequent theoretical analysis of fields of local internal stresses and energies of these configurations are conducted.

2. Experimental materials and procedures

Computing experiment was conducted in computer algebra system Maple version 15. Simulation of tension fields is carried out with using of the explicit form of components of the stress tensor [12, 13]. For the convenience of calculation were considered only wedge components of disclinations. Visualization of stress fields and the spatial distribution of elastic energy is produced using graphical tools of Maple 15. Analysis of the dependence of the energy of disclination configurations (dipole / quadrupole) is performed using numerical integration by Gauss method in the adaptive 30-point variation, at estimates of values of an integration the Kronrod's rule on 61 points was applied.

In the simulation of the crystal representations of the homogeneous isotropic continuum in which the Hooke's law is carried out are used. Independent elastic constants were the shear modulus (G) and Poisson's ratio (ν). The value of the Frank's vector (power of disclinations) ω during computing experiments didn't change and amounted to $\omega \approx 1°$. The last condition is necessary for a geometrical linearization of displacement from disclinations, i.e. in the formulas for the elastic fields are only saved by line ω members. It allows to receive closed analytical relations for elastic fields and energies of rectilinear disclinations [13].

3. Results and discussion

As a result of the conducted electron-microscopic research in works [5, 6] existence of nanostrips of reorientation tens long and few nanometers wide, characterized by high (hundreds of degrees / micrometer) values of elastic curvature of the crystal lattice and high ($\partial P / \partial x \approx 0{,}02$ nm^{-1}) local stress gradients is revealed. On the basis of the analysis results is obtained misorientation scheme (figure 1 c) [6]. The important feature of the found nanostrips is that they break off in a crystal (figure 1 c) and thus they are becoming the zones of the braked shifts and turns. The typical misorientation angles (φ) have values $\approx 0.5° - 2°$ (figure 1 a, b).

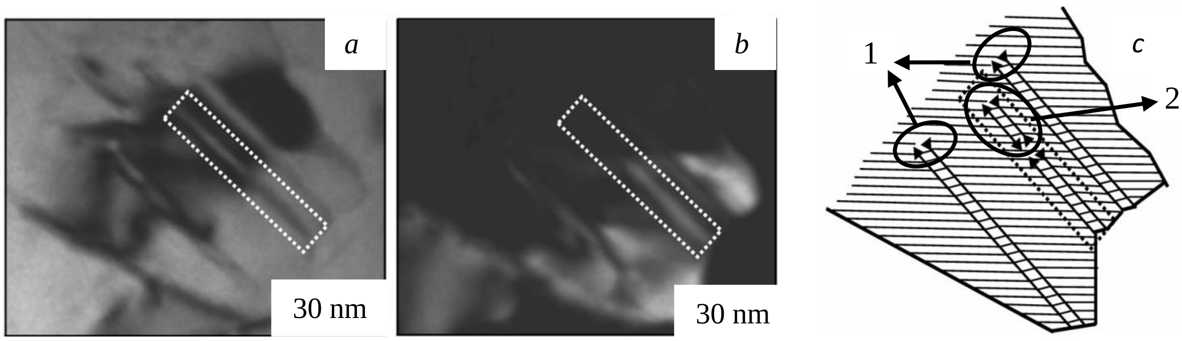

Figure 1. Nanostrips of reorientation in submicrocrystalline nickel after intensive plastic deformation a - bright-field electron - microscope image; b - dark-field image; c - misorientation scheme[5, 6].

On the above mentioned scheme (figure 1 c) the configuration of identified partial disclinations are shown. In particular, dipole (the areas 1 in figure 1 c) and quadrupole (the area 2 in figure 1 c) configurations are presented. From the experiment were found that the characteristic parameters of disclination configurations are the size $l = 3 – 5$ nm and the value of the Frank's vector defined angles of misorientation, $\omega \approx$ $\omega \approx$ 0.5 ° - 2 °.

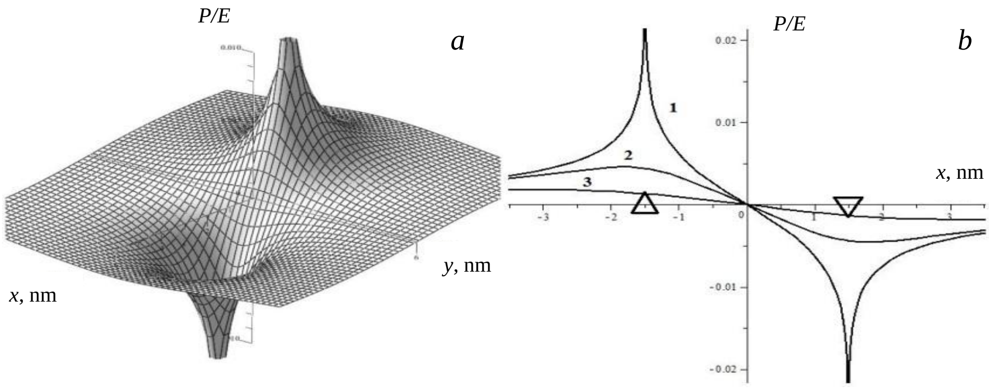

Figure 2. The character of change of pressure $P = (\sigma_{11} + \sigma_{22} + \sigma_{33})/3$ for the nanodipole of partial wedge disclinations with the size $l = 3$ nm and the value of the Frank's vector $\omega \approx 1$ °. a - spatial distribution; b - at different distances from the bedding plane of the dipole $y = 0$ nm (curve 1): at the distance $y = 1$ nm (curve 2); at the distance $y = 3$ nm (curve 3).

Within continual approach using described earlier formalism the analysis of character and magnitude of the stress field of nanodipole with parameters $l = 3$ nm and $\omega \approx 1$ ° in the field of elastic distortions is produced. In figure 2 the spatial distribution of local internal stresses is presented. As can be seen, the stress field is characterized by a complex form with localization in the region of the partial disclinations. It's shown that the maximum stresses and pressure gradients are observed in the bedding plane ($y = 1$ nm) of dipole (figure 2 b). And their values reach the order of $P \approx E / 50$ and $\partial P / \partial x \approx$ 0,02 nm^{-1}. The presented curves in figure 2 b curves indicate rapid decrease of the interaction forces with increasing distance from the bedding plane, due to the effect of shielding of the individual disclinations fields. Figure 2 b shows that, in contrast to the stress field of individual disclination at a distance of $x = 6 - 9$ nm ($2\,l - 3\,l$) almost complete relaxation of the elastic fields of the nanodipole configuration is observed. Thus, the presented nanodipole of partial disclinations really is the concentrator of high tensions in the localized area of the elastic continuum.

In the case of the quadrupole configuration modeling of stress fields was conducted on the equilibrium quadrupole with the size $l = m = 3$ nm, and the value of the Frank's vector $\omega \approx 1$ °. Figure 3 a shows that the field of local internal stresses is symmetric and has four zones of increased stress concentrations corresponding to the locations of partial disclinations. Similarly dipole configurations in the quadrupole are also achieved high (up to $P = E / 50$) values of internal stress fields. In addition, the distinctive feature of the quadrupole configuration is the increase of the values of stress gradients in the bedding plane of dipoles in contrast to the above presented lonely dipole (figure 3 b). It's found that in the quadrupole bounding planes gradients and internal stresses are maximum and reach values $\partial P / \partial x = 0.03$ nm^{-1}. This fact testifies to the presence of an additional screening of interaction between the individual disclination dipole.

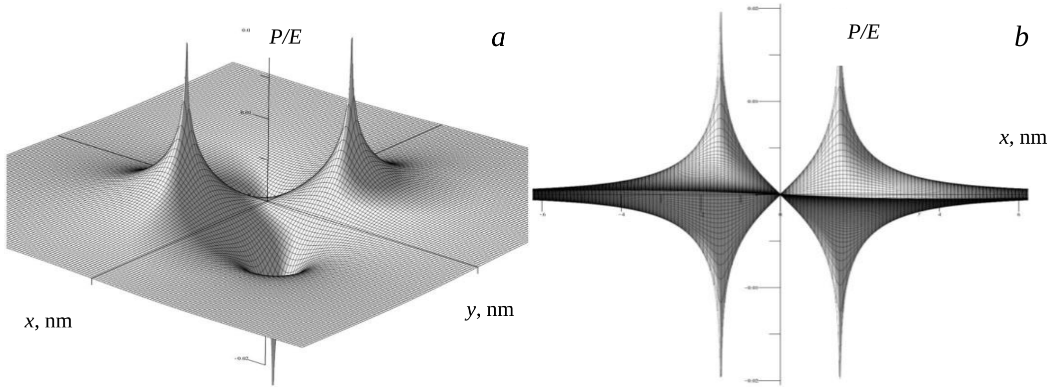

Figure 3. The character of change of pressure $P = (\sigma_{11} + \sigma_{22} + \sigma_{33})/3$ for the quadrupole of partial wedge disclinations with the size l = 3 nm and the value of the Frank's vector $\omega \approx$ 1.a - spatial distribution; b - projection on the plane *x0P* °

Thus, the above presented analysis of the stress distribution demonstrates the possibility of existence of the considered configurations partial disclinations as concentrators of high tensions in the localized area of the elastic continuum. However, to assess probability of the existence of certain disclination configuration requires knowledge of its energy. Due to above told, the analysis of distribution of specific resilient energy in a continuum of dipole and quadrupole configurations (using the formulas [13]) is produced. The results of this analysis are presented in figure 4. It should be noted that the elimination of a logarithmic divergence of energy at large distances is the result of the screening and, thus, energy of dipole and quadrupole systems become independent of the sizes of grain and are defined only by their size. However, the maximal error of calculation of elastic energy distribution is localized in the region of the disclinations, that is seen by the presence of singularities along the line defect (figure 4). A distinctive feature of the quadrupole is that a significant part of the elastic energy is concentrated in its physical volume (figure 4 b), while in the case of the dipole configuration, the area of distribution of elastic energy exceeds its physical size.

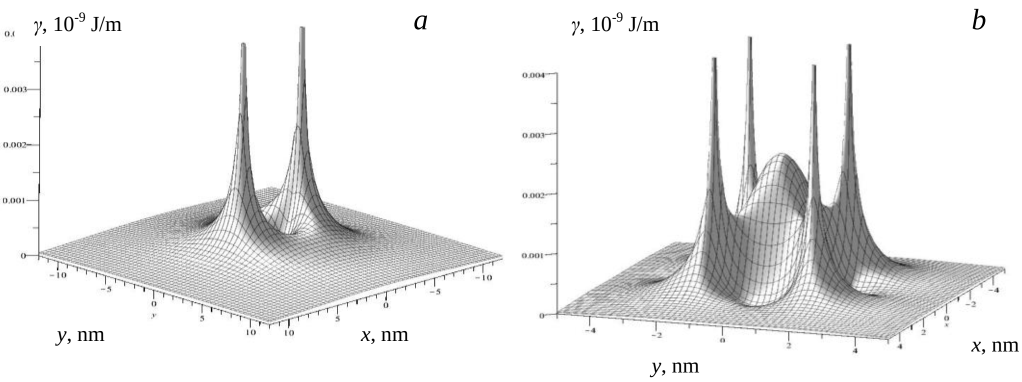

Figure 4. The distribution of the specific elastic energy a - the nanodipole of partial wedge disclinations with the size l = 3 nm and the value of the Frank's vector $\omega \approx$ 1; b - quadrupole partial wedge disclinations with parameters $l = m$ = 3 nm, $\omega \approx$ 1 °.

The analysis of stability considered disclination configurations performed on the basis of estimates of the elastic energy depending on the its size (l). It's shown that after increasing l the proportion of the exchange interaction is reduced that leads to increase in fields of tension and energy (figure 5). As can be seen, for l > 20 cm (figure 5 curve 1) the value of energy for nanodipole system becomes comparable with energy of the separate disclination that testifies to disintegration of system. At the same time, for small values of $l < 6$ nm in the continuum approach the dependence of nanodipole energy has square character and agrees well with analytical expression for the linear energy of the edge dislocation with Burgers vector $\boldsymbol{b} \approx \boldsymbol{l}\,\boldsymbol{w}$ (figure 5 curve 1).

In comparison with the quadrupole configuration (figure 5 curve 2) the value of the dipole energy is order of magnitude larger and more dependent on the its size(figure 5). Thus, in a free elastic continuum (without the presence of internal and external sources of tension), the quadrupole configuration is represented energetically more preferable. This fact indicates the possibility of transformation (disintegration) of the dipole configuration of partial disclinations in the quadrupole.

It's important to note that in the absence of screening by other disclinations systems dipole configuration may be more stable. One of these variants is presented in figure 1. While the central nanodipole is transformed to a quadrupole other dipole configurations near border remain steady.

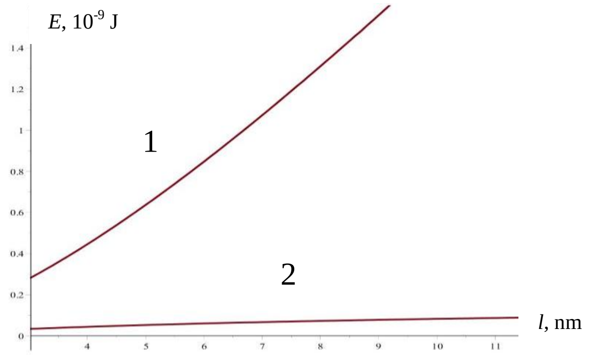

Figure 5. The dependence of the energy for the disclination configuration from the size: 1 - the nanodipole of partial wedge disclinations with the value of the Frank's vector $\omega \approx 1$; 2 - quadrupole partial wedge disclinations with parameters m = const = 3 nm, $\omega \approx 1$ °.

4. Summary

The possibility of using disclination approach within the continuum theory of defects for describing the above presented states on the nanoscale structural level is shown. Based on the study of the force characteristics of dipole and quadrupole configurations of wedge partial disclinations it's established that these configurations characterized by high gradients ($\partial P / \partial x \approx 0.02$ nm^{-1}) of the local stresses in the spatial scales $l < 20$. It's shown that in the energy relation the existence of a quadrupole configuration is more favorable.

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