Analysis of the elastic-stressed state of disclination configurations in the nanograin boundary

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Abstract. Disclination models of grain boundaries in crystals are considered. The features of the spatial distribution of the configuration stress fields depending on number of disclinations and magnitude of the common Frank’s vector are described. The estimate of the energy of the configurations based on the calculations in a wide range of values of the bending-torsion tensor 0.2…1.8 degrees per nanometer was obtained. It was shown that the energy of the equidistant model is higher than the energy of the other two with irregular distribution of disclinations.

1. Introduction

It is known that the main elements of the defective structure of metallic materials are grain boundaries. Depending on the nature of long-range stress fields and excess free energy, a special class of grain boundaries can be distinguished – non-equilibrium boundaries [1-3]. Such boundaries are of great interest for the description and development of ideas about the nature of nanocrystalline materials, which are characterized by the presence of a significant fraction of the grain boundary phase.

Unfortunately, at present, there are only a few works with a quantitative assessment of the parameters of structural states with a high density of defects at various scale levels, and there is a need for conducting complex experimental studies with a theoretical interpretation of the structural elements of the boundary. The generalization of experimental results presented in [4] demonstrates that disclination configurations play a decisive role in the formation of nanocrystalline states in metals and alloys of different classes. Thus, the theoretical description of the grain boundary phase of nanocrystalline materials within the framework of disclination model representations is an important task of modern materials science.

In the present work, a simulation and analytical study of the features of stress fields and the energies of the boundaries of disclination-type grains in nanocrystalline materials is conducted.

2. Experimental materials and procedures

The computing experiment was carried out using the program environment Maple 17. Elastic properties of the modelled media were characterized by modules of elasticity of pure nickel ($E = 204$ GPa $G = 79$ GPa, where $E$ – Young’s modulus, $G$ – shear modulus). Disclination configurations were considered within the framework of the continual method. The charge carriers in these configurations were partial wedge disclinations of the same sign. During modelling the size of the common Frank’s vector did not...
change and was equal to \( \Omega = 10^2 \). To calculate the stress fields and elastic energy, we used the explicit form of the stress tensor components. [5]. In case of wedge disclinations with Frank’s vector \( \omega_z \) directed along axis \( z \) the stresses field have the form:

\[
\chi = \frac{G\omega_z}{4\pi(1-\nu)} r^2 \ln(r),
\]

(1)

\[
\sigma_{xx} = \chi, \quad \sigma_{yy} = \chi, \quad \sigma_{xx} = \chi, \quad \sigma_{xy} = -\chi, \quad \sigma_{zz} = \nu (\sigma_{xx} + \sigma_{yy}).
\]

(2)

Here \( \chi \) – function of stress of Erie, \( \nu \) – Poisson ratio, \( G \) – shear modulus, \( r^2 = x^2 + y^2 \).

The analysis of the energies of disclinational configurations was carried out using the Gauss numerical integration in a 30-point adaptive variation. The integration values were estimated over a set of 61 estimation points using the Kronrod formula.

3. Results and discussion

In the present work, three schemes of disclination distribution of a charge, which can describe structure of borders of nanograins, were considered. The arrangement of linear defects in the first disclination configuration had equidistant character, at which the distance between two disclinations is constant (Figure 1 a). In the second configuration, the distance between disclinations had the irregular exponential character (Figure 1 b). In the third configuration the distance between disclinations charges increased in an arithmetic progression (increase with a constant step), and also had irregular character (Figure 1 c).

Power of disclinations depended only on their quantity \( N \) like \( \omega_i = \Omega / N \). The sizes of the flat disclination concentration varied from several to several tens nanometers, but did not exceed the nanograin size \( R = 100 \) nm. The specified configurations were chosen based on the analytical form of the stress tensor (2).

On the basis of the analysis of elastic stress it was found that fields of stress are mainly localized in the plane of the disclinations (Figure 2). The areas through which the defect lines pass correspond to local peaks, which are characterized by divergence of the stress tensor elements. In the case of a uniform charge distribution, due to the superposition of the stress fields, the maximum pressure values are reached in the center of the disclination configuration and at \( N = 10 \) are \( P \approx E / 55 \) (Figure 2 a). In the exponential disclination scheme, a significant part of the stresses is observed in the region of the maximum density of disclinations and is equal to \( P \approx E / 26 \) (Figure 2 b). For a configuration with an arithmetic progression of the stress field, similarly, as in the case of the exponential configuration, localized in places with maximum density of disclinations (Figure 2 c). These configurations are uncompensated, since they consist of single sign disclinations. For this reason, they do not observe relaxation of stress fields over the entire grain size. The average value of stress gradients for all configurations presented above is \( P \approx E / 35 \). An increase in the number of disclinations \( N \) while maintaining the common Frank’s vector \( \Omega \) leads to a “blurring” of stress fields. Thus, at \( N = 10 \) the maximum pressure values no longer exceed \( P \approx E / 26 \).
The study of the spatial distribution of elastic energy showed that most of the energy in all configurations is concentrated near the lines of disclination type defects (Figure 3). In contrast to the equidistant case, in configurations with an irregular pattern of charge distribution, the features of the superposition of stress fields provide a high density of elastic energy in a region of high density of disclinations (Figure 3 b, c).

Figure 4 shows the dependences of the energies of all the disclination configurations on the value describing the curvature of the crystal lattice – the bending-torsion tensor. It is shown that regardless of the method of constructing configurations these dependencies have a similar character. The energy of the equidistant configuration is slightly lower than the energy of the other two in a wide interval of values of the bending-torsion tensor. This indicates that the equidistant configuration is an energetically
more stable system. Therefore, based on this configuration, it is possible to construct a relatively stable model of the boundary of the nanograin. To build a more non-equilibrium boundary one should use irregular disclination configurations, for example, a configuration with an exponential distribution of disclinations.

![Figure 4](image.png)

**Figure 4.** Comparison of the energies of disclination configurations depending on the magnitude of the component of the bending-torsion tensor. G1 – curve of energy for equidistant configuration, G2 – curve of energy for exponential configuration, G3 – curve of energy for configuration with the arithmetic progression, G4 – energy wedge disclination with Frank's vector $\Omega \approx 10^\circ$.

In the case of increasing the distance between disclinations ($\chi \to 0$), the share of exchange interaction (superposition) decreases, which leads to the degeneration of these configurations into a system of individual noninteracting disclinations (Figure 4). In other case, as the density of the disclination charge increases ($\chi \to + \infty$), there is an asymptotic tendency of the total energy of the configurations to the disclination energy with the with Frank's vector $\omega \approx 10^\circ$.

**4. Conclusion**

The paper discusses disclination configurations that simulate the boundaries in nanocrystalline materials. In the study of the elastic-stress state of these configurations, features of the stress fields were found depending on the number of disclinations and the magnitude common Frank's vector. Based on the performed calculations, the estimate of the configuration energies was obtained in a wide range of values of the bending-torsion tensor, which is equal to $0.2...0.10$ degrees per nanometer. It was found that the energy of the equidistant model is lower than the energy of the other two with irregular distribution of disclinations. This indicates that the equidistant configuration is an energetically more stable system.

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