Change in the Structural State of Grain Boundaries under High-Rate Mechanical Loading

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The molecular-dynamic modeling of the behavior of a three-dimensional crystallite that contains a specific-type grain boundary under shear loading is performed. It is found that the accommodation of displacements of the material grains can be realized owing to structural changes in the intergrain boundaries. The crystal-like structure of the grains can be restored after the external action terminates. The results obtained give deeper insight into the nature of the structural response of the material under mechanical loading at the atomic level.

It is well known that high-rate loading can lead to significant structural changes in real materials [1, 2]. Moreover, owing to the heterogeneous structure, some blocks and grains can undergo large shear strains. It should be noted that a number of unusual nonlinear responses of the material are associated with shear loading. Psakh'e et al. [3, 4] showed that the collective vortex-like motion of the atoms occurs under high-rate shear in the intergrain-boundary region. On a certain interval of shear velocities, the intergrain boundary can propagate at an abnormally high velocity, which can reach 600 m/sec [4]. The results given in [3, 4] were obtained at low temperatures. At the same time, the structural response of the intergrain boundary to high-rate mechanical loading at room or higher temperature can have specific features. Therefore, the present paper deals with the high-rate action on the behavior of a specific-type boundary at room temperature. We chose these boundaries because their properties are sensitive to the temperature [5].

A three-dimensional Al crystallite that contains a specific-type boundary Σ7 was examined. The crystallite dimensions in the directions of the OX, OY, and OZ axes were 167, 65, and 40 at.units, respectively. (As Harrison [6] and Sena [7] pointed out, the use of the atomic system of units is convenient in macroscopic investigations.) The coordinate axes were directed along the following crystallographic directions: the OX axis along (011), the OY axis along (211), and the OZ axis along (111). The crystallite contained over 4 · 10⁵ atoms. The investigation was performed by the molecular-dynamic method with the use of "MONSTER MD" software. The interatomic interaction was calculated within the framework of the pseudopotential method [8].

The grain boundary was located in the middle of the specimen and oriented perpendicularly to the OX axis. The periodic boundary conditions were used in the directions of the OY and OZ axes, whereas the specimen edges were shifted in the OX direction with a constant velocity

\[ V_x = V_z = 0, \quad V_y^l = - V_y^r = -200 \text{ m/sec}, \]

where \( V_y^l \) and \( V_y^r \) are the velocity components at the left and right edges of the specimen, respectively. The investigations were performed at room temperature.

Calculations showed that the structure of the intergrain region changes significantly under the conditions of intense shear loading. The atoms located in the grain-boundary region are displaced from the corresponding atomic planes (Fig. 1).

The form of the radial-distribution functions for the intergrain region is shown in Fig. 2 at the initial moment of time and during loading. A comparison of Figs. 2a and 2b shows that the structure of the
Fig. 1. Projection of the specimen structure onto the $XOZ$ plane at the initial moment of time (a) and $t = 120,000$ at.units (b): solid curves show the grain boundary.

Fig. 2. Functions of the radial distribution of the atoms in the specimen at the initial moment of time (a) and $t = 120,000$ at.units (b).