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Numerical Study of the Influence of Grain Size and Loading Conditions on the Deformation of a Polycrystalline Aluminum Alloy

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Abstract

This work is concerned with numerical simulations of surface roughening in a polycrystalline aluminum alloy. Using 3D finite difference model, high-resolution simulations are conducted. Effects of loading conditions and grain size on surface roughening and mesoscale deformation processes in AL6061-T3 aluminum alloy under quasistatic uniaxial tension are investigated.

Keywords

Polycrystalline Materials, Surface Roughening, 3D Model

1. Introduction

One of the behavioral features of aluminum alloys, limiting their possible use as a material for machine parts, is deformation-induced surface roughness formed on the free surface under wide range of deformation conditions. Despite the increasing number of experimental and computational studies in this area (see, e.g., [1]-[7]), the causes and the mechanisms of surface roughening continue to be debated among researchers. The surface roughening phenomena are shown to be dependent on many microstructural factors such as grain size [1], crystallographic texture [3] [4], etc. Grain anisotropy which causes plastic strain localization and, consequently, surface roughening, has a significant influence on the changes of surface morphology [3].

Real behavior of aluminum alloys is related to the complex multi-level structure of the metal, and the processes occurring within the bulk and on the surface of material depend on a variety of factors. Investigation of the influence of individual factors on the deformation and fracture in the experiment is often not possible. In this regard, numerical simulation is an important addition to the experimental studies. In [8] the evolution of mesoscale deformation in polycrystalline Al6061-T6 alloy containing 280 grains has been analyzed in detail.

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Plastic deformation is shown to arise at the grain boundaries which are sources of stress concentration in material. Localization of stresses and strains is more pronounced near the free surface than in the bulk of material.

This paper continues a series of computational studies of surface roughening phenomena and mesoscale deformation processes in polycrystalline materials [5]-[8]. The influence of boundary conditions (BCs) and grain size on the qualitative characteristics of the surface roughness in polycrystalline AL6061-T3 alloy is analyzed. Microstructural model proposed in [8] is modified to apply periodic BCs. The role of free surface and grain boundaries in the evolution of deformation processes at the mesolevel is discussed. Optimal thickness of the three-dimensional (3D) model for the study of surface roughening is defined.

2. Three-Dimensional Microstructure-Based Simulation

In order to describe the mechanical behavior of a material, we use the mathematical tools of continuum mechanics, assuming that a medium retains its continuity at the meso- and macrolevels in plastic deformation. Total system of equations to describe the elasto-plastic behavior of a material includes equations of motion and continuity, expressions for components of the strain rate tensor and constitutive equations defining the relationship between the stress and strain tensors. The procedure used in the 3D numerical analysis is detailed elsewhere (see, e.g., [9]).

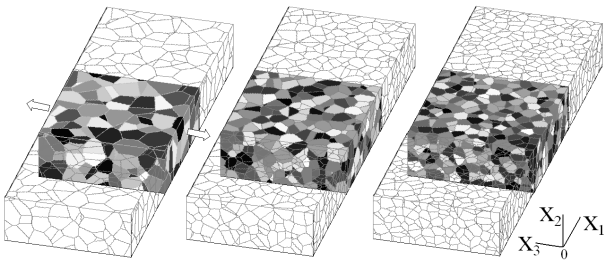
In this work 3D polycrystalline structures are generated by the step-by-step packing method proposed in [9]. Rectangular volume is discretized by a regular mesh of 200 × 75 × 200 cubic cells with a step of 10 μm. As the initial conditions, nucleation centers are distributed randomly within the volume. All grains are assumed to grow according to a spherical law and with the same rate.

Polycrystalline structures, periodic in the X_1-direction, are shown in **Figure 1**. In all three cases, the size of the computational domain is 2000 × 750 × 2000 μm, and the number of grains varies from 200 to 1000. Average grain diameters are 300, 200 and 170 microns, respectively. In order to obtain a periodic structure in a certain direction, an additional condition is checked: if the growing grain goes beyond the surface, its growth continues on the opposite side by parallel transfer. From the equation of spherical volume V, the grain diameter can be expressed as

$$V_g = \sqrt[3]{6V/\pi} = h_m \sqrt[3]{6N_c/\pi}, \tag{1}$$

where N_c is the number of cells approximating the grain, h_m is the step of computational mesh.

A rigorous description of elasto-plastic material behavior calls for crystal plasticity models taking into account explicitly the crystallographic orientation of individual grains and the slip planes, and is based on physics of dislocation interaction [10]. Such models are of fundamental importance for use in describing the behavior of materials with a limited number of slip systems and plastically anisotropic materials. They should be also used when grains rotate significantly because a phenomenological plasticity models based on experimental data and their approximation do not account for the microscale processes in an explicit form. The macroscopically isotropic AL6061-T3 aluminum alloy under study is characterized by fcc lattice and has 12 slip systems, respectively. For the sake of simplicity, assuming that the crystallographic orientation relative to the applied load has no significant effect on the yield stress within the grain, we omit an explicit formulation of crystal plasticity taking an implicit account of the crystallographic orientation of grains through the difference between their elastic and plastic characteristics within ±2 ÷ 5% about average values.



(a) (b) (c)

Figure 1. Polycrystalline models with average grain size of 300 (a); 200 (b); 170 μm (c).

In describing the behavior of polycrystalline aluminum alloys, the Hall-Petch effect has special significance. It should be noted that in this work this effect is intentionally disregarded to separate the impact of the grain size and mechanical properties.

The elastic-to-plastic transition is defined by the von Mises criterion with allowance made for strain-hardening:

$$\sigma_{eq} = 1/2\sqrt{S_{ij}S_{ij}} = \sigma_y^i\left(\varepsilon_{eq}^p\right), \tag{2}$$

where $\sigma_y^i\left(\varepsilon_{eq}^p\right)$ is the strain-hardening function of the *i*-th grain, ε_{eq}^p is the accumulated equivalent plastic strain, S_{ij} is the deviatoric stress tensor. The strain-hardening function for the Al6061-T3 alloy is given in the form of

$$\sigma_y^i = \sigma_0^i + 65\cdot\left(1-\exp\left(-\varepsilon_{eq}^p/0.048\right)\right) \text{ [MPa]}, \tag{3}$$

Here σ_0^i is the initial yield stress of the *i*-th grain. Average values of the shear modulus and the bulk modulus defined in the calculations are 28.4 and 82.0 GPa, respectively. Average value of initial yield stress σ_0^i is 107 MPa. Properties remain constant within each grain, while varying in passing through the grain boundary.

The system of equation is complemented by initial and boundary conditions and solved numerically using the finite difference method [11]. In order to describe loading conditions, let us introduce the Cartesian coordinate system as presented in **Figure 1**. Boundary conditions on $x_3 = 0$ and $x_3 = L_3$ sides simulate uniaxial tension along the X_3-axis:

$$U_3\big|_{x_3=0} = -\upsilon, U_3\big|_{x_3=L_3} = \upsilon, \tag{4}$$

where x_i are the spatial coordinates, $U_3 = \dot{x}_3$ is the velocity vector component, L_i are the sizes of computational domain. The bottom surface is a symmetry plane, its displacements are fixed in the vertical direction and are not constrained in the horizontal plane. On top surface BCs correspond to free surface conditions. On lateral sides $x_1 = 0$ and $x_1 = L_1$ of microvolumes the absence of external forces (free surface) or periodic BCs are applied. Thus the loading scheme used in calculations is shown in **Figure 1**.

3. Calculation Results

Numerical results obtained in calculations are shown in **Figures 2-5**. Surface roughening is shown to be mostly affected by microstructure of the subsurface layer [5]. Basing on this observation, we have determined the mini-

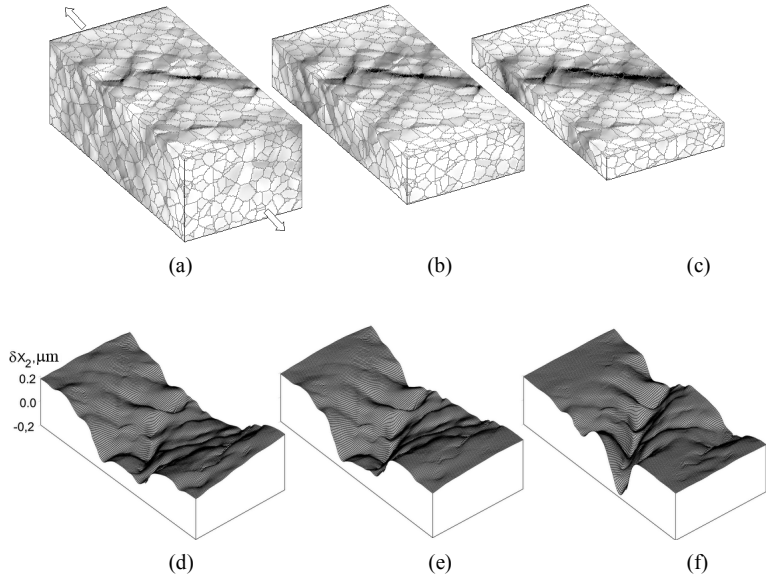


Figure 2. Distributions of equivalent plastic strains ((a)-(c)), and surface roughness patterns ((d)-(f)) in polycrystals of 350 ((a), (d)), 200 ((b), (e)), 100 μm in thickness ((c), (f)), $\varepsilon = 0.3\%$, arrows indicate the direction of tension.

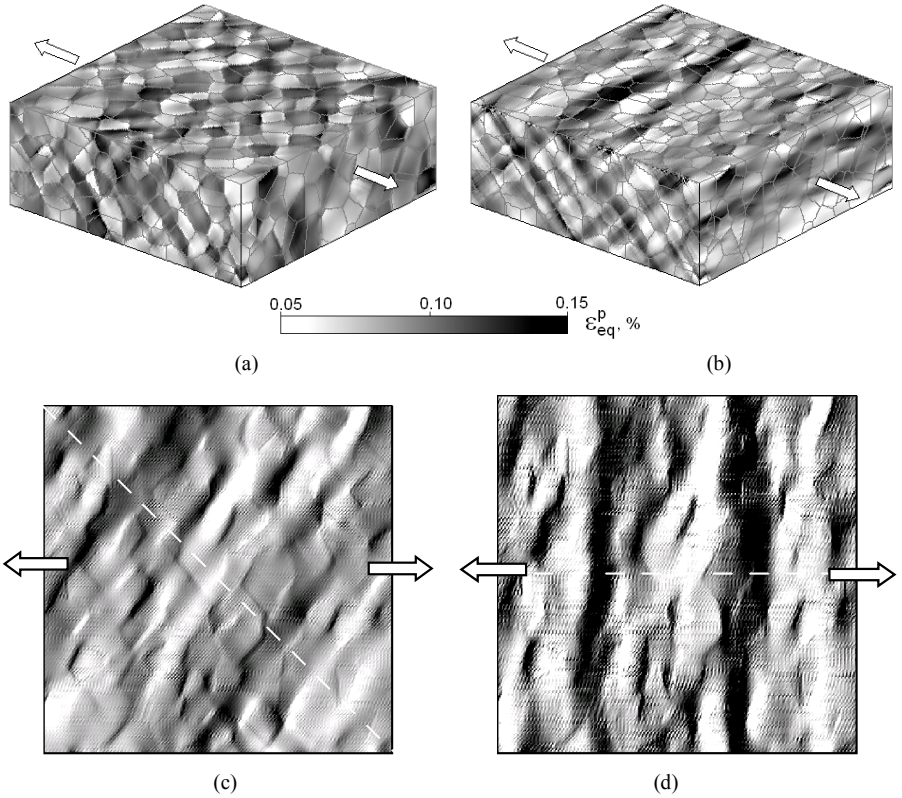


Figure 3. Distributions of equivalent plastic strains ((a), (b)) and surface roughness patterns ((c), (d)) in polycrystals with free lateral surfaces ((a), (c)) and with periodic BCs on lateral surfaces ((b), (d)), $\varepsilon = 0.18\%$.

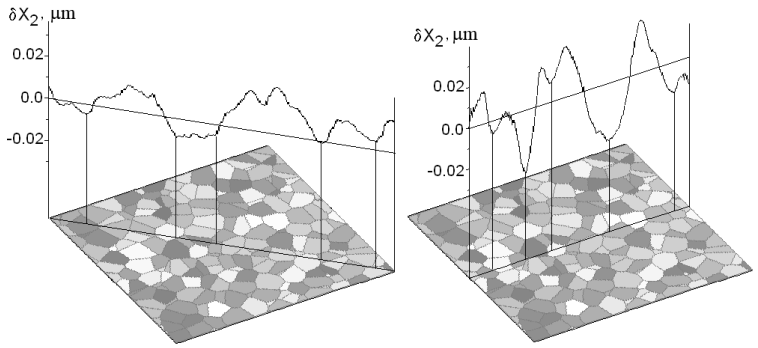


Figure 4. Roughness profiles along the diagonal line (see **Figure 3(c)**) in the polycrystal with free lateral surfaces (a) and along the midline (see **Figure 3(d)**) in the sample with periodic BCs (b), $\varepsilon = 0.18\%$ μm.

mum thickness of the model, needed to reproduce the surface roughening with acceptable accuracy. For doing so, we calculate uniaxial tension of polycrystalline structures of 500 × 350 × 1000, 500 × 200 × 1000, and 500 × 100 × 1000 μm (**Figures 2(a)-(c)**). The lateral $x_1 = 0$ and $x_1 = L_1$ sides are free of loading. Average grain diameter is about 50 μm, so lateral sides in a direction normal to free surface comprises 7, 4, and 2 layers of the grains, respectively.

Analysis of the calculation results shows that the main influence on the deformation processes on the surface has a microstructure lying within 1 - 2 grain diameters. The model that contains only 2 grain layers in thickness fails to adequately describe surface roughness due to influence of the bottom surface (**Figure 2(c)** and **Figure 2(f)**). Using a model of a thickness more than 4 average grain diameters for the considered loading conditions,

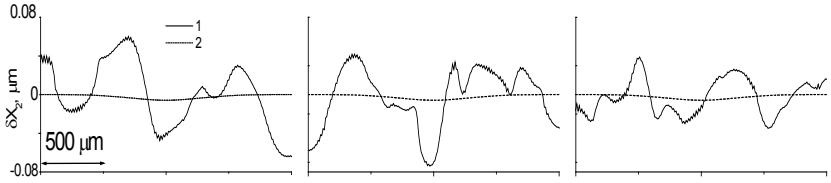


Figure 5. Roughness profiles in polycrystals with average grain size of 300 (a); 200 (b); 170 μm (c) (curves 1); roughness profiles in a homogeneous material (curves 2), ε = 0.22% μm.

we observed that the surface topography varies slightly (cf. **Figure 2(d)** and **Figure 2(e)**). Thus, to investigate the effects of surface roughening, it is recommended to use a model of a thickness of 3 - 4 average grain diameters.

In order to analyze the stress-strain state which is responsible for surface roughening, we have compared the surfaces of a homogeneous isotropic material and a material with internal boundaries. Generally the surface roughening phenomena is related to the microstructure. Due to polycrystalline structure, all components of the stress and strain tensors are nonzero at mesoscale, including the stress tensor component σ_{22} acting across the free surface. In uniaxial tension the stress tensor component σ_{22} exhibits a quasi-periodic distribution of positive and negative values, *i.e.*, the regions exposed to tensile strains alternate with those experiencing compression, compensating each other. Therefore from the macroscopic standpoint, the equilibrium conditions are satisfied. Thus, at mesolevel periodically distributed fields of normal stresses and strains arising in the bulk of the material act from inside towards the surface, resulting in surface roughening. This conclusion was arrived at in our earlier work [12] [13] on the basis of 2- and 3D calculations for a metal matrix composite and a coated material.

To analyze the effects of grain size and loading conditions on the surface roughening, a series of calculations for the microstructures shown in **Figure 1** with different BCs on the lateral sides has been performed. Loading conditions have a significant impact on the surface roughness characteristics. Using 3D matrix-based statistical analysis, authors [2] have experimentally investigated the influence of the loading conditions (uniaxial, biaxial, and plane strain) on the surface roughening in AA5754-O aluminum alloy. In this paper we evaluate the influence of loading conditions on qualitative characteristics of the deformation-induced surface roughness. We consider two idealized cases of BCs: in the first case the lateral sides are free of loading, in the second one they are assigned with periodic BCs that simulate conditions of constrained deformation. The calculations are performed for a model containing 1000 grains (**Figure 1(c)**).

Figure 3 compares the results of calculations for polycrystals with free boundaries and periodic BCs. In both cases, we can observe mesoscopic relief folds, consisting of several smaller ones (**Figure 4**). These computational results are in agreement with experimental findings on aluminum alloys [3] [14]. Qualitative difference is in the orientation of folds and areas of plastic strain localization. When lateral sides are free of external forces, the surface folds and localization bands tend to form at an angle of 45˚ to the axis of tension (**Figure 3(a)** and **Figure 3(c)**), due to the direction of maximum macroscopic shear stress. In the case of periodic BCs, interlacing folds are oriented perpendicular to the loading direction (**Figure 3(b)** and **Figure 3(d)**). In the case of the specimen with free lateral sides, the height of relief folds is smaller, and the width is greater than in case of the sample with periodic BCs (**Figure 4**). In the second case, increase of the surface height data scattering is due to the restriction of deformations in the lateral direction. For both specimens under study, surface roughness profiles demonstrate the presence of several large folds consisting of two or three smaller ones (**Figure 4**). This allows us to class the roughness evolution as a mesoscale phenomenon.

For the study of the grain size effect, we have performed a series of calculations for specimens with an average grain size of 300, 200 and 170 μm (**Figure 1**). It is concluded that the grain refinement gives rise to the decrease of roughness fold height relative to the average level corresponding to the surface of a homogeneous sample, and to the increase of fold number (**Figure 5**). In all cases, the transverse sizes of the folds formed at the early stage of the plastic flow are of 3 - 4 grain diameters.

4. Conclusion

In this paper we have investigated the effect of the loading conditions and grain size on the qualitative characte-

ristics of surface roughness and deformation processes in polycrystalline AL6061-T3 aluminum alloy at the mesoscale under quasi-static tension. It is shown that the increase of grain size leads to the formation of larger relief folds on the surface of polycrystals loaded. Periodic BCs also cause the formation of higher folds with lower period by comparison with the loaded specimen with free lateral surfaces. In order to optimize numerical calculations, we determine the minimum thickness of the specimen for the study of the surface roughness phenomena. It is of 3 - 4 average grain diameters.

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