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Impact of grain boundary character on grain rotation

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Abstract

The capillarity-driven shrinkage of isolated cylindrical grains with structurally different grain boundaries in aluminum was studied by molecular dynamics simulations. Three pairs of grains with ⟨100⟩ tilt and mixed tilt–twist boundaries with the misorientation angles $\theta_0 = 5.45°$, 16.26° and 22.61° were examined. The simulation results showed that the shrinkage of grains with pure tilt boundaries was accompanied by their rotation towards higher misorientation angles. On the contrary, grains with the mixed boundaries did not rotate significantly during their shrinkage. An analysis revealed that for the observed rotational behavior the grain boundary structure is crucial. In contrast to pure tilt boundaries composed of edge dislocations, for mixed tilt–twist boundaries, which are composed of intersecting dislocations with the mixed edge–screw character, the effective mechanisms of dislocation annihilation are available, which allow the respective grains to shrink without rotation.

Keywords: Grain boundary; Grain growth; Grain rotation; Dislocation; Molecular dynamics

1. Introduction

It has been already recognized that, along with dislocation and grain boundary motion, grain rotation is an essential part of microstructure development in polycrystals during plastic deformation as well as in the course of subsequent recrystallization and grain growth during annealing at elevated temperatures [1–6]. It is widely accepted that grains rotate towards a low energy grain boundary configuration associated with the low Σ coincident site lattice orientation relationships [6–8]. This has been also corroborated by atomistic computer simulations by several groups [9–11].

As was theoretically predicted by Cahn and Taylor [12], grain rotation can be induced by grain boundary motion due to the coupling between boundary motion and tangential translation of the adjacent grains, which is proportional to the normal boundary displacement. Since Cahn and Taylor have proposed their approach to describe grain boundary motion, grain translation and grain rotation [12], significant progress was achieved with respect to the theoretical analysis of the shear–migration coupling [12–20] as well as providing experimental evidence of this phenomenon for planar boundaries [21–27]. It has been also experimentally shown that stress-driven boundary migration can be accompanied by grain rotation [28].

The rotation of the isolated grains caused by the coupling effect during their capillarity-driven shrinkage was corroborated by atomistic computer simulations [29–31] and phase-field modeling [32]. However, in situ transmission electron microscopy observations on the shrinkage of island grains in thin films of Al [33] and Au [34,35] did not provide any evidence of grain rotation.

Previous atomistic simulations, where grain rotation during shrinking the island grain was studied [11,29–31], were performed for grains with tilt grain boundaries. A purely tilt grain boundary with a low index rotation axis, however, is a very specific model case. In a real polycrystal most boundaries are not pure tilt or pure twist but rather of

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general type. Their structure is more complex than that of pure tilt boundaries, which are (or can be described as) composed of edge dislocations. The dynamic behavior of grains with random boundaries can therefore be very different from that of grains with pure tilt boundaries. In fact, in the recent experiments and simulations it was found that the change of grain boundary geometry from pure tilt to mixed tilt–twist is crucial for migration and faceting of low angle boundaries in aluminum [36,37]. In the current paper we report on the results of atomistic simulations, which demonstrate that grain rotation during capillarity-driven grain shrinkage is not a universal feature, but confined to the grains with pure tilt boundaries, and does not occur for the grains with random/mixed boundaries.

2. Applied atomistic simulation method

For an analysis of the behavior of the isolated/embedded grains with different pure tilt and mixed tilt–twist boundaries molecular dynamics (MD) simulations were employed. The large-scale atomic/molecular massively parallel simulator (LAMMPS) code [38] was utilized. Aluminum was used as a model material. The atomic interactions were described by the second nearest-neighbor modified embedded atom method (2NN MEAM) potential for Al developed by Lee and coworkers [39–41]. The configuration used in these MD simulations was composed of a cylindrical crystal/grain embedded in a differently oriented crystalline matrix. The capillary-driven shrinkage of such grain misoriented with respect to the matrix by different angles θ around a common $\langle 100\rangle$ axis was studied. Three pairs of grains with pure tilt and mixed tilt–twist boundaries with the misorientation angles $\theta_0 = 5.45°$, 16.26° and 22.61° were examined (Table 1). The grains with tilt boundaries were misoriented around the [100] axis aligned parallel to the z-axis of the simulation box (Fig. 1). The boundaries of these grains retain their pure tilt character over the entire circle/length. For computing the grains with the mixed boundaries the common [100] rotation axis was additionally rotated counterclockwise by an angle of about $\xi \approx 20°$ ($\xi \equiv \mathrm{acos}([100]\cdot\bar{c}/\|c\|)$) around the crystallographic direction parallel to the x-axis of the simulation box. At the inclination $\psi = 0°$, therefore, these boundaries had a tilt–twist character with the 20° twist component. With increasing inclination ψ the twist component ξ decreases down to zero at $\psi = 90°$ (Fig. 1).

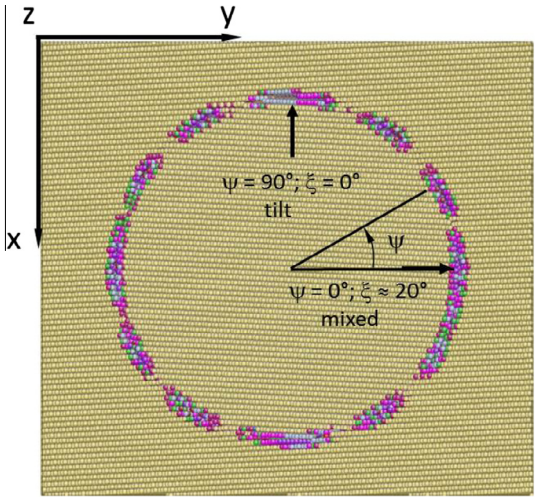

Fig. 1. Cross-section of the simulation box with the embedded cylindrical grain with the 5.5° $\langle 100\rangle$ mixed tilt–twist (see Table 1) boundary. The grain and the matrix are rotated by $\pm\theta/2$ (here $\theta_0 = 5.45°$) around the common [100] axis tilted by an angle $\xi \approx 20°$ around the x-axis. For grains with the pure tilt boundary (not shown) the common [100] axis is aligned parallel to the z-axis.

Periodic boundaries conditions were used on all the surfaces of the simulation box. Before the MD simulation was performed, the energy of the system was minimized by the conjugate-gradient algorithm. Subsequently, damped dynamics were applied to fully relax the grain boundary. The isothermal–isobaric (NPT) ensemble was used for the time integration with a time step of 0.2 fs. All simulations were performed at 400 °C. To avoid stresses caused by thermal expansion and loss of free volume due to grain boundary elimination, the pressure tensor of the simulation box was controlled to zero during the simulation run. Grain rotation during shrinkage was not prohibited to allow the natural development of the system. The change of the grain volume with time was tracked by using an orientation-dependent order parameter for the atoms, as defined in Ref. [42]. In order to warrant the accuracy of the measured properties of the simulated systems, snapshots were regularly saved in intervals of 0.01 ns. The obtained configurations were subsequently quenched

Table 1
Parameters of the performed simulations. The sizes of the simulation box Δx, Δy, Δz and radius r of the cylindrical grain are given in units of the lattice parameter for aluminum (4.05 Å). The three mutually orthogonal vectors $\bar{a}$, $\bar{b}$ and $\bar{c}$ represent the crystallographic directions of the matrix grain that are parallel to the x-, y- and z-axes of the simulation box, respectively. The corresponding axes of the cylindrical grain can be defined in terms of the components of these vectors as $\langle a_i - a_j a_k\rangle$, $\langle b_i b_j - b_k\rangle$, $\langle c_i c_j - c_k\rangle$ for the tilt and mixed grain boundaries.

Boundary	θ_0 (°)	Δx	Δy	Δz	$\bar{a}$	$\bar{b}$	$\bar{c}$	r
Tilt	5.45	42.04	42.04	16	$\langle 0121\rangle$	$\langle 0\bar{2}\bar{1}1\rangle$	$\langle 100\rangle$	15.76
Mixed	5.45	42.04	45.35	56.08	$\langle 0121\rangle$	$\bar{1}7\bar{4}22$	$\langle 52\bar{2}\bar{1}1\rangle$	15.76
Tilt	16.26	42.42	42.42	16	$\langle 017\rangle$	$\langle 0\bar{7}1\rangle$	$\langle 100\rangle$	15.90
Mixed	16.26	42.42	45	21.21	$\langle 017\rangle$	$\langle \bar{5}\bar{1}\bar{4}2\rangle$	$\langle 20\bar{7}1\rangle$	16.87
Tilt	22.61	45.89	45.89	16	$\langle 015\rangle$	$\langle 0\bar{5}1\rangle$	$\langle 100\rangle$	17.11
Mixed	22.61	45.89	49.29	27.92	$\langle 015\rangle$	$\langle \bar{2}\bar{5}1\rangle$	$\langle 13\bar{5}1\rangle$	17.11