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An analytical model for stress-induced grain growth in the presence of both second-phase particles and solute segregation at grain boundaries

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Abstract—A theoretical framework that incorporates the influence of second-phase particles and solute segregation at grain boundaries (GBs) on stress-induced GB migration and grain rotation is formulated in the present paper. In our work, we modified the well-established Cahn–Taylor model to account for the drag stresses generated by second-phase particles and by solute atoms segregated at GBs. The theoretical framework is then implemented to rationalize GB migration and grain rotation using experimental data from a previously published study on stress-induced grain growth in the presence of both second-phase particles and solute segregation at GBs. The calculated grain growth results are generally consistent with the experimental data, providing support to the proposed theoretical model, despite the various assumptions involved. Moreover, the influence of second-phase particles and solute segregation at GBs on GB migration and grain rotation was also investigated using the model, and our results suggest that both second-phase particles and solute atoms segregated at GBs reduce the velocities of GB migration and grain rotation as compared to those in the case of high-purity Al.
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Keywords: Grain growth; Grain boundary migration; Grain rotation; Second-phase particles; Grain boundary segregation

1. Introduction

Grain growth has been the topic of many investigations over the past few decades, and despite the vast amount of theoretical and experimental studies, many important questions remain unanswered [1–8]. It is well established that the underlying mechanisms that govern grain growth primarily involve grain boundary (GB) migration [1–4] and grain rotation (followed by coalescence) [5–8]. The driving forces for GB migration and grain rotation stem from two sources: (i) internal structures, i.e., surface tension due to GB curvature and gradient in dislocation densities between neighboring grains that cause GB migration [1,2] and net torque due to a reduction in GB energy that triggers grain rotation [5,9–12]; and (ii) externally applied stresses [3,4,6–8].

Internal structure driven GB migration (for reviews, see Refs. [1,2]) and grain rotation [5,9–12] have been well documented. Recently, stress-induced GB migration and grain rotation have been extensively investigated using molecular dynamics (MD) simulations [13–21], and in situ [3,4, 6–8,22–24] and ex situ [25–29] transmission electron microscopy (TEM) observations have confirmed the occurrence of stress-induced GB migration and grain rotation. Furthermore, MD simulations [15,17–21] and experimental studies via optical microscopy [30,31] and TEM [23,24] have revealed that, during stress-induced grain growth, there exists a coupling effect between grain translation (sliding) along a GB caused by shear stress along the GB and GB migration, the former giving rise to grain rotation in the case of a curved GB [19,32]. The coupling phenomenon has also been studied by theoretical modeling [32–34].

Inspection of these and other published studies, however, reveals that theoretical [13–18,21] and experimental [3,4,6–8,22–29] efforts relevant to stress-induced GB migration and grain rotation involve mostly single-phase materials and consequently, material systems containing second-phase particles have received very limited attention [35]. As a consequence, an important question remains unanswered. That is, what is the interaction between second-phase particles at GBs and stress-induced GB migration and grain rotation? In addition, inspection of the published theoretical investigations [13–18] indicates that only very limited studies [21] address the effect of solute

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atoms segregated at GBs on stress-induced grain growth. Interestingly, despite the fact that electrodeposited materials, which almost always contain a high level of impurities as solute atoms segregated at GBs [8,25,27,36,37], are widely used as model materials to study stress-induced GB migration and grain rotation, the interactions between GB segregation and stress-induced GB migration and grain rotation are seldom discussed [35,38].

Most recently, Lin et al. experimentally studied the stress-induced grain growth phenomenon in the presence of both second-phase particles and solutes segregated at GBs during hot extrusion of an ultra-fine-grained (UFG) 5083 Al (an Al–Mg–Mn–Cr–Fe alloy) synthesized via the consolidation of mechanically milled powders [35]. The results show that second-phase particles and solute segregation at GBs generate such high resistance forces that grain growth was essentially inhibited during annealing of the UFG 5083 Al at 400 °C for a prolonged period of 5 h in the absence of an externally applied stress. In contrast, the average grain size increased by a factor of ~2.7 during hot extrusion of the UFG 5083 Al at 400 °C, suggesting that the externally applied stresses originating from the state of stress imposed during extrusion overcame these resistance forces, enabling the operation of GB migration and grain rotation and thus the occurrence of grain growth.

In view of the above discussion, it is the objective of the present study to quantify the influence of second-phase particles and solute segregation at GBs on GB migration and grain rotation during stress-induced grain growth. To accomplish this goal, a theoretical framework is first formulated by incorporating the drag stresses generated by second-phase particles and by solute atoms segregated at GBs into the well-established Cahn–Taylor model [32] and then implemented to rationalize stress-induced grain growth phenomenon reported in Ref. [35]: (i) to analyze and discuss stress-induced grain growth during hot extrusion and (ii) to quantify the influence of second-phase particles and solute atoms segregated at GBs on stress-induced GB migration and grain rotation. In order to provide proper context to the present study, the experimental results reported in Ref. [35] are reviewed in Section 2.

2. Published experimental results on stress-induced grain growth phenomenon in UFG 5083 Al containing both second-phase particles and solute segregation at GBs [35]

An UFG 5083 Al (chemical composition: Mg 4.50, Mn 0.70, Cr 0.16, Fe 0.20, Ni 0.019, Si 0.13, Cu 0.014, C 0.019, O 0.45, N 0.004, Al balance, wt.%) used as the model material for the study of stress-induced grain growth was prepared by hot isostatic pressing (HIPing) of mechanically milled pre-alloyed 5083 powders. In order to study stress-induced grain growth, the UFG 5083 Al was extruded at 400 °C with area reduction ratio of 10. The extrusion process was estimated to last ~36 s, with an associated deformation time of ~2.9 s and a strain rate of ~0.8 s^{-1}. It is noted that heat can be generated during the plastic deformation process, including extrusion, which is closely related to the strain rate [39]. Inspection of the published studies shows that the temperature rise due to the adiabatic heating effect was reported to be 2–27 °C for strain rates from 1.7×10^{-4} to 1.7×10^{-1} s^{-1} in an Al–Mg alloy [40] and 13–24 °C for strain rates from 5×10^{-3} to 5×10^{-1} s^{-1} in a 6010 Al alloy [41]. Based on 0.8 s^{-1} of the strain rate during extrusion in the present study, the temperature rise is estimated to be less than 30 °C, which is expected to have a very limited effect on grain growth relative to that at 400 °C.

The microstructure of the as-HIPed 5083 Al is characterized by ultra-fine equiaxed grains with average grain size $\overline{d} = 244$ nm (a grain size (d) is denoted by the area-equivalent circle diameter of a grain in a TEM view field). During extrusion, the average grain size increased to $\overline{d} = 647$ nm (equiaxed grains), indicative of significant grain growth during extrusion. Microstructural analysis revealed that GB migration and grain rotation (followed by coalescence) as two operative mechanisms for stress-induced grain growth were activated during extrusion. In the extruded 5083 Al, measurement of the solute concentrations at GIs and GBs via atom probe tomography showed that all of alloying elements are segregated at GBs. The measured concentrations of solutes at GBs are presented as follows (at.%): Mg 5.3283 ± 0.0347, Mn 0.1150 ± 0.0077, Cr 0.0293 ± 0.0034, Fe 0.1054 ± 0.0062, Ni 0.0266 ± 0.0032, Si 0.0702 ± 0.0051, Cu 0.0440 ± 0.0040, C 0.0334 ± 0.0036, O 0.1110 ± 0.0088 and N 0.0226 ± 0.0030. The GB energy per unit area at 400 °C was lowered from $\gamma_0 = 0.229$ J m^{-2} for pure Al to $\gamma = 0.144$ J m^{-2} for the 5083 Al by the solute segregation at GBs. The second-phase particles in the as-HIPed and extruded 5083 Al primarily include four types: $Al_{12}Mg_2(CrMnFe)$, $Al_{12}(FeMn)_3Si$, $Al_6(CrMnFe)$ and MgO. During extrusion, the volume fraction, size and distribution of the second-phase particles remain almost unchanged. The volume fraction (f) and the average size ($\overline{l}$) of the second-phase particles were assessed to be $f = 3.68\%$ and $\overline{l} = 30$ nm, respectively. The dislocation densities in the as-HIPed and extruded 5083 Al were estimated to be $\sim 2.4 \times 10^{14}$ and $\sim 7.7 \times 10^{13}$ m^{-2}, respectively.

3. Theoretical model

It has been well established that the velocities of GB migration (v_n) and/or of grain rotation (v_t) provide indications as to whether GB migration and/or grain rotation occur, leading to grain growth or not [1,20]. Based on this viewpoint, a theoretical model used to investigate grain growth must quantify v_n and v_t. In the experimental study reported in Ref. [35], the mechanisms underlying the stress-induced grain growth include both GB migration and grain rotation; moreover, the two mechanisms are coupled to each other as discussed in Section 1. Hence, in order to properly rationalize the stress-induced grain growth phenomena reported in Ref. [35], a theoretical framework that involves the coupling effect of GB migration and grain rotation is required. Cahn and Taylor originally formulated a unified theoretical model (referred to as "the Cahn–Taylor model" in the discussion that follows) that can be implemented to investigate coupled grain translation along the GB (grain rotation in the case of curved GB) and GB migration [32]. More recently, the model was reviewed and detailed by Trautt and Mishin; furthermore, the formulas in the Cahn–Taylor model have been validated by their MD simulations [20].

In the Cahn–Taylor model, a cylindrical grain investigated is assumed to be embedded in an outer grain, and the shear stress along the GBs is the sole externally applied stress, as shown in Fig. 1a [20,32]. In the present study,

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