Kinetics of grain boundary migration in nanocrystalline Al

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In the classical model of grain growth, it is tactically assumed that grain boundary migration velocity is linearly dependent on curvature. This relationship has been found to be consistent with both experimental and simulation results for bicrystals. However, recent experimental observations and theoretical works seem to imply that the relationship is much more complex in polycrystalline materials.

In this work, we determined the velocity and curvature of approximately 12000 grain boundaries from molecular dynamics simulations of the annealing of randomly textured nanosized polycrystalline Al. The grain boundary kinetics was studied at different scales and compared with theoretical predictions. At the grain level, that is, attributes averaged over all grain boundaries of a grain, the kinetics behavior showed a linear correlation of curvature and velocity. When studying grain-boundary-level behavior (i.e., attributes of individual grain boundaries are considered), we found a clear correlation between the sign of the grain boundary curvature and the direction of migration. Nevertheless, considering all the grain boundaries, the correlation coefficient between the magnitude of velocity and curvature was found to be low although a strong linear correlation was observed for a subset of high angle, long-lived, initially large grain boundaries with uniform curvature distribution and similar 5 crystallographic degrees of freedom. Furthermore, some grain boundaries that are close in crystallographic space showed different kinetics. This elucidates the complexity of grain boundary migration in the nanocrystalline ensemble as a result of complex dependence of grain boundary mobility and energy on grain boundary character, and the existence of other driving forces that affect the behavior of grain boundary migration. Among others, defect distributions and variation in stress distribution between neighboring grains are found to play a role in the grain boundary migration process.