The Mechanism of Grain Growth in $SrTiO_3$

Hadas Sternlicht[1,2], Wolfgang Rheinheimer[3], Alex Mehlmann[2], Avner Rothchild[2], Michael J. Hoffmann[3], Wayne D. Kaplan[2]

[1]School of Engineering, Brown University, Providence, Rhode Island, USA.

[2]Department of Materials Science and Engineering, Technion – Israel Institute of Technology, Haifa, Israel.

[3]Karlsruhe Institute of Technology, Institute of Applied Materials, Karlsruhe, Germany.

Grain boundary motion is a well-known phenomenon and one of the fundamental processes which define microstructural evolution, and thus many of the properties of polycrystalline materials. Although methodologies to study grain boundary migration kinetics have been established, and grain boundary mobility (velocity normalized by the driving force) can be experimentally measured, the atomistic mechanism by which a grain boundary moves is unknown. Understanding the mechanism of grain boundary motion is important for both fundamental and applied issues related to microstructural evolution of materials, such as the role of grain boundary atomistic structure on growth, and controlling the grain size of polycrystalline material systems in order to optimize their engineering properties.

Following the terrace ledge kink (TLK) model, grain boundaries were described as stepped planes which move by step-motion along the boundary plane during grain growth. The concept of steps at grain boundaries includes line defects; such that steps can have both a step and a dislocation character (so called disconnections). In the past, high symmetry grain boundaries (in bicrystals) were (almost) exclusively studied, since their atomistic structure can be determined. However, these make up a small portion of available boundaries and don't necessarily exist in nature or represent the general case.

The present work focuses on the atomistic mechanism by which *general* grain boundaries migrate. To do this, aberration corrected electron microscopy was employed to characterize disconnections at grain boundaries in a model system ($SrTiO_3$). The main goal of the research was to correlate between experimentally determined grain boundary mobility and an atomistic mechanism, while identifying specific grain boundary disconnections. General grain boundaries in $SrTiO_3$ were studied *ex-situ*, and compared to thin films of $SrTiO_3$ which were studied *in-situ*. The step and dislocation components of the identified disconnections were found to be anisotropic and of the same nature at boundaries annealed at a variety of conditions. The existence of steps in both *in-situ* and *ex-situ* experiments indicates that they are active during grain boundary motion. As such, step motion is very likely associated with the mechanism of grain growth in general grain boundaries.