Disconnections and the Mechanism of Grain Growth

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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 can be experimentally measured, the atomistic mechanism by which a grain boundary moves was unknown. Understanding the mechanism of grain boundary motion is important for both fundamental and applied issues related to microstructural evolution of materials, such as 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 named disconnections, which can have both a step and a dislocation character. In the past, high symmetry grain boundaries 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 $SrTiO_3$ acting as a model system. 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 disconnections in both *in-situ* and *ex-situ* experiments indicates that they play an active role during grain boundary motion. As such, anisotropic disconnection motion is the mechanism by which general grain boundaries migrate in $SrTiO_3$.

In agreement with the results acquired in $SrTiO_3$, anisotropic disconnections were also detected *ex-situ* in β-$Yb_2Si_2O_7$ acting as a promising ceramic for environmental barrier coatings (EBCs) for ceramic-matrix composite (CMC) components in the hot-section of gas-turbine engines. In addition to the various requirements an EBC must satisfy, EBCs must be resistant to high-temperature attack by calcia-magnesia-aluminosilicates (CMASs) ingested by the engine in the form of sand, dust, ash, *etc.* For this reason, the disconnections were studied before and after the interaction with CMAS glass.