Atomic Structural Features of Grain Boundary Complexions in Alumina

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Grain boundaries in polycrystalline microstructures are often decorated with dopants that are added intentionally, or impurities that are acquired during processing and service. The nature of the foreign substances profoundly influences various materials properties including diffusional transport, interfacial fracture, oxidation, corrosion and creep resistance. In many metallic and ceramic systems interfaces with various types of segregation, from sub-monolayer to thick microscopic films, have been observed. Recently, these interface phases have been considered as thermodynamically distinct three dimensional phases, called *Grain Boundary Complexions*.[1-2] In the current work, alumina has been chosen as a model system to study the various boundary complexion types and its relationship with boundary mobility.

Grain growth kinetics measurements in hot pressed dense yttrium-doped and yttrium-silicon co-doped polycrystalline alumina showed boundary mobility varying over 6 orders of magnitude between 1200 °C and 2000 °C. Additionally, six different regimes of boundary mobility were observed. Microstructures corresponding to these distinct boundary mobility regimes were identified and quenched from the annealing temperatures to preserve the grain boundary structure. Thin specimens of the specimens were examined with high resolution transmission electron microscopy, which showed interface types of progressively increasing disorder. Representative specimens each of these distinct grain boundaries were selected for studying the atomic structural environment of the dopants by synchrotron x-ray absorption fine structure spectroscopy (XAFS) at Y K-edge.[3] As the dopant (yttrium) preferentially segregates to the grain boundary, the local structure of yttrium gave the same of the grain boundary phases. The various grain boundary types identified were (i) boundaries with sub-monolayer adsorption of dopants, (ii) clean boundaries with no adsorption, (iii) boundaries with bilayered segregation of dopants, (iv) boundaries with a quasi-amorphous interface phase, (v) boundaries with thin amorphous intergranular films, and finally (vi) boundaries with thick wetting glassy films. The presentation aims to focus on the relationship between the boundary mobility and the structural features of the interface complexions from complementary studies of electron microscopy and synchrotron XAFS.

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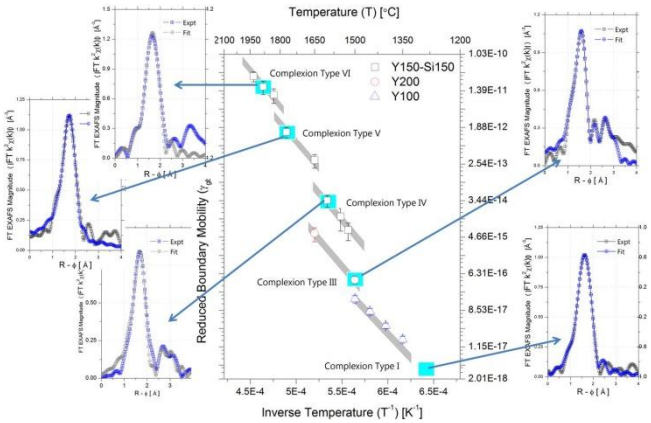

Figure 1: Boundary mobility and Y K-edge EXAFS features of Y-doped and Y-Si co-doped alumina. The middle panel shows the reduced boundary mobility over a wide temperature regime and distinct regimes of mobility. The XAFS features of the interface types (complexions I, III, IV, V, & VI), corresponding to the blue squares, are indicated.