THESIS **DEFENSE**

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Interpreting Macroscale Conductivity Behavior of Ceria-based Oxides via Nanoscale Quantification of Grain Boundaries

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Location:
Hill Hall 300

Abstract: Non-stoichiometric oxides, which exhibit advantageous electronic and ionic conductivity, are used in a number of technologically relevant areas including gas separators, solid oxide fuel cells and electrolysis cells. Grain boundaries dramatically limit the charge transport and therefore the overall efficiency of these devices. The limited conductivity is typically attributed to composition and chemistry changes within a few nanometers from the interface, due to the different defect formation energies at grain boundaries compared to the bulk. In the following, macroscopic electrical properties of two non-stoichiometric ceria-based oxide systems are related to individual grain boundary compositional and chemical variations, primarily through correlative atom probe tomography (APT) and transmission electron microscopy (TEM).

First, a robust technique using the scanning transmission electron microscope (STEM) is developed to automatically analyze grain orientation, an important factor in grain boundary segregation. Second, segregation of oxygen vacancies and cation species were quantified at multiple high angle grain boundaries and at phase boundaries in a dense dual-phase ceramic membrane consisting of $BaCe_{0.8}Y_{0.2}O_{3-\delta}$ - $Ce_{0.8}Y_{0.2}O_{2-\delta}$. No trend between misorientation and segregation could be determined. Finally, direct measurements of individual grain boundary composition, electronic structure, and electrostatic potential were systematically investigated and compared between two doping levels in ceria solid solutions: $Ce_{0.09}Y_{0.01}O_{2-\delta}$ and $Ce_{0.9}Y_{0.1}O_{2-\delta}$. It was found that the potential was positive for the 1% doped sample, while a negative potential was measured and corroborated by three techniques in the 10% doped sample. While most of the measurements of ceria solid solutions in literature assume a positive grain boundary potential, these results suggest that this is not necessarily always the case.

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