Size Dependence of Electrical and Thermal Transport Properties in Oxides

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ABSTRACT

The awareness of environmental factors, limited energy resources, and increasing energy demands have driven the search for both improved utilization of our fossil energy and new alternative energy resources. These new energy technologies are preferably cleaner, cheaper, smaller and more efficient than those currently being employed, for instance fuel cells, lithium-ion batteries, thermoelectrics. Nanocrystalline oxide conductors may exhibit significantly altered physical properties, which offer opportunities for technological innovations. This is particularly true in the oxide semiconductors, which have unusual optical, electrical, and magnetic properties. In addition, the size plays a critical role in the electrical, diffusive and defect properties of electroceramics. In this presentation, we consider the size dependence of the defect formation, electrical conductivity, thermopower, and magnetization in several technologically important oxides for energy conversion and storage system.

In nanocrystalline undoped CeO_2, decreasing the grain size results in an increase in the electrical conductivity, which was attributed to an increase in both carrier density and mobility because of larger surface/volume fraction in finer grain specimens. On the other hand, there exist discrepancies in the role of size on the transport properties of doped CeO_2 and ZrO_2, which are key ionic-conductor components in solid oxide fuel cells. In bulk nanocrystalline doped CeO_2 and YSZ, both size and chemical impurities play a role in oxide-ion transport in grain and grain boundary regions. In thermoelectric devices, unlike most conventional intermetallic thermoelectric materials, oxide thermoelectrics possess a low content of toxic elements, resistance to oxidation, and potential cost effectiveness, in addition to their chemical stability. Hence, oxide thermoelectric materials enable the use of waste heat from steam generating plants, fuel cells, or vehicles to generate "clean" electrical power. Our work on doped In_2O_3 demonstrated that high electrical conductivity and thermopower can be achieved simultaneously in bulk materials. Thermoelectric devices with $Ca_3Co_4O_9$ as the p type legs and doped In_2O_3 as the n type legs have been assembled as a prototype lab device, which possessed a performance five time better than reported recent results (Funahashi, et al., J. Appl. Phys. **99** (6), 066117 (2006)). In nanocrystalline films, enhanced thermopower can be achieved, while maintaining sufficient electrical conductivity.

To further illustrate the size effect, I will discuss the size dependence of physical properties in a few additional nanocrystalline oxides, including ZnO, MnO_2, and Fe_3O_4.