ABSTRACT

Oxides Surfaces and Novel Electronic Properties

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The scope of this thesis extends to the study of surface structures and electronic properties in a number of complex oxides. The c(6×2) surface reconstruction on $SrTiO_3$ (001) was solved using a combination of plan view transmission electron microscopy imaging, atomic resolution secondary electron imaging, and density functional theory calculations. This work provided fundamental insights on the effects of dielectric screening in secondary electron generation. A thorough analysis on the limitation and functionality of transmission plan view imaging showed that the kinematical approximations used in the separation of top and bottom surfaces is only valid in thin samples ($\sim$ 5 nm or less for $SrTiO_3$). The presence of an inversion center in the surface structure also made separation of the top and bottom surfaces more robust.

Surface studies of two other oxides, $KTaO_3$ and $NdGaO_3$, provided understanding on the mechanism of surface heterogeneity and segregation. In the case of $KTaO_3$, selective ion sputtering and the loss of K resulted in large stoichiometric variations at the surface. Annealing of such samples led to the formation of a potassium deficient tetragonal phase ($K_6Ta_{10.8}O_{30}$) on the surface. A similar phenomenon was also observed in $NdGaO_3$.

Exploratory surface studies of the rare earth scandates ($ReScO_3$, Re = Gd, Tb, Dy) led to the observation of large flexoelectric bending inside an electron microscope. Thin rods of these scandates bent by up to 90° under a focused electron beam; the bending was fully reversible. Ex-situ measurements of flexoelectric coefficient performed by another graduate student, Christopher Mizzi, confirmed that the scandates have a large flexocoupling voltage (∼42 V).

Electronic structure of the lanthanide scandates was studied using temperature dependent X-ray photoelectron spectroscopy and hybrid density functional theory calculations. The amount of charging under X-ray illumination was greatly reduced with increasing temperature owing to the presence of oxygen vacancies and surface band gap reduction. These results also indicated that the 4f-electrons are active components of the valence band electronic structure. We believe that the lanthanide scandates are a rich playground of material properties and have potential for applications in electronic and nano-mechanical devices.

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