MAR12-2011-000217

Abstract for an Invited Paper
for the MAR12 Meeting of
the American Physical Society

Interdiffusion, Unintentional Doping and Electronic Reconstruction at Polar/nonpolar Oxide Interfaces[1]

SCOTT CHAMBERS, Pacific Northwest National Laboratory

The observation of conductivity at the interface of insulating polar and non-polar perovskites (general form ABO_3) has sparked considerable interest worldwide, with much of the work to date being focused on the $LaAlO_3/SrTiO_3(001)$ heterojunction. Many attribute the interface conductivity to an electronic reconstruction alleviating the polar discontinuity via a film-to-interface charge transfer. However, the possibility of dopant- and/or defect-mediated conductivity cannot be ruled out, especially when the interfaces are not atomically abrupt. Electronic reconstruction requires an electric field within the film to facilitate the charge transfer process. However, x-ray photoemission spectroscopy studies reveal little or no electric field in the LAO film either above or below the critical thickness for conductivity, calling into question the validity of the electronic reconstruction model. In order to gain deeper insight into the electronic properties, it is worthwhile to manipulate the interface by changing the B-site cation in the polar perovskite. There are no low-lying d–derived bands in $LaAlO_3$ Therefore, if conductivity occurs, it ought to be driven by either the wholesale transfer of charge from the $LaAlO_3$ O2p-derived band into the STO (i.e. electronic reconstruction), or unintentional doping and/or defect creation. By replacing Al with a transition metal cation, we inject a new degree of freedom into the band structure – partially occupied $d$orbitals – and, thus, enable other mechanisms of charge redistribution. We have explored this concept by placing Cr(III) at the B-site and describe the electronic properties of epitaxial $LaCrO_3$/STO(001) heterojunctions. To minimize defect creation, the films were deposited using molecular beam epitaxy (MBE), in which the incoming atom energies are very low (<0.1 eV). Core-level and valence-band x-ray photoemission spectra measured for MBE-grown $LaCrO_3/SrTiO_3(001)$ yield band offsets and potential gradients within the $LaCrO_3$ sufficient to trigger an electronic reconstruction to alleviate the polarity mismatch. Yet, the interface is insulating. Based on first principles calculations, we attribute this unexpected result to interfacial cation mixing combined with charge redistribution within CrO_2 layers, enabled by low-lying d states within $LaCrO_3$, which suppresses an electronic reconstruction.

---

[1] This work was supported by the U.S. Department of Energy, Office of Science, Division of Materials Sciences and Engineering under Award #10122 (film growth) and Division of Chemical Sciences under Award #48526 (photoemission measurements and modeling).