Surface Investigations of Pure and Sn-Doped In_2O_3 (111) and (100)

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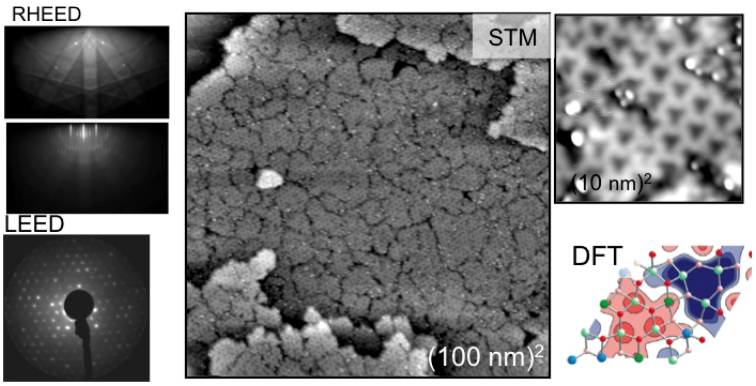
Tin-doped Indium Oxide (ITO) is a transparent conducting oxide that finds wide use in a variety of technical areas such as gas sensing, solar cells, and organic light-emitting diodes. While the surface properties of this material play a key role in these and many other applications, surprisingly little information exists about its fundamental surface characteristics.

We will present results from our multi-technique (LEED, XPS, UPS, RHEED, and STM) surface studies of epitaxial ITO films, grown on Yttria-stabilized Zirconia, and discuss geometric models that are derived from atomically-resolved STM images and DFT calculations [1, 2]. Surface polarity appears to play a major role in the stability and surface structure of ITO films.



The (111) surface of the bixbyite structure is non-polar and ITO(111) surfaces are essentially bulk-terminated with a 1x1 periodicity, see the figure at the left. The apparent topology in STM images is dominated by the physical corrugation. The (100) surface is polar, and atomically-resolved STM images show a rich structure that can be reconciled with a dimerization of surface O atoms that is predicted by theoretical calculations, as well as adsorbates at specific lattice sites.

First results on (undoped) In_2O_3 single crystals will also be discussed. The as-grown samples have the form of small cubes with (100)-oriented facets. They are pale yellow at room temperature and show a reversible darkening upon heating in UHV to a temperature below 500°C. While the LEED pattern is sharp and compatible with the one from epitaxial thin films, STM shows a significant disorder in the atomic-scale surface structure. Measurements of step height distributions show that, for sputtered/annealed surfaces, terminations with mixed types of In atoms are preferred, while this preference disappears when the surface is exposed to an oxygen plasma.

[1] E. Morales, et al., New J. Phys., 10 (2008) 125030;
[2] E. Morales and U. Diebold, Appl. Phys. Lett., 95 (2009) 253105