Soft X-ray Emission Study of Tin-Doped Indium Oxide (ITO) and It's Components

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Beamline(s): **X1B**

Introduction: Tin-doped indium oxide (In_2O_3:Sn otherwise known as ITO) is an increasingly important material for the electronics industry. The reasons for it's importance are closely linked to the fact that it is one of a group of transparent conducting oxides. Aside from it's technological uses as a thin film in many devices such as flat panel displays, a comparison of spectra obtained from ITO and spectra from pure tin oxide and indium oxide is of interest in terms of the information obtained concerning the band structure of this applied material. Furthermore the electronic structure of the binary transition metal oxides can be probed by soft x-ray emission spectroscopy and suitably doped ITO may prove interesting to study the variation of hybridization.

Methods and Materials: Soft X-ray emission (SXE) spectroscopy is a sensitive tool which allows the user to probe a material on an element-specific basis and obtain local partial densities of states (LPDOS) of the valence band of the material under study. The high-intensity soft x-ray undulator beamline X1B is ideally suited for use with this photon in-photon out spectroscopy. The outgoing photon is detected using a specially designed soft x-ray emission spectrometer equipped with a microchannel plate array where readout is by a resistive anode encoder..

ITO is normally used in technological applications with a ratio of 90% In_2O_3 to 10% SnO_2. In this study a similar stoichiometric sintered mixture of indium oxide and tin oxide is used as a sample, typical of the precursor from which thin films are grown by e-beam evaporation. In_2O_3 is a semiconductor with a band gap 3.75eV and forms in the bixbyite crystal structure. Few band structure calculations exist for indium oxide or for tin-doped indium oxide (ITO) except as pertains to the optical and electrical characteristics resultant from the doping.

Results: The preliminary data presented here shows both the soft x-ray absorption (SXA) spectra and various soft x-ray emission (SXE) spectra acquired at the positions indicated on the soft x-ray spectrum from the ITO precursor sample. Highlighted in the inset graph in **Figure 1** is a peak in the SXE spectrum at a binding energy of approximately 16eV which agrees well with the binding energy calculated by Mi et al.

Conclusions: The observed soft x-ray emission spectra of indium oxide, tin oxide and ITO (tin doped indium oxide) have highlighted the progression of the hybridization of the metal 4d orbital with the ligand (oxygen) 2p orbital in binary transition oxides such as these and CdO. This further demonstrates that soft x-ray emission is a sensitive and direct measurement of such hybridization effects.

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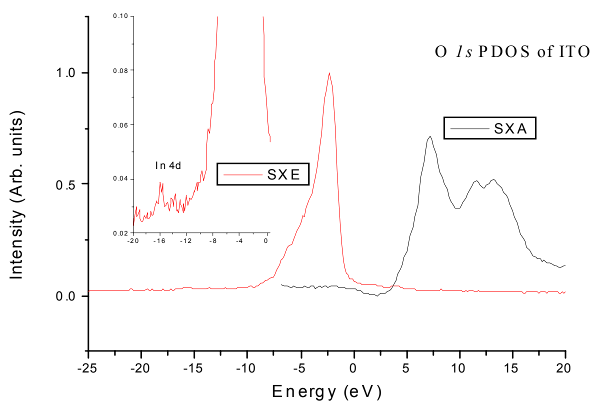

Figure 1. Pictured here is the O *K* soft X-ray emission (SXE) spectrum of ITO combined with the O *K* soft x-ray absorption (SXA) spectrum. The zero is set to be the valence band maximum (VBM). The graph inset shows a highlighted portion of the SXE spectrum showing a peak at 16eV binding energy corresponding to a hybridization peak of the O *2p* with the In *4d*.