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PII: S0040-6090(16)00100-0
DOI: doi: 10.1016/j.tsf.2016.02.010
Reference: TSF 35010

To appear in: *Thin Solid Films*

Received date: 2 April 2015
Revised date: 2 February 2016
Accepted date: 3 February 2016

Please cite this article as: D. Schmeißer, J. Haeberle, Intrinsic localized gap states in IGZO and its parent single crystalline TCOs, *Thin Solid Films* (2016), doi: 10.1016/j.tsf.2016.02.010

# Intrinsic localized gap states in IGZO and its parent single crystalline TCOs

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**Abstract**

We report on the X-ray absorption data for Indium-Gallium-Zink-Oxide thin films, amorphous ZnO films, amorphous $SnO_x$ films, and single crystalline $In_2O_3$, $Ga_2O_3$, ZnO, and $SnO_2$ data. These absorption data probe the empty conduction band states explicitly. Also they allow for an elemental assignment using resonant excitation to derive the contributions of each metal ion. We find that the lowest states appear right at the Fermi energy and result from configuration interaction induced charge transfer states which we consider as intrinsic gap states.

## Introduction

The transparent conductive oxide (TCO) family [1] of materials contains the Ga and In substituted ZnO compounds; often called Indium-Gallium-Zinc-Oxides (IGZO). Thin films of IGZO can be prepared and are used in thin-film transistor technologies. Their transport properties are outstanding as carrier mobilities up to 46 $cm^2/Vs$ [2] can be achieved. According to the Hosono model [1] these can be attributed to the overlap of the spatially large 5s wave function of In which enable band like states in the conduction band (CB) even in amorphous thin films. Certainly, this model does not explain the observed small effective masses of around 0.3 referred to the free electron mass ($m_e$). However, it seems to be in line with calculations based on density functional theory (DFT) in such that the lowest unoccupied states in the CB indeed are from the s-orbitals while the O2p derived states mainly contribute to the occupied valence band (VB) states (see literature for ZnO in [3], for $In_2O_3$ in [4], and for $Ga_2O_3$ in [5] .

Here we report on X-ray absorption spectroscopy (XAS) data which probe the empty conduction band (CB) states explicitly. Using resonant excitation we derive the contributions of each metal ion. We compare the data for IGZO thin films, amorphous ZnO films, amorphous $SnO_x$ films, and single crystalline $In_2O_3$, $Ga_2O_3$, ZnO, and $SnO_2$ data. We find that all XAS data are very similar and discuss that the lowest CB states are formed by configuration interaction (CI) induced gap states (CIGS).