O 30: Focussed session: Transparent conductive oxides II (jointly with HL, DS)

Time: Tuesday 11:15–13:15 Location: WIL B122

Topical Talk O 30.1 Tue 11:15 WIL B122
Experimental Electronic Structure of In_2O_3 and Ga_2O_3 — •Christoph Janowitz — Brandenburgische Technische Universität Cottbus — Humboldt Universität zu Berlin, Institut für Physik

Transparent conducting oxides (TCO's) pose a number of serious challenges. Besides the strive for high quality single crystals and thin films their application has to be preceded by a thorough understanding of their peculiar electronic structure. It is of fundamental interest to understand why materials transparent up to the UV spectral regime behave also as conductors. In this talk two binary oxides -In_2O_3 and Ga_2O_3 from the group of TCO's showing the smallest respectively largest optical gap- will be explored experimentally. The investigations on the electronic structure were performed on high quality n-type single crystals showing carrier densities of 10^{19} cm^{-3} (In_2O_3) and 10^{17} cm^{-3} (Ga_2O_3). Subjects addressed are the determination of the band structure along the high symmetry directions, effective masses and fundamental gap by angular resolved photoemission (ARPES). Also by resonant ARPES and a combination of X-ray photoemission and X-ray absorption complementary information on the orbital character of the valence- and conduction band regime and on the band gap are obtained. The observations are discussed by reference to calculations of the electronic structure and models for the conductivity mechanism.

Topical Talk O 30.2 Tue 11:45 WIL B122
Transparent Electronics Using Oxide Materials — •Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II

We discuss all-oxide transparent electronic devices, such as diodes, photodiodes, transistors and inverters, based on rectifying, transparent Schottky contacts from metal oxides, transparent semiconducting oxides and transparent substrates. In particular, MESFET devices are presented with crystalline and amorphous oxides as channel, exhibiting low operation voltage and voltage swing. Inverters built from such transistors exhibit high gain (>200). Directions of further research will be discussed.

Topical Talk O 30.3 Tue 12:15 WIL B122
Optical properties of undoped and doped ZnO — •Axel Hoffmann and Markus R. Wagner — Institut für Festkörperphysik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

A spectroscopic study of optical transitions and lattice dynamics of ZnO under the influence of external fields is reviewed. A comparative study of different ZnO single crystals and doped and undoped ZnO films reveals pronounced differences in the free and bound exciton luminescence which can be related to different impurity centers and strain levels. A correlation between the localization energies of excitons bound to the same chemical element in the neutral and ionized charge state is reported. The properties of the shallow impurity bound excitons are compared to defect related deeply bound excitons. The lattice dynamics of ZnO crystals are studied by Raman spectroscopy under the influence of external pressure. A variety of important material parameters is derived including high precision values of the hydrostatic pressure coefficients and Grüneisen parameters of all Raman active modes. For the Born transverse effective charge, an incorrect pressure dependence in the literature is discovered and revised. Raman measurements of ZnO single crystals under uniaxial pressure are reported. In combination with the hydrostatic pressure measurements on the same samples, the first experimental determination of the phonon deformation potentials of all Raman active modes in ZnO is achieved.

O 30.4 Tue 12:45 WIL B122
Thermodynamic stability, stoichiometry and electronic structure of bcc-In_2O_3 surfaces — •Peter Agoston and Karsten Albe — TU Darmstadt, Petersenstr. 32, 64287 Darmstadt

The thermodynamic stability of all experimentally observed low index surfaces of bcc-indium oxide (In_2O_3) have been investigated by means of density functional theory calculations. The effect of a changing environment has been studies as well as the influence of hydrogen and water. It is found that the (001) surfaces have the most complex behavior. For this surface additionally the effects due to dopants (Sn) as well as the in-plane lattice strain has been studied. Finally, scanning tunneling microscopy images are presented and discussed in the light of previous experiments.

O 30.5 Tue 13:00 WIL B122
Growth and characterization of In_2O_3 single crystals — •Valentina Scherer, Peter Hlawenka, Christoph Janowitz, Alica Krapf, Helmut Dwelk, and Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin

The scientific interest in transparent conducting oxides (TCOs) such as ZnO, Ga_2O_3, In_2O_3 and SnO_2 increases significantly. However, information on the electronic structure and the doping behaviour is very scarce. This is in part due to the challenging problem of growing high purity single crystals and substrates for homoepitaxy, which also limits the attainable progress in device production. High quality In_2O_3 single crystals were grown using the chemical vapor transport method (CVT). The crystals were of body centered cubic bixbyite-type structure with a lattice parameter $a = 10.12$. The temperature-dependent resistivity, Hall-constant, and mobility were measured and an electron density in the range of $\sim 10^{19} cm^{-3}$ was determined. The crystals were then investigated using high resolution photoemission and transport measurements. Emission from the valence band and the partially filled conduction band at the Γ-point yielded a direct band gap of ~ 3 eV. The weak conduction band emission near the Fermi edge enabled a Fermi-map and the determination of the Fermi surface. The obtained results are in good agreement with theoretical band structure calculations and with the previously experimental results of the thin films.