DS 48: Oxide Semiconductors for Device and Energy Applications II (Joint session of DS and HL, organized by DS)

Time: Thursday 15:00–16:45 Location: H11

DS 48.1 Thu 15:00 H11

How Seebeck coefficient measurements help determine oxide transport properties — •Alexandra Papadogianni[1], Oliver Bierwagen[1], Mark E. White[2], James S. Speck[2], Zbigniew Galazka[3], Kelvin H. L. Zhang[4], Yingge Du[4], and Scott A. Chambers[4] — [1]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, D-10117 Berlin, Germany — [2]Materials Department, University of California, Santa Barbara, California 93106, USA — [3]Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, D-12489 Berlin, Germany — [4]Pacific Northwest National Laboratory, Richland, Washington 99352, USA

Measuring the Hall effect is a common and convenient method to investigate the electrical transport properties of thin samples, providing us with an estimate of integral sheet carrier concentration. In low-mobility p-type semiconducting oxides, such as the Sr-doped $LaCrO_3$, however, Hall measurements fail. For such instances, studying thermoelectric properties, namely the Seebeck coefficient, can be a simple alternative, which provides us with the carrier type and volume carrier concentration. A combination of Seebeck and Hall measurements can moreover be used for estimating the actual thickness of a carrier system within a semiconductor. As an example, an application on n-type SnO_2 shows how this method can help distinguish bulk carriers, with homogeneous depth distribution, from sheet carriers accumulated within a thin layer.

DS 48.2 Thu 15:15 H11

Metal incorporation and reaction-kinetics for the molecular beam epitaxial growth of $(Ga_xIn_{1-x})_2O_3$ — •Patrick Vogt and Oliver Bierwagen — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5–7, 10117 Berlin, Germany

This contribution presents the metal incorporation and reaction-kinetics study of the plasma-assisted molecular beam epitaxial (MBE) growth of the transparent semiconducting oxide alloy $(Ga_xIn_{1-x})_2O_3$. By using MBE, an impinging Ga- (Φ_{Ga}), In- (Φ_{In}), and oxygen-flux (Φ_O) react amongst others to $(Ga_xIn_{1-x})_2O_3$ on a heated, single-crystalline substrate under ultra-high vacuum conditions. The data obtained were measured *in-situ* by a laser reflectometry (LR) set-up and a line-of-sight quadrupole mass spectrometer (QMS) or *ex-situ* by energy dispersive X-ray spectroscopy (EDX). The LR allowed measuring the growth-rate (ρ), the QMS enabled identifying the species that desorbed off the substrate which are not incorporated into the alloy, and the EDX measurements revealed the In incorporation x and the reciprocal Ga incorporation 1-x.

We present the growth rate dependencies of the binary grown In_2O_3 and Ga_2O_3 as function of growth temperature (T_G). Furthermore, we show the dependence of ρ and x for the ternary grown alloy on T_G, the metal-to-oxide ratio ($r_{MeO} = (\Phi_{In} + \Phi_{Ga})/\Phi_O$) , and the In-to-Ga ratio ($r_{InGa} = \Phi_{In}/\Phi_{Ga}$).

The measured discrepancy of ρ for the binary grown oxides compared to x for the ternary grown alloy can be explained by the different adhesion energies for In and Ga on the $(Ga_xIn_{1-x})_2O_3$ surfaces.

DS 48.3 Thu 15:30 H11

Application of Cr_2O_3 and Cr_2O_3:Mg as a Buffer Layer in Organic Solar Cells — •Daragh Mullarkey[1], Elisabetta Arca[1], Linda Cattin[2], Jean Christian Bernède[3], and Igor Shvets[1] — [1]School of Physics and CRANN, Trinity College Dublin, University of Dublin, Ireland — [2]Université de Nantes, Institut des Matériaux Jean Rouxel, France — [3]Université de Nantes, MOLTECH-Anjou, France

The use of undoped Cr_2O_3 and p-type Cr_2O_3:Mg as an anode buffer layer in organic solar cells is explored. The effects of buffer layer thickness, roughness, and growth conditions on the properties of the solar cell were studied. These effects were investigated for solar cells grown on both indium tin oxide and fluorine doped tin oxide. In both cases, Cr_2O_3 and Cr_2O_3:Mg were found to improve the efficiency of the solar cell.

The band offsets between the anode material and the buffer layer, as well as between the buffer layer and the organic absorber were studied by X-ray Photoelectron Spectroscopy (XPS) and Ultra Violet Photoelectron Spectroscopy (UPS). The efficiency of the solar cells is discussed in terms of the experimentally determined band alignment.

DS 48.4 Thu 15:45 H11

TiO2 laminated Silicon microstructures based stable photocathode for water splitting — •Chittaranjan Das[1], Massimo Tallarida[2], and Dieter Schmeisser[3] — [1]Angewantde Physik / Sensorik ,BTU Cottbus-Senftenberg, Germany — [2]ALBA-Barcelona — [3]Angewantde Physik / Sensorik ,BTU Cottbus-Senftenberg, Germany

The photoelectrochemical (PEC) water splitting is one of the most efficient ways to obtain hydrogen from water using solar power which can be used as carbon free fuel. The PEC device can bedesigned using semiconducting material that will convert solar radiation to H2. Silicon can be one of the best choices for PEC due to its success in solar cells technology. There are certain issues with Si such as stability in electrochemical medium [1] and higher surface reflectance (25%) which limits the Si as an ideal candidate for PEC technique [2].

In the present work we addressed these issues by surface structuring and laminating the surface with metal oxide. The microstructuring of Si was done by electrochemical method. The Si microstructure photocathode was stabilized by thin layer of ALD grown TiO2 film. The microstructuring and lamination of Si photocathode by ALD layer of TiO2 decreased the reflectance ofthe surface and shift the onset potential towards anodic direction by 350 mV with a prolonged stability over 60 hours[3].

[1] C. Levy-Clement, J. Electrochem. Soc 1991, 12, 69 [2] J. Oh, et al. Energy Environ. Sci., 2011, 4, 1690 [3] C. Das, et al. Nanoscale 2015,7, 7726

DS 48.5 Thu 16:00 H11

Optical and Magneto-Optical Investigation of Normal and Disordered $ZnFe_2O_4$ in Relation to Magnetic Properties — •Vitaly Zviagin[1], Peter Richter[2], Yogesh Kumar[1], Israel Lorite[1], Michael Lorenz[1], Dietrich R.T. Zahn[2], Georgeta Salvan[2], Pablo Esquinazi[1], Marius Grundmann[1], and Rüdiger Schmidt-Grund[1] — [1]Universtät Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, Germany — [2]Technische Universtät Chemnitz, Semiconductor Physics, Reichenheiner Str. 70, Germany

We present the magneto-optical dielectric tensor of normal and disordered $ZnFe_2O_4$ grown at different temperatures on MgO (100) and $SrTiO_3$ (100) substrates by pulsed laser deposition. Optical transitions in the diagonal element of the dielectric function, obtained by spectroscopic ellipsometry, are identified as transitions from O_{2p} to Fe^{3+} 3d and 4s bands. Via the off-diagonal element, obtained by magneto-optical Kerr effect spectroscopy, the observed features are confirmed to be similar to the mentioned transitions. One transition in particular, namely a transition from O_{2p} to tetrahedrally coordinated Fe^{3+} cation, located at $\sim$ 3.5 eV, suggests disorder of the normal crystal structure. Its amplitude is highest for the sample grown at the lowest temperature in both the diagonal and off-diagonal elements of the dielectric tensor. Furthermore, the overall magnetic response, measured by SQUID, is highest for the sample grown at the lowest temperature, suggesting that the presence of Fe^{3+} on the tetrahedral sites is directly related to the ferrimagnetic order of the crystal due to the dominating nature of the oxygen mediated coupling between the two lattice sites.

DS 48.6 Thu 16:15 H11

Monitoring Proton Diffusion in Thin Films of Tungsten Oxide — •Simon Burkhardt[1], Sabrina Darmawi[1], Matthias T. Elm[1,2], and Peter J. Klar[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen — [2]Physikalisch-Chemisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 17, 35392 Gießen

The reversible change of the optical properties of materials due to the electrochemical insertion of ions is called electrochromism. Tungsten-VI oxide (WO_3) and its electrochromic properties have been intensively studied since 1969 as a model system which nowadays can be found in applications like smart window systems or other coated glasses. However fundamental questions concerning the colouration mechanism are still under discussion. A combination of electrochemical proton insertion and *in situ* UV/Vis-transmission spectroscopy is applied to provide new insights. With the developed set up it is not only possible to investigate the time-dependence of the colouration behaviour, but it

also allows a spatially resolved analysis of the colouration process and thus the ion diffusion in electrochromic thin films. To investigate the diffusion of protons, thin films of WO_3 are deposited on TCO-coated substrates via electron beam evaporation and coated with a structured PMMA layer to enable local ion insertion. Significant differences in the colouration behaviour of amorphous and crystalline WO_3 films can be observed which will be compared with a simulation of lateral 1D diffusion processes.

DS 48.7 Thu 16:30 H11

Oxygen Vacancies in the Ultrathin SiO_2 Interfacial Layer of High-K/Metal Gate CMOS Devices — •Florian Lazarevic[1,2], Roman Leitsmann[1,2], Philipp Plänitz[1], and Michael Schreiber[2] — [1]MATcalc, AQcomputare GmbH, Annaberger Str. 240, 09125 Chemnitz, Germany — [2]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany

We study oxygen vacancy defect levels in ultrathin SiO_2 layers in metal-oxide-semiconductor devices. First principles calculations were performed to model a $Si/SiO_2/HfO_2$ gate stack and a SiO_2 bulk reference system. The extremely thin SiO_2 layer thickness and dissimilar structural and electronic properties of the adjacent layers (namely Si and HfO_2) result in a degeneration and stabilization of certain SiO_2 bulk defects. We find that partial H passivation of the vacancies additionally stabilizes defects energetically which are related to the leakage current in CMOS devices. Furthermore the incorporation of F atoms has a large influence on the stability of H passivated SiO_2 defects.