

HL 35: New Materials: Optoelectronic and Photovoltaic Applications

Time: Wednesday 9:30–10:45

Location: H13

HL 35.1 Wed 9:30 H13

Characterization of $\beta - Ga_2O_3$ single crystals — ●JAN STEHR¹, ALBRECHT HOFSTAETTER¹, DETLEV HOFMANN¹, BRUNO K. MEYER¹, and REINHARD UECKER² — ¹I. Physikalisches Institut, Justus-Liebig-Universität, Heirich-Buff-Ring 16, D- 35392 Giessen — ²Leibniz-Institut für Kristallzüchtung, Max-Born-Strasse 2, D- 12489 Berlin

Ga_2O_3 is a wide band gap semiconductor with potential applications as transparent conducting oxide (TCO). $\beta - Ga_2O_3$ is typically an n-type conducting material due to oxygen vacancies, which act as shallow donors. To control the electrical properties of the material it is thus necessary to study defects and impurities in the material.

A $\beta - Ga_2O_3$ crystal was investigated by optical measurements and magnetic resonance spectroscopy. The band gap energy determined by UV-VIS spectroscopy is 4.6 eV parallel to the b-axis and 4.3 eV parallel to the c-axis at room temperature; we followed its dependence down to liquid helium temperature. By electron paramagnetic resonance we observe 3 signals (Signal A, B and C). Signal A consist of 8 lines with equal intensity therefore $I = 7/2$ is attributed to Co. Signal B shows a single line and is anisotropic, the g-value moves in angular dependent measurements from $g=2.4$ to $g=1.5$. Signal C with $g=1.96$ is the well known resonance of the oxygen vacancies causing the shallow donors in Ga_2O_3 .

HL 35.2 Wed 9:45 H13

Alternative bufferlayers for CIGS solarcells. — ●A. BELEANU, T. GRUHN, C.G.F. BLUM, B. BALKE, and C. FELSER — Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, Mainz, Germany

Cadmium sulfide is a highly efficient buffer layer material in $Cu(In,Ga)(S,Se_2)$ [CIGS] solar devices [1], but for environmental reasons and possible gains in efficiency there is a great interest in replacing CdS by a cadmium-free alternative buffer layer. Using standard density functional theory (DFT) methods possible candidates like $LiZnP$ and $LiCuS$ have been proposed as alternative buffer layers. The experimental verification of the DFT results was quite challenging due to the fact that $LiCuS$ was an unknown and completely new material. In a first step, we tried to synthesised $LiCuS$ through solid state reactions in a corundum crucible. After optimizing the parameters and successfully synthesising the material its properties were investigated. In a second step, huge amounts of $LiCuS$ and $LiZnP$ were synthesised and pressed using Spark Plasma Sintering as 3 inch targets. $LiCuS$ and $LiZnP$ films were grown by radio-frequency magnetron sputtering from these target and their properties as an alternative buffer layer in CIGS solar cells were investigated. The 1:1:1 stoichiometry of the films was delivered from in-situ XPS measurements. Absorption measurements show a band gap of ≈ 2.0 eV which is in good agreement with the theoretical estimates. [1]T. J. Coutts, *Thin Solid Films*, 90 (1982) 451-460. *This work was financially supported by the BMU project comCIGS.*

HL 35.3 Wed 10:00 H13

Systematic ab initio study of half-Heusler materials for optoelectronic applications — THOMAS GRUHN and ●CLAUDIA FELSER — Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg University, 55099 Mainz

The development of new, optimized optoelectronic devices depends crucially on the availability of semiconductors with tailored electronic and structural properties. At the moment, the majority of applications is based on a rather small set of semiconducting materials, while many more semiconductors exist in the huge class of ternary compounds. Especially, the class of 8-electron half-Heusler materials comprises a large number semiconductors with various properties.

With the help of ab initio density functional theory we have studied essentially all 8-electron half-Heusler compounds that are of technological relevance. For more than 650 compounds we have determined the

optimum configuration by varying the lattice constant and permuting the elements over the sublattices. Within this exceptionally large data set we have studied the band structure and the lattice constants as a function of the electronegativities of the elements, the arrangement of the atoms, and the atomic radii. The results are used to select suitable materials for the buffer layer in thin-film solar cells with a $Cu(In,Ga)Se_2$ (CIGS) absorber layer. Considering the bandgap and the geometrical matching with the CIGS film, we have obtained a set of 29 compounds that are promising materials for cadmium-free CIGS buffer layer. The authors gratefully acknowledge financial support by the DfG (Research Unit 559).

HL 35.4 Wed 10:15 H13

Nanosecond switching in GeTe phase change memory cells — ●GUNNAR BRUNS¹, PHILIPP MERKELBACH¹, CARL SCHLOCKERMANN¹, MARTIN SALINGA¹, MATTHIAS WUTTIG¹, THOMAS HAPP², JAN BORIS PHILIPP³, and MICHAEL KUND³ — ¹I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — ²Qimonda Dresden GmbH & Co. OHG, Königsbrücker Strasse 180, 01099 Dresden, Germany — ³Qimonda AG, Bibbergerstr. 93, 82008 Unterhaching, Germany

While phase change materials have already successfully been applied in rewriteable optical data storage, they are also promising to form the basis for novel non-volatile electronic data storage devices. To understand the underlying mechanism of these so-called Phase Change Memories (PCM) it is mandatory to gain a deeper insight into the switching process between the high resistive amorphous (RESET state) and the low resistive crystalline phase (SET state).

The electrical switching behavior of GeTe-based phase change memory devices is characterized by time resolved experiments. SET pulses with a duration of less than 16 ns are shown to crystallize the material. Depending on the resistance of the RESET state, the minimum SET pulse duration can even be reduced down to 1 ns [1]. This finding is attributed to the increasing impact of crystal growth upon decreasing switchable volume. Using GeTe or materials with similar crystal growth velocities, hence promises nonvolatile phase change memories with DRAM(dynamic random access memory)-like switching speeds.

[1] G. Bruns et. al., *App. Phys. Lett.* 95, 043108 (2009).

HL 35.5 Wed 10:30 H13

Valence and core excitations in $Li_{(1-x)}FePO_4$ — ●MICHAEL KINYANJUI^{1,2}, PETER AXMANN², MARGRET WOHLFAHRT-MEHRENS², PHILIPPE MOREAU³, FLORENT BOUCHER³, and UTE KAISER¹ — ¹University of Ulm, Albert Einstein Allee 11, 89081 Ulm, Germany — ²Centre for Solar Energy and Hydrogen Research, Helmholtzstr. 8, 89081 Ulm, Germany — ³Institut des Matériaux Jean Rouxel, UMR6502, CNRS - Université de Nantes, 2 rue de la Houssinière, B.P.32229, 44322 Nantes cedex, France

$LiFePO_4$ is a potential cathode material for Li ion batteries applications. However, its electronic properties and the mechanism by which lithium ions are extracted or inserted into the lattice are still unclear. The electronic properties of $LiFePO_4$ and $FePO_4$ have been investigated using valence electron energy loss spectroscopy (VEELS), core-loss EELS and *ab initio* calculations. The VEELS spectra of $FePO_4$ show interband transitions between 0-20 which are not observed in $LiFePO_4$ VEELS spectra. Using the calculated imaginary part of the dielectric function, the interband transitions were assigned as rising from valence states with mainly O-2p character. The core-loss spectra in $FePO_4$ show a pre-edge peak that is observed above the threshold of the main O-K edge. This is not observed in $LiFePO_4$. The position of the pre-edge peak is determined by a charge transfer process which shifts the position of the Fe 3d bands with respect to the conduction band with the extraction of lithium ions from the $LiFePO_4$ lattice. Therefore $FePO_4$ can be considered to be a charge-transfer insulator while the $LiFePO_4$ is a typical Mott-Hubbard insulator.