HL 7: "New" Materials and New Physics in "Old" Materials I

Time: Monday 9:30–11:30 Location: EW 015

HL 7.1 Mon 9:30 EW 015

Electronic and optical properties of Copper Oxides from first principles — •Markus Heinemann, Bianca Eifert, and Christian Heiliger — I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Germany

The copper oxide phases Cupric oxide (CuO), Cuprous oxide (Cu_2O), and Paramelaconite (Cu_4O_3) are of rising interest in the field of optoelectronics and solar technology. We investigate the phase stability of these copper oxide phases in different temperature and pressure domains within the framework of density functional theory. An *ab initio* approach to the LDA+U method is employed to calculate the electronic structure of all phases from first principles. Further, we study the optical properties of these materials by calculating the dielectric function. The results are compared to experimental measurements of sputtered Cu_2O thin films.

HL 7.2 Mon 9:45 EW 015

Deposition of copper oxide by a modified Radio-Frequency Ion Thruster (RIT) as Ion-Beam-Sputter-Source — •Martin Becker, Philipp Hering, Angelika Polity, Davar Feili, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

Radio-Frequency-Ion-Thrusters, as designed for propulsion applications, are also qualified for thin film deposition and surface etching, because different gas mixtures, extraction voltages and rf power can be applied.

Copper oxide thin films were grown by ion beam sputter deposition using a 4 inch ceramic cuprous oxide target. Different aspects of the thin film growth and properties of the copper oxides were investigated in relation to growth parameters such as substrate temperature, supplied rf power and flux of oxygen.

Results of first investigations on thin films grown by this methodology will be compared to those obtained by "cold" rf-sputtered samples post-annealed in nitrogen atmosphere. Analysis of structural, optical and electrical properties will be shown.

HL 7.3 Mon 10:00 EW 015

Optical and electrical properties of different copper oxide phases deposited by magnetron sputtering — •Daniel Reppin, Angelika Polity, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

Copper oxides Cu_xO_y are attractive materials for solar cell applications; that is due to the fact that the bandgaps of the different oxides lie in the range from 1.6 eV (CuO) to 2.17 eV (Cu_2O). Beside these two "main" phases of copper-oxide there are at least two phases which are more or less discussed in the literature: the metastable Cu_4O_3 and Cu_3O_2 known from low temperature oxidation experiments.

We will show that it is possible to obtain the different copper oxides by magnetron sputtering under different oxygen flows without substrate heating. A correlation will be given for structural, optical and electrical properties with the phase changes between the copper oxides. The obtained properties of the films will be discussed in terms of phase purity and stoichiometry.

HL 7.4 Mon 10:15 EW 015

Network of SnO2 nanowires for gas sensing application — •Elise Brunet, Giorgio Cataldo Mutinati, Stephan Steinhauer, and Anton koeck — Health & Environment Department, Molecular Diagnostics, AIT Austrian Institute of Technology GmbH, 1220 Vienna, Austria

SnO2 is an n-type semiconductor particularly used in metal oxide gas sensors, whose principle relies on changes of electrical conductance due to interactions between the surrounding gas and the sensing layer. We present a gas sensor device, whose sensing layer is reduced to a bundle of SnO2 nanowires. The surface to volume ratio is increased, which enlarges the number of interactions between the gas molecules and the SnO2 surface and improves the sensitivity of the sensor device.

A SnO2 thin film is deposited by spray pyrolysis on SiO2/Si substrates coated with CuO. The SnO2 film is then cleaved in two pieces, which are glued together on a support plate with a distance of about 150 micrometers. A thermal treatment of this assembly at 900°C in Ar-atmosphere results in the growth of single crystalline SnO2 nanowires on each of the two SnO2-coated substrates. The nanowires grown on the edges are long enough to interconnect and bridge the gap between the two substrates. The sensing performance of this network of SnO2 nanowires is investigated in the presence of small concentrations of CO, CO2, H2 and H2S in the low ppm range and compared with those of a single nanowire sensor device.

HL 7.5 Mon 10:30 EW 015

Switchable nanothermochromic VO_2 diffraction gratings defined by site selective ion implantation — •Johannes Zimmer, Hubert Krenner, Helmut Karl, and Achim Wixforth — Institut für Physik, Universität Augsburg, Universitätsstr. 2, 86159 Augsburg

The metal-insulator transition (MIT) of vanadium dioxide has been studied in great detail over the past 50 years, showing both structural and electronic phase changes. The bulk materials electric conductivity rises drastically at T=68°C, when heated from the isolating phase at room temperature to the metallic phase. Additionally optical properties of VO_2 exhibit significant changes during the MIT on sub-picosecond timescales. We examined the near-infrared thermochromic behaviour of VO_2 nanocrystals, which were synthesised by high-dose ion implantation through optically structured masks. Fused silica was chosen as matrix material for the fabrication of the diffractive optical elements, leaving the VO_2 crystals inert to structural degradation when undergoing the MIT. Two different processes were used to define diffraction gratings containing VO_2 nanocrystals. The first was direct implantation of VO_2 through masks into the host material and the second was site-selective bombardement of already synthesised nanocrystals, with argon ions in order to suppress the metallic phase in those regimes. While undergoing the phase transition, the gratings showed switching in diffraction efficiencies by factors of 3 for the directly synthesised gratings and more than one order of magnitude for the Ar-deactivated gratings. All gratings show broad thermal hysteresis extending down to room temperature.

HL 7.6 Mon 10:45 EW 015

Low-temperature photocarrier dynamics in single-layer MoS_2 — •Tobias Korn, Gerd Plechinger, Stefanie Heydrich, Johannes Schmutzler, Michael Hirmer, and Christian Schüller — Institut für Experimentelle und Angewandte Physik, Universität Regensburg

The dichalcogenide MoS_2, which is an indirect-gap semiconductor in its bulk form, was recently shown to become an efficient emitter of photoluminescence as it is thinned to a single layer [1], indicating a transition to a direct-gap semiconductor due to confinement effects. Here, we present scanning Raman and time-resolved photoluminescence studies of few- and single-layer MoS_2 flakes [2]. Scanning Raman spectroscopy reveals the intensity and spectral position of the characteristic Raman vibration modes of the flake. Photoluminescence (PL) measurements are performed on single-layer areas of a flake. We clearly see two PL peaks at low temperatures, which we may assign to bound and free exciton transitions. Time-resolved PL traces reveal photocarrier recombination on the few-picosecond timescale at low temperatures. For temperatures above 150 K, we observe a longer-lived component of the PL, which we attribute to increased carrier-phonon interaction at higher temperatures.

[1] K. F. Mak et al., Phys. Rev. Lett. **105**,136805 (2010).
[2] T. Korn et al., Appl. Phys. Lett. **99**, 102109 (2011).

HL 7.7 Mon 11:00 EW 015

Electronic and vibrational properties of single- and few-layer MoS_2 — •Gerd Plechinger, Stefanie Heydrich, Johannes Schmutzler, Franz-Xaver Schrettenbrunner, Jonathan Eroms, Dieter Weiss, Christian Schüller, and Tobias Korn — Institut für experimentelle und angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany

The layered transition-metal dichalcogenide MoS_2 has attracted great interest because of good optical properties and as alternative to graphene for nanoelectronic applications. With the transparent tape liftoff method, single- and few-layer MoS_2 flakes were prepared. By annealing the samples in vacuum, photoluminescence peak intensity positions varying by about 20 meV at room temperature, were made uni-

form. Low temperature photoluminescence measurements on single-layer MoS_2 flakes show an additional low-energy peak. It can be attributed to a surface-bound exciton, because samples with a HfO_2 or Al_2O_3 coating do not show the low-energy peak.

In Raman-measurements, we have identified an interlayer shear mode at $30\,cm^{-1}$ in bulk material. We observed a decrease in wavenumber with decreasing layer number. By scanning an area on the sample, we can distinguish regions of different layer numbers by mapping the spectral position of the shear mode.

HL 7.8 Mon 11:15 EW 015

Atomically thin layers of transition metal dichalcogenides investigated by ab initio methods — •Kerstin Hummer and Georg Kresse — University of Vienna, Computational Materials Physics, Vienna, Austria

The advances in the fabrication of atomically thin layered materials has enabled investigations of new physical properties inherent to low dimensional structures. Transition metal dichalcogenides (TMX_2) crystallize in a quasi-two-dimensional structure that allows for low dimensional structuring. Among them, the prototype material molybdenum disulfide (MoS_2), has attracted intense interest because of its distinct electronic and optical properties that enable its application in photovoltaics and photocatalysis. A key issue regarding the applicability in efficient opto-electronic devices is the energy gap that should match the solar spectrum (1-3 eV). Bulk TMX_2 with TM = Mo, W and X = S, Se, Te have band gaps between 1 and 1.5 eV, but their fundamental gaps are indirect and thus optically forbidden. However, a transition from an indirect to an direct gap semiconductor was achieved in MoS_2, when going from bulk to atomically thin layers.

In this work, we present density functional theory studies of thin layer TMX_2 with TM = Mo, W and X = S, Se, and Te. Accurate band structures are obtained with the modified Becke-Johnson exchange potential in combination with LDA correlation. Particular emphasis is put on the variation of the band gap with layer thickness as well as the influence of the substrate present in experiment.