HL 47: Oxide Semiconductors II

Time: Friday 9:30–11:30 Location: POT 81

HL 47.1 Fri 9:30 POT 81

Origin of Resistive Switching in $SrTiO_3$ — •Wahib Aggoune[1], Christian Carbogno[1], Martin Albrecht[2], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft and IRIS-Adlershof of the Humboldt-Universität zu Berlin. — [2]Leibniz-Institut für Kristallzüchtung, 12489 Berlin.

Memristors may play a key role for the next generation of non-volatile memory devices. They are typically realized using materials that allow to switch between a low- and a high-resistance state. This effect has been recently observed in $SrTiO_3$ thin films, whereby a pronounced dependence of the switching properties on the growth conditions was found [1,2]. To shed light on the underlying atomistic mechanisms, we performed density-functional theory calculations and carefully analyzed the critical effects of different exchange-correlation functionals. We explored the most stable defects (vacancies, interstitial, substitutional) under Ti-*rich* conditions. The study reveals that the formation of a Ti_{Sr} antisite defect is energetically favorable and also induces a spontaneous polarization. It can be further stabilized by an additional nearby Sr-vacancy (Ti_{Sr}+V_{Sr}). Furthermore, such a defect complex increases the observed polarization. We discuss these results with respect to the experimentally observed resistive switching by analyzing the electronic properties and the polarization as well as the energy barriers for switching it.

[1] A. Baki, *et al.*, *Sci. Rep.* **11**, 7497 (2021).
[2] K. Klyukin, *et al.*, *Phys. Rev. B* **95**, 035301 (2017).

HL 47.2 Fri 9:45 POT 81

Second harmonic generation of blue series excitons in Cu_2O — •Andreas Farenbruch[1], Dietmar Fröhlich[1], Heinrich Stolz[2], Dmitri R. Yakovlev[1,3], and Manfred Bayer[1,3] — [1]Experimentelle Physik 2, TU Dortmund, Dortmund, Germany — [2]Institut für Physik, Universität Rostock, Rostock, Germany — [3]St. Petersburg, Russia

Excitons are Coulomb-bound complexes of electrons and holes in semiconductors with a discrete hydrogen-like energy series. The yellow exciton series in Cu_2O involves excitations between the highest valence and lowest conduction band and it presents an ideal platform for investigations of exciton physics with Rydberg states up to a principal quantum number of n=28. Excitations, that involve the same valence band but the second lowest conduction band belong to the so-called blue series. Access in linear optical spectroscopy to these states is hard to achieve due to the high absorption in this spectral range. Optical second harmonic generation (SHG) is therefore a suitable investigation method. By analyzing the measured polarization dependence of the SHG signal and comparing it with group theoretical simulations, the magneto-Stark and Zeeman effects are identified as the SHG mechanisms involved. The 1S, 2S and 2P excitons and magneto-excitons up to n=8 in magnetic fields up to 10 T are detected. By analyzing their magnetic-field shift and polariton effect, key properties such as the energies of the exciton resonances, the Rydberg energy, the band gap, the reduced exciton mass, the anisotropy of the conduction band mass and the exciton radius are obtained for the blue exciton series.

HL 47.3 Fri 10:00 POT 81

Electrical and thermoelectrical properties of the two-dimensional electron gas in polar discontinuity doped BaSnO3/LaInO3 heterostructure — •Fazeel Zohair, Georg Hoffmann, and Oliver Bierwagen — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 7, Berlin, Germany

Transparent semiconducting oxides (TSOs) are key players for optoelectronic devices, among which high frequency applications benefit from electrical properties of two-dimensional electron gases (2DEGs) . In this contribution we demonstrate the electrical and thermoelectric properties of the 2DEG at the interface between a nonpolar perovskite oxide BaSnO3 and a polar perovskite oxide LaInO3, grown by plasma assisted molecular beam epitaxy. The electrical and thermoelectric properties are analyzed using Seebeck measurements and van der pauw-Hall measurements. Integrating the charge carrier concentrations from both measurements, we were able to deduce the thickness of the charge carrier system.

HL 47.4 Fri 10:15 POT 81

Analysis of thickness distributions for combinatorial pulsed laser deposition — •Clemens Petersen, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig Felix-Bloch-Institut, Leipzig, Deutschland

Recently combinatorial deposition methods have increasingly gained scientists* attention, due to the high experimental throughput and resource-wise efficiency they offer in materials discovery. This enables fast screening of material properties of multinary material systems using just a single sample. By employing pulsed laser deposition with our segmented target approach [1] we successfully realized the deposition of α-$(Al_xGa_{1-x})_2O_3$ with continuous composition spread over the whole composition range on a single 2-inch sapphire wafer [2]. Accompanied by the usage of high-throughput measurements such as spectroscopic ellipsometry and x-ray diffraction, the characterization of the material systems' physical properties with high chemical resolution and comparably low efforts becomes feasible. By employing the plasma plume expansion model suggested by Anisimov *et al.* [3] and the resulting spatial material-deposition distribution we calculate binary growth rates as function of position enabling us to predict film thickness and composition locally. Thereby the deposition of group III sesquioxides can be described exceptionally well. We further show that the binary distributions can be used to predict the combinatorial deposition of ternary alloys with high precision. [1] H. von Wenckstern *et al.*, pss(b), Vol. 257, 1900626 [2] A. Hassa *et al.*, pss(b), Vol. 258, 2000394 [3] S. I. Anisimov *et al.*, Phys. rev. B, Vol 48, 12076.

15 min. break

HL 47.5 Fri 10:45 POT 81

Cloud in cell scheme based stochastic modelling of $BiFeO_3$ memristor for circuit simulations — •sahitya yarragolla[1], nan du[2,3], torben hemke[1], xianyue zhao[2,3], ziang chen[2], and thomas mussenbrock[1] — [1]Chair of Applied Electrodynamics and Plasma Technology, Ruhr University Bochum, Germany — [2]Institute for Solid State Physics, Friedrich Schiller University Jena, Jena, Germany — [3]Department of Quantum Detection, Leibniz Institute of Photonic Technology , Jena, Germany

In recent years, analog memristive devices have been extensively investigated for neuromorphic computing and hardware security applications. It is found that these devices show excellent properties such as long retention time, intrinsic stochasticity, and fast switching. However, the switching mechanism in these devices from the physics point of view is still under discussion. Therefore, in this work, we focus mainly on understanding the resistive switching based on the transport of oxygen vacancies in the interface-type Au/$BiFeO_3$ (BFO)/Pt/Ti memristive devices using a 1D cloud-in-a-cell model. The proposed model combines the advantages of both 1D concentrated and 3D distributed models in a single model. The model is stochastic and computationally less expensive, making it suitable for circuit simulations. The calculated I-V characteristics of BFO memristor using the proposed are in excellent agreement with the experimental results. Furthermore, the response of the BFO memristor to changes in electrical properties, temperature and retention characteristics are analyzed, and the results show reasonable agreement with experimental findings.

HL 47.6 Fri 11:00 POT 81

Comparing processing strategies for Indium oxide field-effect transistors — •Fabian Schöppach, Clemens Petersen, Holger von Wenckstern, and Marius Grundmann — Felix Bloch Institute for Solid State Physics, Universität Leipzig, Germany

Indium oxide (In_2O_3) combines promising physical properties such as high carrier mobility and transparency in the visible. However, due to its tendency to form an electron accumulation layer on its surface (SEAL), the use of In_2O_3 in active devices is generally difficult. We use the published strategies, compensating Mg doping [1] and oxygen plasma treatment [2], to suppress SEAL formation and allow the films to be used in FET devices. In addition, In_2O_3 as sesquioxide is a very robust material that resists classical patterning processes such as wet chemical etching.

We identified two different fabrication strategies to structure our films laterally: Plasma-assisted etching and using a wet-chemical soluble sacrificial layer. In this work, both strategies are compared re-

garding additionally necessary processing steps and the final devices' performance. We used In_2O_3 films grown by pulsed laser deposition. For the source and drain contacts, gold was deposited via inert ambient sputtering. Schottky gate diodes were fabricated in a reactive sputtering process, which is a prerequisite for obtaining electrically rectifying contacts to In_2O_3 [3].

[1] Schmidt, et al. physica status solidi (b) 252.10, 2304–2308 (2015)
[2] Michel, et al. ACS Appl. Mater. Interf. 11, 27073–27087 (2019)
[3] von Wenckstern, et al. APL Materials 2.4, 046104 (2014)

HL 47.7 Fri 11:15 POT 81

Charge carrier diffusion and localization in metal oxide photoabsorbers — •Hannes Hempel, Markus Schleuning, Klaus Schwarzburg, Rainer Eichberger, Roel van de Krol, Moritz Kölbach, Fatwa F. Abdi, and Dennis Friedrich — Helmholtz-Zentrum Berlin, Germany

Long diffusion lengths of photo-excited charge carriers are crucial for high power conversion efficiencies of photoelectrochemical and photovoltaic devices. However, in metal oxids are effects such as (multiple-)trapping, carrier localization and polaron formation can lead to time-varying mobilities and lifetimes that are not accounted for in the conventional analysis. Therefore, here, a generalized analysis is presented that determines the diffusion length directly from the integral of a photoconductivity transient, regardless of the nature of carrier relaxation. This approach is presented on amorphous silicon, a prototype of disordered materials, and BiVO4, one of the most studied photoanode materials for solar water splitting. Our generalized analysis allows monitoring the temporal evolution of the charge carrier displacement, which converges for both materials after ˜100 ns to a diffusion length of a few tens of nanometers. For BiVO4, the obtained diffusion length is significantly shorter than the typical thin film thickness, which rationalizes the photocurrent loss in the corresponding photoelectrochemical device. Finally, we probe several metal other prominent metal oxide photoabsorbers, namely Fe2O3, FeVO4, CuFeO2, α-SnWO4, BaSnO3, and CuBi2O4, and find sings of carrier localization on the nanometer scale, which limits the charge carrier diffusion.