DS 10: Oxide Semiconductors for Novel Devices (Focussed Session): Session II

The class of semiconducting oxides includes low temperature processed amorphous thin films for bendable electronics and display technology as well as highly crystalline materials such as the wide band group-III sesquioxides being interesting for UV and DUV photo sensors, power electronics and even memristors. This session sets a focus on physical properties of such oxides, their growth methods and heterostructures for demonstrator devices. This focus session is supported by the Leibniz ScienceCampus GraFOx.

Organized by

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Time: Monday 15:00–18:15 Location: E 020

DS 10.1 Mon 15:00 E 020

Defect and interface formation in $SrTiO_3$ homoepitaxial thin film growth — •Laura Bogula, Toni Markurt, Martin Albrecht, and Jutta Schwarzkopf — Max-Born-Str. 2, 12489 Berlin, Germany

$SrTiO_3$ represents a model system for perovskite materials and is therefore in the focus of fundamental research. Despite many studies, its functional properties and the correlation to atomic defects are not fully understood so far. Moreover, in many $SrTiO_3$ based devices next to the structural quality of the epitaxial film itself also the interface between substrate and film plays a crucial role. Therefore, we have performed a systematic investigation of the influence of different growth and pregrowth conditions on the resulting interface and the structural quality of homoepitaxial films grown by pulsed laser deposition (PLD). Transmission electron microscopy and x-ray diffraction techniques as well as reflection high-energy electron diffraction are applied to characterize films and interfaces. By varying substrate temperature, chamber pressure and oxygen content the optimal growth conditions for a stoichiometric, point defect-poor interface and film structure are specified. We found that on the one hand a high oxygen partial pressure during heat-up prior to film growth leads to an unfavourable surface reconstruction of the substrate causing a non-stoichiometric substrate/film interface. On the other hand, the formation of point defects in the film is correlated to the energetic ion bombardment during film growth which is reduced with a high process pressure.

DS 10.2 Mon 15:15 E 020

The electric field dependence of the permittivity of $SrTiO_3$ — •Julian Stoever, Laura Bogula, Toni Markut, Jos Boschker, Jutta Schwarzkopf, Martin Albrecht, and Klaus Irmscher — Leibniz Institute for Crystal Growth, Max-Born-Str. 2, 12489 Berlin, Germany

Resistive switching in $SrTiO_3$ belongs to the interesting applications in the fast growing field of oxide electronics. Oxygen vacancy diffusion due to high electric fields in the depletion layer of $SrTiO_3$ Schottky diodes is a commonly used model to describe the resistive switching behaviour. The dependence of the permittivity on the electric field strength has been rarely taken into account for $SrTiO_3$ resistive switching devices. The permittivity of $SrTiO_3$ is strongly dependent on the temperature and the electric field. Additionally, capacitance-voltage and current-voltage characteristics show deviations of the C^{-2}-V relation and the thermionic-emission model, respectively. Theoretical models were developed that assume a non-linear dielectric response of the crystal [Reich et al. Phys. Rev. B, 91 11 (2015)]. Another approach is the introduction of a low-permittivity interlayer, as it was done by Yamamoto et al. [Jpn. J. Appl. Phys. 37 4737 (1998)]. To verify the theoretical approaches, fundamental measurements of the permittivity are necessary. We performed permittivity measurements at different temperatures and electric fields on plate capacitor structures made of insulating $SrTiO_3$. The results will be compared with the behaviour of the Schottky diodes and are important for characterization methods like deep level transient spectroscopy.

DS 10.3 Mon 15:30 E 020

Theoretical description of the current conduction thorough the Schottky barrier in SrTiO3/Pt based resistive switching devices — •Carsten Funck[1], Christoph Bäumer[2], Regina Dittmann[2], Rainer Waser[1,2], and Stephan Menzel[2] — [1]Institute für Werkstoffe der Elektrotechnik II, RWTH Aachen University, 52064 Aachen, Germany — [2]Peter Grünberg Institut (PGI 7), Forschungszentrum Jülich, 52425 Jülich, Germany

The current transport across Schottky contacts is widely investigated in many fields of semiconductor technology. Often this current transport is described with a certain conduction mechanism, which connects the electrical current with an analytical equation. This analytical expressions are frequently used to explain the experimental current through resistive switching devices. Especially, the Schottky emission theory is often applied to $SrTiO_3$ based thin film Schottky contacts. However, this proceeding leads often to physical inconsistencies. Therefore we developed an atomistic fully quantum mechanical model based on density functional theory combined with the non-equilibrium Green's function formalism. This model will be underlined by single band transport simulations. As a conclusion of these models we will show that the often applied Schottky emission theory is insufficient to describe the electrical current in Nb:$SrTiO_3$/$SrTiO_{3-x}$/Pt based resistive switching devices. In contrast it will be shown that a thermally assisted tunneling process is responsible for the current transport across the interface, which crosses over into a direct tunneling for higher voltages.

DS 10.4 Mon 15:45 E 020

Pulse kinetic study on HfO_2/TiO_2- bilayer resistive switching memories — •Felix Cüppers[1], Alexander Hardtdegen[1], Susanne Hoffmann-Eifert[1], Moritz von Witzleben[2], and Ulrich Böttger[2] — [1]PGI-7, Forschungszentrum Jülich GmbH, Germany — [2]IWE II, RWTH Aachen University, Germany

Memristive devices based on ultrathin metal oxide layers are promising candidates for future information technology applications. Bilayer oxide stacks of HfO_2/TiO_2 exhibit enhanced switching stability [1] compared to the respective monolayers. However, the origin of the stability is not fully understood. Effects under discussion comprise the intrinsic current limitation by the titanium oxide layer as well as a change in the temperature management during switching. Furthermore, the influence of the intrinsic series resistor on the switching kinetics of the bilayer cell needs further exploration.

In this study, electrical characterization by pulse measurements of bilayer oxide stacks of HfO_2/TiO_2 is done. By variation of time, voltage, state resistance and pulse geometry, different regimes of cell performance are identified and characterized. These results allow a deeper understanding of the kinetics of resistively switching oxide bi-

layer stacks. [1] A. Hardtdegen et al., "Internal Cell Resistance as the Origin of Abrupt Reset Behavior in HfO_2-Based Devices Determined from Current Compliance Series" *2016 IEEE 8th International Memory Workshop (IMW)*, Paris, 2016, pp. 1-4.

DS 10.5 Mon 16:00 E 020

Electrode Influence on the Resistive Switching Performance in HfOx based RRAM Devices — •Benjamin Krah[1], Stefan Petzold[1], Ulhas Sharath[1], Eszter Piros[1], Tom Blomberg[2], Eric Jalaguier[4], Marko Tuominen[2], Hessel Sprey[3], Sophie Bernasconi[4], Etienne Nowak[4], Philipp Komissinskiy[1], Erwin Hildebrandt[1], and Lambert Alff[1] — [1]TU Darmstadt, Darmstadt, Germany — [2]ASM Microchemistry Ltd., Helsinki, Finland — [3]ASM Belgium, Leuven, Belgium — [4]CEA Leti, Grenoble, France

Resistive switching random access memory (RRAM) is an intensively investigated candidate for DRAM and FLASH replacement. The resistance of an insulator, sandwiched between two electrodes, can be modified by an applied voltage generating a soft breakdown of the dielectric. Hafnium oxide (HfO2) based dielectrics are of high interest due to their proven CMOS compatibility. Recently, we have shown in a simple model device how to achieve all reported switching modes, including conductance quantization [1]. Here, we investigate in the same model device (Pt/HfO2/bottom electrode (BE) and Pt/HfOx/BE) the influence of electrode material on the switching variability and performance. As only additional parameter, the oxygen stoichiometry HfOx is varied. The tested bottom electrodes include TiN, TiWN, WN and W due to their applicability in the semiconductor industry. We found that strong oxygen getter electrodes tend to increase the switching variability and to reduce the reliability. The choice of electrode, therefore, is a crucial parameter for switching performance.

[1] S. U. Sharath et. al., Adv. Funct. Mater. 27, 1700432 (2017)

DS 10.6 Mon 16:15 E 020

Ab initio study of oxygen vacancy formation and migration in HfO_2 under electric field — •Marta Gibertini, Daniel Wortmann, Gustav Bihlmayer, Shigeru Tsukamoto, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Among the storage devices investigated so far, resistive random access memories (ReRAMs) stand out because of the high-speed/high-density properties and the low energy required for the writing/rewriting circles. A deep understanding of the role played by point defects and dopants is important for an optimization of the device functionality. We present a density functional theory (DFT) study aimed at investigating the formation energies and the migration energy barriers of oxygen vacancies in monoclinic HfO_2. We look at the dependence of these properties in bulk and film systems on the magnitude of an external electric field. We also study the influence of Yttrium dopants on the diffusion. The nudged elastic band method is applied and the DFT calculations are performed with the electronic structure code jüRS, a real-space finite-difference implementation of the projector augmented wave (PAW) method. The real-space formalism is chosen because it allows a flexible treatment of the boundary conditions, and therefore, it is favourable for the application of an external electric field in terms of a capacitor model. - The work is supported by DFG - SFB 917 (Nanoswitches)

DS 10.7 Mon 16:30 E 020

Filament growth and resistive switching in hafnium oxide memristive devices — •Sven Dirkmann[1], Jan Kaiser[1], Christian Wenger[2], and Thomas Mussenbrock[3] — [1]Ruhr-Universität Bochum, Lehrstuhl für Theoretische Elektrotechnik, 44780 Bochum, Germany — [2]IHP, 15239 Frankfurt (Oder), Germany — [3]BTU Cottbus-Senfenberg, Lehrstuhl für Theoretische Elektrotechnik, 03046 Cottbus, Germany

Memristive nanostructures are devices that change their resistance when a voltage is applied to them and maintain their resistance when removing this voltage. In particular, HfO2 based RRAM devices are under investigation due to their scalability ($<$ 10 nm), simple fabrication , fast switching speeds and their compatability with CMOS technology. Here, we report on the resistive switching in TiN/Ti/HfO2/TiN memristive devices. A resistive switching model for the device is proposed, based on important experimental and theoretical findings and validated using 2D and 3D kinetic Monte Carlo simulations. The model is coupled to a field solver and different current transport mechanisms as direct tunneling, trap assisted tunneling, ohmic transport, and transport through a quantum point contact have been taken into account. Important parameter, difficult to measure in experiments, as the shape of the conductive filament, width of the filament constriction, current density and temperature distribution, are calculated. We find that the numerical results are in excellent agreement with experimentally obtained data. This work is funded by the German Research Foundation DFG in the frame of Research Unit FOR2093.

15 min. break.

DS 10.8 Mon 17:00 E 020

Molecular beam epitaxy of Ga2O3 homoepitaxial (010) thin films — •Piero Mazzolini[1], Charlotte Wouters[2], Martin Albrecht[2], and Oliver Bierwagen[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany

Due to some of its peculiar properties like its intrinsic wide bandgap (Eg = 4.8 eV) and the possibility to tune its transport properties, gallium oxide is recently attracting large interest especially in the field of power electronic devices. Nonetheless, the future application of Ga2O3 is connected to the possibility to obtain a deep control of its functional properties, i.e. limiting/controlling the presence of defects (e.g. doping). We here present a study on homoepitaxially grown β-Ga2O3 thin films via molecular beam epitaxy on (010)-oriented β-Ga2O3 substrates. We thoroughly study the effect of the in-situ surface cleaning, growth T and metal-to-oxygen flux ratio. The quality of the deposited gallium oxide homoepitaxial thin films is determined employing different in-situ (e.g. RHEED) and ex-situ (e.g TEM, AFM, XRD) characterization techniques.

DS 10.9 Mon 17:15 E 020

Thermal Conductivity of β-Ga_2O_3 Bulk and thin Films — •Martin Handwerg[1], Robin Ahrling[1], Rüdiger Mitdank[1], Günter Wagner[2], Zbigniew Galazka[2], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Leibniz Institute for Crystal Growth, 12489 Berlin, Germany

The transparent conductive oxide β-Ga_2O_3 is of huge interest for high power electronics and optoelectronics because of its high band gap ($E_G \approx 4.7eV$). Knowledge of the thermal conductivity is crucial to design stable applications.

Here, we investigate the thermal conductivity of thin MOVPE grown polycristalline β-Ga_2O_3 films on sapphire-substrates and single-crystalline, electrically conductive β-Ga_2O_3 films on insulating Mg-doped Czochralski-grown β-Ga_2O_3 substrates.

In order to measure the thermal conductivity of films and substrates, we used multiple aspects of the 3ω-method: the differential 3ω-method with a separate measurement of the substrate; a variation of multiple heater lines with different line widths and a 2ω approach.

We observe a reduction of the bulk thermal conductivity in dependence of the crystallinity and film thickness. This reduction can be explained with the reduced mean free path of the phonons due to the film thickness and grain sizes. This result, as well as an observed electrical conductivity reduction with decreasing film thickness, leads to a limitation of thermally influenced applications with films thinner than $\approx$ 150 nm or the need of an improved thermal management.

DS 10.10 Mon 17:30 E 020

Electronic Raman scattering in β-Ga_2O_3 — •Andreas Fiedler[1], Manfred Ramsteiner[2], Zbigniew Galazka[1], and Klaus Irmscher[1] — [1]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5−7, 10117 Berlin, Germany

Currently, β-Ga_2O_3 is in the research focus as a material for power electronic devices because of its anticipated high electric break down field ($\approx$ 8 MV/cm). For such applications, doping control is of outermost importance. Here we report on Raman spectroscopy investigations of highly n-type doped β-Ga_2O_3 single crystals. For degenerate material ($n > 3 \times 10^{18}$ cm^{-3}), we observe Raman lines at about 282 cm^{-1} (with a shoulder at 255 cm^{-1}) and at about 564 cm^{-1}, which cannot be assigned to first-order scattering by phonons. These lines exhibit only a weak temperature dependence and are essentially independent of the shallow donor species (Sn or Si). We attribute the doping induced Raman features to electronic Raman scattering caused

by excitation of electrons from an effective-mass like donor impurity band into the conduction band. This assignment is based on the fact that the peak position of the low-frequency line coincides with the ionization energy of effective-mass like donors (≈ 36 meV) and the occurrence of the Raman signals only for doping concentrations exceeding the Mott criterion. Consequently, the high-frequency Raman line at 564 cm^{-1} (= 2 × 282 cm^{-1}) is explained by second-order electronic Raman scattering.

DS 10.11 Mon 17:45 E 020

Analysis of the conductivity anisotropy of β-Ga_2O_3 using Van der Pauw measurenemts — •Christian Golz[1], Zbigniew Galazka[2], Fariba Hatami[1], W. Ted Masselink[1], and Oliver Bierwagen[3] — [1]Department of Physics, Humboldt-Universität zu Berlin, Newton-Str. 15, D-12489 — [2]Leibniz Institute for Crystal Growth, Max-Born-Str. 2, D-12489 — [3]Paul-Drude-Institute, Hausvogteiplatz 5-7, D-10117

Using Van der Pauw measurements, the conductivity anisotropy of β-Ga_2O_3 was analyzed. The structural asymmetry due to the monoclinic lattice structure of β-Ga_2O_3 translates into anisotropic properties like optical absorption and thermal conductivity. Due to an anisotropic effective mass and anisotropic scattering rates (e. g. due to anisotropic phonon modes), conductivity might be anisotropic as well. Square shaped β-Ga_2O_3 high quality bulk samples oriented in several surface orientations with lithographically processed contacts were analyzed for temperatures between 10 K and 375 K. The results were translated into the conductivity tensor (both diagonal and off-diagonal elements) by comparing them to finite element simulations of the potential in each sample and calculation of a two-dimensional conductivity tensor in the coordinate system of the sample edges. Less than 5% anisotropy were found at and above room temperature, where isotropic conductivity is within the experimental error. Larger anisotropies were found at low temperatures (about 30% at 10 K) and for a samples having a large number of low-angle grain boudaries (anisotropy above a factor of 20 at 50 K, but only 12 % at 365 K).

DS 10.12 Mon 18:00 E 020

Carrier mobility in crystalline MOVPE-Ga2O3-films — •Rüdiger Mitdank[1], Robin Ahrling[1], Martin Handwerg[1], Günter Wagner[2], Zbigniew Galazka[2], and Saskia F. Fischer[1] — [1]AG Novel Matirials, Institut für Physik der Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany

We demonstrate the results of Hall- and van-der-Pauw measurements for Si-doped ß-Ga2O3 MOVPE layers with a thickness 30nm < t < 230 nm between T = 50 K and 300 K. The homoepitaxial layers were grown on isolating substrates with Mg-doping. At high temperature T, the mobility is dominated by scattering of electrons at polar optical phonons, at low T by scattering at ionized impurities. A mobility limit for T = 300K and t >100nm of 140 (cm*cm)/Vs was found in the case of pure electron-phonon interaction. For t < 100 nm the mobility decreases strongly. The reduction of the carrier mobility due to surface scattering and propagation of electron waves in thin films is discussed.