DF 10: High- and low-k-dielectrics (jointly with DS)

Time: Wednesday 9:30–11:30 Location: EB 407

DF 10.1 Wed 9:30 EB 407

High dielectric constants due to charge order induced electrical heterogeneity — •Stephan Krohns[1], Pit Sippel[1], Holger Kirchhain[1], Stefan Riegg[1], Peter Lunkenheimer[1], Armin Reller[2], and Alois Loidl[1] — [1]Experimental Physics V, University of Augsburg — [2]Resource Strategy, University of Augsburg

One of the most imminent challenges of modern materials science is the development of new materials with less critical elements that have comparable or better functionalities than those currently used. We illustrate an interdisciplinary approach by applying it to the prototypical example of materials with extremely high dielectric constant to validate the innovative potential in a very early stage of research.[1]

Not only the validation of the economic and technical potential of high dielectric constant materials are in the focus of interest, but also the mechanisms generating this dielectric phenomena. Most of the materials exhibiting those effects, among them numerous transition-metal oxides[2], have complex ground states emerging from strong electronic correlations. $La_{15/8}Sr_{1/8}NiO_4$ for example shows a very high dielectric constant up to gigahertz frequencies at room temperature and it seems that charge order induced electrical heterogeneity can be the origin. To scrutinize that, we also thoroughly investigate the structural, magnetic and dielectric properties of various isostructural $La_{2-x}(Ba,Ca,Sr)_xNiO_4$ compounds especially emphasizing the contribution of electronic phase separation to the permittivity.

[1] S. Krohns *et al.*, Nat. Mat. **10**, 899 (2011). [2] P. Lunkenheimer *et al.*, Eur. Phys. J. Special Topics **180**, 61 (2010).

DF 10.2 Wed 9:50 EB 407

Bilayer gate dielectric stacks of cerium oxide and titanium oxide for nanoelectronics — •Meng Meng Vanessa Chong[1,2], Kam Chew Leong[2], Pooi See Lee[1], and Ing Yoong Alfred Tok[1] — [1]School of Materials Science and Engineering, Nanyang Technological University, Block N4.1, Nanyang Avenue, Singapore 639798 — [2]Global Foundries Singapore Pte. Ltd., Singapore 528830

Numerous materials systems are under consideration as potential replacements for SiO2 as the gate oxide material for sub-0.1 micron CMOS technology. Many properties have to be considered in selecting a suitable material because of emerging issues with high-k technology development. Though, many dielectrics appear favorable in some of these areas, but very few materials are promising with respect to all the required properties.

This work focuses on the rare earth oxide - CeO2 as alternative dielectric as it has small lattice mismatch with Si and high k-values. This study also shows the integration of a high-k passivation layer (TiO2) to suppress the formation of undesirable interfacial layer. Physical characterizations are done to determine the stoichiometry, surface roughness and interface quality.

In addition, temperature dependent measurements are done to identify the different conduction mechanisms such as Poole-Frenkel emission. Identification of various leakage constituent is important for estimation and reduction of leakage power. Furthermore, in-depth electrical analysis helps to determine the quality of the film and dielectric interface.

DF 10.3 Wed 10:10 EB 407

High quality REO thin films from wet chemical deposition — •Maraike Ahlf[1,2], Meng Meng Vanessa Chong[2,3], Mathias Wickleder[1], Alfred Ing Yoong Tok[2], Pooi See Lee[2], and Katharina Al-Shamery[1] — [1]University of Oldenburg, IRAC, Germany — [2]Nanyang Technological University, MSE, Singapore, Singapore — [3]Global Foundries Ltd., Singapore

The aggressive scaling in microelectronics leads to the need of new high performance thin film materials as gate oxides in MOS devices. High leakage currents suffered for conventionally used SiO_2 when scaling down to sub 22 nm requires alternative high κ dielectrics. REOs are potential candidates to replace SiO_2 due to their ecellent electrical properties. This necessitates the synthesis of new RE precursors and deposition methods to achieve impurity free films, since conventionally used techniques suffer from problems such as C impurities from the organic precursors used and formation of interfacial layers or byproducts due to high process temperatures. Results of an unconventional, low temperature, patented, wet chemical approach which is easy to realize and integrate into device production to deposit Nd_2O_3 ultra thin, high quality gate stacks will be presented. The constitution and annealing dependent crystallization behavior on Si and the deposition mechanism of inorganic designer RE-precursors has been investigated with XPS, XRD, AFM and HRTEM. CV and IV measurements show κ values as twice as high and leakage currents down to 10 orders of magnitude lower than conventionally SiO_2. Various current conduction mechanisms can be understood from varying temperature measurements.

DF 10.4 Wed 10:30 EB 407

Epitaxial growth of $Ba_{0.6}Sr_{0.4}TiO_3$ on highly conductive $SrMoO_3$ thin films by Pulsed Laser Deposition — •Aldin Radetinac, Philipp Komissinskiy, and Lambert Alff — Institut für Materialwissenschaften, Technische Universität Darmstadt, Petersenstraße 23, 64287 Darmstadt, Germany

High-quality thin films and heterostructures of dielectric and conducting oxides are necessary for realization of all-oxide tunable capacitors. Here we present epitaxial $Ba_{0.6}Sr_{0.4}TiO_3/SrMoO_3$ (BST/SMO) heterostructures grown by Pulsed Laser Deposition (PLD) on single crystal $SrTiO_3$ (100) and $GdScO_3$ (110) substrates. 80 nm thick highly conducting (001) SMO films with a resistivity below 100 $\mu\Omega$cm are deposited in argon atmosphere at $5x10^{-4}$ Torr [1]. A 5 nm thick initial epitaxial BST buffer layer is grown at low oxygen pressure of 10^{-5} Torr and flow of 0.7 sccm. The buffer layer prevents oxidation of the SMO film to $SrMoO_4$ and allows further deposition of the fully oxidized paraelectric BST at oxygen pressure of $5x10^{-4}$ Torr and 0.9 sccm flow. To our knowledge this study shows for the first time how metastable materials like SMO can be incorporated in oxide electronic devices. The work is supported by the GRK 1037 (TICMO) project of the DFG.

[1] A. Radetinac, K. S. Takahashi, L. Alff, M. Kawasaki and Y. Tokura, Appl Phys Express 3 (7) (2010)

DF 10.5 Wed 10:50 EB 407

***P*-type conductivity in oxygen deficient HfO_{2-x} thin films grown by Reactive Molecular Beam Epitaxy** — •Erwin Hildebrandt[1], Jose Kurian[1], Mathis Müller[1], Thomas Schroeder[2], Hans-Joachim Kleebe[1], and Lambert Alff[1] — [1]Institute of Materials Science, Technische Universität Darmstadt, Germany — [2]IHP, Frankfurt(Oder), Germany

Highly oxygen deficient thin films of hafnium oxide HfO_{2-x} were grown using reactive molecular beam epitaxy on *c*-cut sapphire substrates. The oxygen content and, thus, oxygen vacancy concentration was engineered by controlled oxidation using RF-activated oxygen during growth. Hafnium oxide, a high-k dielectric insulator in its stoichiometric form, turns into a *p*-type semiconductor above a threshold of oxygen vacancies with up to 6 times 10^{21} charge carriers per cm^3. The introduction of oxygen vacancies reduces the optical band gap from 5.7 eV for stoichiometric HfO_2 by more than 1 eV. The absence of crystalline and/or amorphous metallic hafnium phases was proven by X-ray diffraction and a tilting series using High-Resolution Transmission Electron Microscopy. We suggest the formation of an oxygen vacancy induced *p*-type defect band within the energy gap as the origin of the observed *p*-type conductivity [1].

[1] E. Hildebrandt, J. Kurian, M. M. Müller, T. Schroeder, H.-J. Kleebe, and L. Alff, Appl. Phys. Lett. **99**, 112902 (2011).

DF 10.6 Wed 11:10 EB 407

Hydrogen Impurity in Y_2O_3: an *Ab – Initio* and a μSR perspective — •Estelina L. Silva, Apostolos Marinopoulos, Rui Vilão, and Ricardo Vieira — CEMDRX and CFC, Physics Department, University of Coimbra, P-3004-516 Coimbra, Portugal

Density functional calculations were performed for interstitial hydrogen in Y_2O_3, by employing the semi-local GGA-PBE and the hybrid HSE06 exchange-correlation functionals. It was observed that the lowest energy H^0 and H^- configurations prefer to relax in the interstitial, vacant O, sites. For these charge systems, two different geometrical configurations (interstitial vacant Y and bond O-H type) also occur as higher-energy metastable sites. In contrast, the H^+ equilibrium state was found only when a O-H bond is formed. The overall results for the formation energies, obtained by employing the two functionals are consistent, for which amphoteric behavior was found for hydrogen

after considering the lowest-energy structures for each charge state. To compare results with μSR measurements, the formation energies of the metastable configurations were also evaluated. The results are consistent with the μSR data, where the co-existence of the observed diamagnetic signal is attributed to a shallow donor-like muonium and the paramagnetic signal to an acceptor-like deep muonium configuration.

For the interstitial configurations, of the neutral and negative charge systems, a defect level was found in the gap and positioned slightly above the valence band maximum, whereas for the bond O-H site, the defect level is located above the middle of the band gap, closer to the conduction band.