DS 15: High-k and Low-k Dielectrics (joint session with DF)

Time: Tuesday 11:15–12:15 Location: H 0111

DS 15.1 Tue 11:15 H 0111

Broadband dielectric response of doped rutile: intrinsic or extrinsic colossal dielectric constants? — •Martin Wohlauer, Stephan Krohns, Peter Lunkenheimer, and Alois Loidl — Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg (Germany)

Materials exhibiting so-called colossal effects have an enormous potential for future use in correlated electronics, including capacitors for energy storage and integrated circuits. The search for functional ceramics showing colossal dielectric constants (CDC) is still an active field of research[1]. Different phenomena, e.g., charge-order or internal as well as external electrical heterogeneities can lead to CDCs[2]. For the most prominent ceramic, $CaCu_3Ti_4O_{12}$, the mechanism giving rise to a dielectric permittivity of up to 10^5 is of extrinsic nature, e.g. interface polarisation. The discovery of CDCs in indium- and niobium-doped rutile at room temperatures recently also attracted high scientific interest[3]. In this talk, broadband dielectric measurements on various doped rutile ceramics will be presented. The results will be thoroughly discussed, especially emphasizing the contributions of external and internal interface effects influencing the permittivity. We demonstrate, that extrinsic interface effects are responsible for the CDCs in doped rutile.

[1]S. Krohns *et al.*, *Nat. Mat.*, **10**:899 (2011).
[2]P. Lunkenheimer *et al.*, *Eur. Phys. J. Special Topics*, **180**:61 (2010).
[3]W. Hu *et al.*, *Nat. Mat.*, **12**:821 (2013).

DS 15.2 Tue 11:30 H 0111

Structuring and interface manipulation of ultra-thin silicate films on a $Si(001)$ surface — •Shariful Islam[1], Karl Hofmann[2], and Herbert Pfnür[1] — [1]Institut für Festkörperphysik (ATMOS), Leibniz Universität Hannover — [2]Inst. f. Bauelemente der Mikroelektronik, Leibniz Universität Hannover

The dielectric-substrate interface plays a very important role on the growth condition and on the chemical, structural and kinetic properties of dielectric layers. Some very important properties like the sharpness of the interface, trap densities and band alignment also influenced by the cleanliness of substrate surface. We found the crystalline high-k silicate $(Ba_{0.8}Sr_{0.2})_2SiO_4$ and Ba_2SiO_4 to have dielectric constants ~ 18 and ~ 20 respectively. We studied the silicates elaborately both on structured and unstructured $Si(001)$ surface after depositing both at room and at high temperature ($650°C$). In addition to the spectroscopic measurements (XPS, SPA-LEED, EELS, AFM and TEM) we performed electrical measurements (C-V & I-V) of the silicate as an alternate gate dielectric in a MOS diode to study the dielectric-substrate interface in detail. The crystalline orthorhombic Ba_2SiO_4 grown here has a band gap of $E_G = 5.7$eV, an interface trap density $D_{it} \sim 10^{12}eV^{-1}cm^{-2}$, very low hysteresis < 0.5mV, band offset > 2eV, leakage current $< 6\ mA/cm^2$ at $+1$V; additional structural and electrical properties will be discussed.

DS 15.3 Tue 11:45 H 0111

k-restore Process with Plasma Enhanced Fragmentation for Damaged ULK Materials — A DFT and MD Study — •Anja Förster[1,5], Christian Wagner[2], Jörg Schuster[1], Sibylle Gemming[3,4], and Stefan Schulz[1,2] — [1]Fraunhofer ENAS, Chemnitz — [2]Center for Microtechnologies, TU Chemnitz, Chemnitz — [3]Institute of Physics, TU Chemnitz, Chemnitz — [4]Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [5]cfaed, TU Dresden, Dresden

Because of their low dielectric constant (k-value) ultra-low-k (ULK) materials are used for isolating the interconnects in integrated circuits. However, during the manufacturing process the k-value lowering methyl groups are replaced by hydroxyl groups and hydrogen atoms. This process is called OH- and H-damage.

In our simulation study we use fragmented silyation molecules (OMCTS, DMADMS) to repair the OH-and H-damages and restore the k-value of the ULK material by reinserting lost methyl groups. The fragmentation of DMADMS and OMCTS is investigated as a function of the reaction temperature using DFT on the PBE/DNP-level.

The repair behavior of the so obtained fragments are studied with two model systems: an assortment of small ULK-fragments and a silica cluster. We show that larger repair fragments with two and three methyl groups are energetically favorable.

DS 15.4 Tue 12:00 H 0111

Dissipative hydrogen two-level systems in Al_2O_3 — •Hazem Abu-Farsakh[1,2], Luke Gordon[1], Anderson Janotti[1], and Chris G. Van de Walle[1] — [1]Materials Department, University of California, Santa Barbara — [2]Prince Sultan University, Riyadh, Saudi Arabia

Superconducting qubits based on Josephson tunnel junctions are promising candidates for quantum computing. A limiting factor for their performance is the resonant absorption by two-level systems (TLSs) in the dielectric material. However, the microscopic nature of these TLSs has not been identified. In this work we propose that hydrogen interstitial atoms are the main source of TLSs in Al_2O_3. Using *ab-initio* calculations employing hybrid functionals we identify H binding sites and show that a hydrogen atom forms a H-bond in Al_2O_3 and feels a double potential well, resulting in a tunneling effect. We map the three-dimensional potential energy of an interstitial H atom and calculate its tunneling frequency by solving the corresponding Schrödinger equation. Our results show that the tunneling of H atoms gives rise to a resonant absorption in the 10 GHz region, in agreement with experimental observations. This work was supported by IARPA.