DS 21: High-k and Low-k Dielectrics (jointly with DF)

Time: Tuesday 13:45–15:15 Location: GER 38

DS 21.1 Tue 13:45 GER 38

Nondestructive Hard X-ray Photoelectron Spetroscopy Study of Resistive Switching TiN/Ti/HfO_2/TiN RRAM Cells — •Małgorzata Sowińska[1], Sebastian Thiess[2], Christian Walczyk[1], Damian Walczyk[1], Christian Wenger[1], Mindaugas Lukosius[1], Wolfgang Drube[2], and Thomas Schroeder[1] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]P09 beamline at Petra III (DESY), Notkestrasse 85, 22607 Hamburg, Germany

Resistive switching metal-insulator-metal (MIM) diodes present a promising approach for back-end-of-line (BEOL) integration of embedded nonvolatile memory (NVM) cells in Si integrated circuits. Research in our group focused on TiN/Ti/HfO_2/TiN devices and one-resistor (1R) as well as one-transistor, one-resistor (1T1R) architectures were successfully processed under Si CMOS BEOL conditions. Switching characteristics in sweep as well as pulse mode were electrically investigated to study NVM characteristics (retention, endurance etc.). To unveil the microscopic origin of the switching mechanism, the Ti/HfO_2 interface was studied by nondestructive Hard X-ray Photoelectron Spectroscopy (HAXPES) studies at the recently constructed P09 beamline at Petra III (Hamburg). Results on RRAM cells in as-deposited, ON and OFF, as well as hard breakdown state will be presented.

DS 21.2 Tue 14:00 GER 38

Improvement of dielectric properties of $Sr_xZr_{(1-x)}O_y$ grown by Molecular Beam Deposition and Sputtering — •Matthias Grube[1], Dominik Martin[1], Walter M. Weber[1], Thomas Mikolajick[1,2], Lutz Geelhaar[3], and Henning Riechert[3] — [1]Namlab gGmbH, 01187 Dresden — [2]Lehrstuhl für Nanoelektronische Materialien, TU Dresden, 01062 Dresden — [3]Paul-Drude-Institut für Festkörperelektronik, 10117 Berlin

Following the demand of replacing conventional dielectrics in the semiconductor industry, a material screening for new high-k dielectrics with nanometer-scale thicknesses is required. Among the many investigated potential materials are ZrO_2 as well as laminates and mixtures of ZrO_2 with HfO_2, Ta_2O_5 and Al_2O_3. We concentrated our efforts to the growth and characterisation of ZrO_2 with the admixture of SrO to form $Sr_xZr_{(1-x)}O_y$. We employed the molecular beam deposition technique (MBD) in a co-deposition regime for this purpose. The capability of MBD for high-k material screening was verified by comparison to deposition via sputtering a stoichiometric $SrZrO_3$ target. The investigated test structures were metal-insulator-metal capacitors (MIM) with a TiN bottom electrode on n^{++}-Si substrates. I-V and C-V measurements revealed a k-value of 19 for amorphous $Sr_xZr_{(1-x)}O_y$ grown by either MBD or sputtering. After surpassing a crystallisation temperature of approximately 650°C the k-value increases to 30 while the dielectric changes into a polycrystalline film with a cubic phase. A comparison of MBD and sputtering of ZrO_2 and $Sr_xZr_{(1-x)}O_y$ will be presented in detail.

DS 21.3 Tue 14:15 GER 38

Phase equilibria at Si-HfO_2 and Pt-HfO_2 interfaces from first principles thermodynamics — •Rampi Ramprasad[1] and Hong Zhu[2] — [1]University of Connecticut, Storrs, USA; Fritz-Haber-Institut der MPG, Berlin, Germany — [2]University of Connecticut, Storrs, USA

In this work, two types of interfaces found in the emerging technologically important high-k MOSFETs have been studied. The phase diagrams of Si-HfO_2 and Pt-HfO_2 interfaces as a function of temperature and oxygen pressure have been determined using first principles thermodynamics (FPT), i.e., by combining conventional density functional theory results with thermodynamics [1]. The vibrational and configurational entropic contributions to the free energies of the condensed phases are explicitly included in this treatment. We demonstrate that the predictions of the FPT approach are in quantitative agreement with experiments for the classes of interfaces considered here. In particular, under UHV conditions, we show that FPT methods predict the correct Si-HfO_2 silica-like interface configurations. Likewise, we also show that an interfacial oxygen coverage of 0.5-1.0 monolayer is favored under UHV conditions at the Pt-HfO_2 interface before rapid oxidation of Pt may be expected (for higher oxygen pressures). These results have important implications both for the applicability of FPT methods for the considered classes of interfaces as well as for high-k dielectrics-based electronic devices in which such interfaces are expected.

[1] H. Zhu, C. Tang and R. Ramprasad, Phys. Rev. B, in print (2010).

DS 21.4 Tue 14:30 GER 38

Bottom-up Modeling of the Elastic Properties of Organosilicate Glasses and their Relation to Composition and Network Defects — •Jan M. Knaup[1,2], Han Li[3], Joost J. Vlassak[3], and Efthimios Kaxiras[1,2,3] — [1]Department of Physics, Harvard University, Cambridge MA, USA — [2]EPFL, Lausanne, Suisse — [3]School of Engineering and Applied Sciences, Harvard University, Cambriudge MA, USA

Organosilicate glasses (OSG), also known as SiCOH or carbon-doped oxide are used as low-k inter-metal dielectrics for integrated circuits. The material must fulfill two conflicting requirements: It has to have low density to reduce the dielectric constant and be mechanically stable enough to withstand mechanical stress during subsequent production steps. Experimental advances in improving their mechanical and electrical properties have not yet been theoretically examined at the ab initio level, due to the relatively large model sizes necessary for amorphous materials. We employ the density-functional based tight-binding (DFTB) method to achieve an accurate description of OSG properties at different compositions. We analyze the influence of composition and topological defects on the density and bulk modulus of non-porous OSG. We find that the dependence of density and stiffness on chemical composition is of different nature. This difference is traced to a transition between different mechanisms of elastic deformation in silica glass and in silicon hydrocarbide, which is also the reason for different sensitivity to topological defects in the two materials.

DS 21.5 Tue 14:45 GER 38

Local I-V characteristics of high-k ultra-thin ZrO_2- and $ZrO_2/Al_2O_3/ZrO_2$-films. — •Dominik Martin[1], Matthias Grube[1], Elke Erben[1], Johannes Müller[2], Wenke Weinreich[2], Uwe Schroeder[1], Lutz Geelhaar[3], Walter Weber[1], Thomas Mikolajick[1,4], and Henning Riechert[3] — [1]namlab Gmbh, D-01187 Dresden — [2]Fraunhofer-CNT, D-01099 Dresden — [3]Paul-Drude-Institut für Festkörperelektronik, D-10117 Berlin — [4]Chair of Nanoelectronic Materials, 01062 Dresden, Germany

In order to produce ultra thin ZrO_2-films, with a dielectric constant high enough to satisfy industry demands, it is necessary to reach the tetragonal crystalline phase. This can be achieved either by high temperature deposition or by a post deposition annealing step. Both however induce high leakage currents. Small amounts of Al_2O_3 can be incorporated in ZrO_2 to reduce leakage current. To get more insight into the charge carrier transport mechanisms involved, a thickness series of ultra thin ZrO_2- and $ZrO_2/Al_2O_3/ZrO_2$-films were deposited by ALD and subjected to different rapid thermal annealing processes. These layers were examined by GI-XRD, TEM, I-V-, C-V-Spectroscopy and conductive atomic force microscopy. Thus, leakage currents are reduced to $3.2 \cdot 10^{-8} \frac{A}{cm^2}$ at 1 V while maintaining the high k value (CET=1 nm at 1V for a 10 nm film) . CAFM studies demonstrate how the crystallization effects the charge transport mechanisms on the mesoscopic scale. Local I-V curves acquired on amorphous films and at grain boundaries in nanocrystalline films in yield lower breakdown voltages and higher leakage currents at crystallite grain boundaries.

DS 21.6 Tue 15:00 GER 38

Post-etch cleaning mechanisms at ultra low k surfaces — •Roman Leitsmann[1], Oliver Böhm[1,2], Philipp Plänitz[1], Christian Radehaus[1], Michael Schreiber[2], and Matthias Schaller[3] — [1]GWT-TUD GmbH, Material Calculations, Chemnitz, Germany — [2]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz — [3]Globalfoundries Dresden Module Two GmbH & Co. KG, Germany

The usage of materials with an ultra low dielectric constant is necessary due to the decreasing feature size of integrated circuits, which results in smaller distances between the conduction layers, and hence to an increasing resistance capacitance delay. However, the application of such ultra low k (ULK) materials is connected to several problems.

For example a fluorocarbon film at the ULK-surfaces at the sidewalls of trenches or vias is formed during the etch process. To remove this film a post-etch cleaning procedure have to be applied. In this study we investigate the cleaning efficiency of diluted HF using state of the art density functional theory. In particular different desorption mechanisms of CF-polymer fragments will be discussed in detail.