

## DF 13: Dielectric and ferroelectric thin films and nanostructures III

Time: Thursday 14:00–17:00

Location: EB 107

DF 13.1 Thu 14:00 EB 107

**Current transport mechanism in metal/HfO<sub>2</sub>/metal structures** — ●CHRISTIAN WALCZYK<sup>1</sup>, THOMAS SCHROEDER<sup>1</sup>, CHRISTIAN WENGER<sup>1</sup>, JAROSLAW DABROWSKI<sup>1</sup>, MINDAUGAS LUKOSIUS<sup>1</sup>, SERGEJ PASKO<sup>2</sup>, and CHRISTOPH LOHE<sup>2</sup> — <sup>1</sup>IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany. — <sup>2</sup>AIXTRON AG, Kackertstr. 15-17, 52072 Aachen, Germany.

The metal-insulator-metal (MIM) capacitor integration into BiCMOS technology is governed by the efforts toward increasing the capacitance density, reducing the leakage current density and improving the voltage linearity. In particular, achievement of an acceptable leakage current density in BEOL MIM capacitors is still a challenge. To get around this critical problem, high-k dielectrics have been introduced. Among various candidates, HfO<sub>2</sub> has been investigated due to its high dielectric constant, low leakage current and chemical stability<sup>1</sup>. Despite the considerable efforts for HfO<sub>2</sub>, its current transport mechanism in MIM structures needs further investigations. Based on experimental results of the temperature dependence of the leakage current, we studied the current transport mechanism and energy band diagrams. The leakage current was measured in the temperature range of 200 - 400 K. The slope of an Arrhenius plot yielded activation energies in the range of  $E_a = 0.2$  eV. In particular, we obtained a trap level at  $\phi_{PF} = 0.4$  eV below the HfO<sub>2</sub> conduction band which contributes to Poole-Frenkel conduction.

[1] M. Houssa et al., Materials Science and Engineering R51, (2006).

DF 13.2 Thu 14:20 EB 107

**Characterisation of thin tantalum oxide films** — ●KATRIN BRUDER<sup>1</sup>, ACHIM WALTER HASSEL<sup>1</sup>, and DETLEF DIESING<sup>2</sup> — <sup>1</sup>Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf — <sup>2</sup>Institut für physikalische Chemie, Universität Duisburg-Essen, 45141 Essen

Metal-Insulator-Metal (MIM, consisting of tantalum– anodic tantalum oxide–platinum) contacts were investigated by means of IV characteristics and impedance spectroscopy. With impedance spectroscopy it is possible to determine the capacitance, the metals resistivities and the tunnel resistance. The latter one is a function of the bias voltage, while the capacitance and metals resistivities remain constant. The tunnel resistivity was found to have a maximum at a bias  $U_{max}$  slightly different from 0 V. This shift was investigated as a function of the film thickness ( $d = 4$  nm to 12 nm) and the temperature in the range from  $T = 58$  K to 350 K. The measurements were compared to simulations. These simulations show, that for an explanation of this shift, asymmetrical barriers and tunneling through the valence band has to be considered.

DF 13.3 Thu 14:40 EB 107

**Hyperfeinwechselwirkung in dünnen Schichten von HfO<sub>2</sub>** — ●MICHAEL STEFFENS<sup>1</sup>, REINER VIANDEN<sup>1</sup> und ANDRE STESMANS<sup>2</sup> — <sup>1</sup>Helmholtz - Institut für Strahlen- und Kernphysik, Nußallee 14-16, 53115 Bonn, Germany — <sup>2</sup>Dept. of Physics, Celestijnenlaan 200D, 3001 Leuven, Belgium

Das „high- $\kappa$ “-Dielektrikum HfO<sub>2</sub> soll als Nachfolger von SiO<sub>2</sub> als Gate-Oxid in MOSFET-Strukturen eingesetzt werden. In dieser Technologie gefertigte Chips haben bereits Marktreife erreicht. Durch diesen Übergang wird der Weg für eine weitere zukünftige Leistungssteigerung im Sinne des Mooreschen Gesetzes ermöglicht. Zwar wurde HfO<sub>2</sub> in den vergangenen Jahren intensiv studiert, vollständig verstanden sind seine Eigenschaften jedoch nicht.

Die Hyperfeinwechselwirkung des Hf in 100 nm dünnen Schichten HfO<sub>2</sub> wurde mit der gestörten  $\gamma$ - $\gamma$ -Winkelkorrelation (PAC) untersucht. Die PAC eignet sich besonders für die Bestimmung der lokalen Umgebung eines Sondenkerns im Material. Die PAC-Sonde <sup>181</sup>Hf wird durch Neutronenaktivierung des natürlich in den Proben vorkommenden <sup>180</sup>Hf erzeugt. Die Filmproben sind mit ALCVD und MOCVD auf einem einkristallinen (100)Si-Substrat gewachsen.

An verschiedenen thermisch behandelten Proben wurden PAC-Messungen durchgeführt. Die Ergebnisse eines isochronen Aushilfprogramms und temperaturabhängiger Messungen werden gezeigt und im Vergleich zum Verhalten von gleichbehandeltem reinem HfO<sub>2</sub> diskutiert. Schwerpunkt ist dabei die Kristallstruktur der Schichten und ihr Verhalten unter Temperatureinflüssen.

DF 13.4 Thu 15:00 EB 107

**Atomic vapour deposition of Sr-Ta-O films for MIM applications** — ●MINDAUGAS LUKOSIUS<sup>1</sup>, CHRISTIAN WENGER<sup>1</sup>, SERGEJ PASKO<sup>2</sup>, IOAN COSTINA<sup>1</sup>, JAROSLAW DABROWSKI<sup>1</sup>, ROLAND SORGE<sup>1</sup>, HANS-JOACHIM MÜSSIG<sup>1</sup>, and CHRISTOPH LOHE<sup>2</sup> — <sup>1</sup>IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — <sup>2</sup>AIXTRON AG, Kackertstr. 15-17, 52072 Aachen, Germany

Metal-Insulator-Metal (MIM) capacitors are widely used in ICs for Radio-Frequency (RF) applications. Advanced RF-technologies require further reduction in feature size combined with several significant materials challenges: according to the International Roadmap for Semiconductors for wireless communication technologies, the capacitance density should be higher than 5 fF/\*m<sup>2</sup>, capacitance variation and leakage current should be minimized and quality factor should be maximized [1]. These requirements imply the replacement of silicon oxide-based dielectrics with new high-k materials. Sr-Ta-O thin films are of interest for applications as high-k dielectric in MIM capacitors in CMOS back-end of line (BEOL) due to their high permittivity.

Depositions of strontium tantalate films were performed by Atomic Vapor Deposition (AVD) technique. We observed that the process pressure has a considerable influence on the stoichiometry of the deposited Sr-Ta-O films as well as on some electrical properties.

[1] RF and Analog/Mixed-Signal Technologies for Wireless Communications, ITRS (Semiconductor Industry Association, Palo Alto 2006 update ).

DF 13.5 Thu 15:20 EB 107

**Surface preparation of TiN electrodes for subsequent HfO<sub>2</sub>-based high-k dielectrics deposition.** — ●PETER DUDEK, GRZEGORZ LUPINA, THOMAS SCHROEDER, and HANS-JOACHIM MUESSIG — IHP-Microelectronics, Im Technologiepark 25, 15236 Frankfurt (Oder) / Germany

High-k dielectrics combined with compatible metal electrodes are significant material research approaches to scale down dynamic random access memories (DRAM). Accordingly, TiN-based electrodes require strict control of the surface chemistry to avoid the presence of performance limiting interfacials<sup>1</sup>. Recent studies show an interfacial layer present on the TiN electrode forming TiN/TiON<sub>x</sub>/TiO<sub>2</sub> materials stack. Different etching methods for interface removal have been applied and characterised by x-ray photoelectron spectroscopy (XPS) and atomic force microscopy (AFM). Direct comparison of high-k dielectric properties on treated and as-deposited TiN electrode is the objective of research.

[1] Schroeder et al. J.Appl.Phys. 102, (2007).

DF 13.6 Thu 15:40 EB 107

**Growth of HfO<sub>x</sub> thin films by reactive molecular beam epitaxy** — ●ERWIN HILDEBRANDT, JOSE KURIAN, and LAMBERT ALFF — Institut für Materialwissenschaft, TU Darmstadt

Thin films of hafnium oxide were grown on single crystal *r*-cut and *c*-cut sapphire by reactive molecular beam epitaxy. The conditions for the growth of single oriented hafnium oxide thin films have been established. Hafnium oxide thin films were characterized by x-ray diffraction and optical absorption measurements. It was found that hafnium oxide thin films grown on *r*-cut sapphire were (001) oriented whereas, on *c*-cut sapphire, hafnium oxide films showed different orientations depending on the growth temperature and oxidation conditions. The hafnium oxide films grown at higher temperature and under strong oxidation conditions yielded (001) oriented films on *c*-cut sapphire whereas slightly weaker oxidation condition leads to (111) oriented hafnium oxide films. The bandgap deduced from optical absorption measurement carried out on hafnium oxide films grown under optimized conditions agreed well with the values reported in literature. A range of oxygen deficient thin films of hafnium oxide were also grown on single crystal sapphire substrates in order to investigate the effect of oxygen vacancies on dielectric properties of hafnium oxide. The oxygen deficient thin films of hafnium oxide show a decrease in bandgap with increase in oxygen deficiency.

DF 13.7 Thu 16:00 EB 107

**Investigation of (SrO)<sub>x</sub>(ZrO<sub>2</sub>)<sub>(1-x)</sub> high-k dielectrics deposited by molecular beam deposition** — ●MATTHIAS GRUBE<sup>1</sup>,

OLIVER BIERWAGEN<sup>2</sup>, DOMINIK MARTIN<sup>1</sup>, LUTZ GEELHAAR<sup>2</sup>, and HENNING RIECHERT<sup>2</sup> — <sup>1</sup>namlab gGmbH, D-01187 Dresden — <sup>2</sup>Qimonda, D-81730 Munich

Thin high-k dielectrics will be essential for metal-insulator-metal capacitors in future dynamic random access memory. Focused on this necessity, we investigated thin amorphous films of  $\text{ZrO}_2$  and  $(\text{SrO})_x(\text{ZrO}_2)_{(1-x)}$  grown by molecular beam deposition. As substrates, we used  $\text{n}^{++}$ -Si-wafers which were covered with a pre-deposited 5 nm-thin TiN layer. Current-voltage and capacitance-voltage measurements were performed to determine the electrical properties of the dielectrics.

The  $\text{ZrO}_2$  films were grown by three different methods, either in ultra-high vacuum or with an additional supply of  $\text{O}_2$ , and employing either Zr or  $\text{ZrO}$  targets. A k-value of 23 - 28 was extracted from a thickness-series, which is consistent with the value for amorphous  $\text{ZrO}_2$ .

$(\text{SrO})_x(\text{ZrO}_2)_{(1-x)}$  was grown by co-evaporating SrO and  $\text{ZrO}_2$ . For as-grown films with  $x \approx 0.6$ , a k-value of about 6 was extracted. This is significantly lower than the tabulated value. Preliminary experiments for  $x \approx 0.4$  indicate a more reasonable value of  $k \approx 20$ . In addition, post-deposition annealing experiments were performed, which improved the properties of the films. Their density was increased, and their capacitance equivalent thickness was reduced to 50% and less.

DF 13.8 Thu 16:20 EB 107

**Computer-simulated Fullerene-based dielectric materials: Ways to improve the properties of the generated ultralow-k structures** — ●KOSTYANTYN ZAGORODNIY, HELMUT HERMANN, and MANFRED TAUT — Leibniz Institute for Solid State and Materials Research, IFW Dresden, PF 270116, D-01171 Dresden, Germany

Insulating low-k dielectric materials are needed to minimize crosstalk between metal interconnects in microelectronic products. The continuous shrinking of device dimensions of ultra-large-scale integrated (ULSI) chips imposes strong demands on the backend of the line (BEoL) interconnect structures. The International Technology Roadmap for Semiconductors (ITRS) indicates that the k values need

to be reduced to 2.0 for the 45 nm technology node or below in the next few years. Additionally to extremely low dielectric constants, new insulating materials must have also suitable mechanical properties. We have recently proposed the model for new ultralow-k dielectrics as an ordered three-dimensional network consisting of two components: C60 Fullerenes as nodes and bridge molecules as edges connecting the nodes. In the present work we analyze the generated structures in order to improve mechanical and electronic properties. Substituting of the bridge molecules and varying the ways of connecting them to the C60 molecule the mechanical and electronic properties of the model can be affected. Classical and quantum-chemical methods are used to optimize the structures and to calculate its properties. Possible improvements and the limitations are discussed.

DF 13.9 Thu 16:40 EB 107

**Molecular Beam Epitaxy of crystalline oxides on Si for C-MOS and for the monolithic integration of semiconductors on Silicon** — ●GUILLAUME SAINT-GIRONS<sup>1</sup>, CLÉMENT MERCKLING<sup>1</sup>, MARIO EL-KAZZI<sup>1</sup>, LOIC BECERRA<sup>1</sup>, PHILIPPE REGRENY<sup>1</sup>, GILLES PATRIARCHE<sup>2</sup>, LUDOVIC LARGEAU<sup>2</sup>, VINCENT FAVRE-NICOLIN<sup>1</sup>, and GUY HOLLINGER<sup>3</sup> — <sup>1</sup>INL/UMR5270, site ECL, 36 av. Guy de Colongue, 69134 Ecully cedex, France — <sup>2</sup>LPN-UPR20/CNRS, Route de Nozay, 91460 Marcoussis, France — <sup>3</sup>CEA/DRFMC/SP2M, 17 rue des Martyrs 38054 Grenoble and UJF, BP53, 38041 Grenoble cedex 9, France

In this contribution, a detailed description of the growth mechanisms and structural properties of high-k  $\text{Al}_2\text{O}_3$ ,  $\text{Gd}_2\text{O}_3$  and amorphous  $\text{LaAlO}_3$  on Si will be presented. On the basis of these studies, relevant oxide/Si systems will be proposed that fulfill the requirements of future C-MOS systems. In particular, very promising electrical characteristics have been obtained showing that the (amorphous  $\text{LaAlO}_3$ )/Si system is compatible with ITRS recommendations in terms of EOT and leakage current. Moreover, it will also be shown that InP/oxide heterointerfaces present a quasi-ideal compliant behavior that opens the way to the monolithic integration of III-V heterostructures on Si for advanced micro and optoelectronic applications.