Functional Thin Films and Surfaces
Room Pacific F-G - Session C2-1-ThA

Thin Films for Electronic Devices I

Moderators: Dr. Julien Keraudy, Oerlikon Balzers, Oerlikon Surface Solution AG, Liechtenstein, **Dr. Jörg Patscheider**, Evatec AG, Switzerland

1:20pm **C2-1-ThA-1 An Imperfect High k Dielectric (O Vacancies, Contamination) Can Give a Perfect MIM Device*, Christophe Vallee, N. Tokranova, K. Beckmann,*** SUNY College of Nanoscale Science and Engineering, USA*; N. Cady,* SUNY college of Nanoscale Science and Engineering, USA **INVITED**

The reduction of high k dielectric thicknesses below 10 nm gives rises to new potential application of these materials due to unexpected "resistance switching"which is a phenomenon by which some electrical insulators display a change of resistance upon application of a dc bias voltage.Increasing the voltage across an insulator inevitably leads to breakdown, which corresponds to an abrupt resistance decrease. In some circumstances, it is possible to restore a high value of resistance by applying a voltage of opposite polarity. Switching between a low and high resistance state can be repeated by voltage sweeping, leading to a hysteresis loop in the current-voltage (I-V) characteristic. Resistance switching is observed in a variety of metal oxides thin films. In recent years this phenomenon has attracted interest for the fabrication of memory devices ("resistive memory") and for the fabrication of voltage-controlled resistors ("memristors"). At present, physical mechanisms at the origin of resistance switching are based on field-enhanced electrode diffusion into the oxide (in that case the devices are named "conductive bridging memories" or CBRAM) and voltage-controlled creation and annihilation of oxygen vacancies (named "OXRAM" devices).

Within this presentation we will discuss the use of high k dielectrics and their fabrication for metal-insulator-metal (MIM) devices such as linear MIM capacitors, resistive memories, and MIM diodes. We will also discuss the use of resistive switching for neuromorphic computing and compute-in-memory applications, and the integration of resistive memory devices with CMOS. Whatever the device, due to the very small thickness of the high k dielectric, it seems obvious that the electrode materials as well as the interfaces between the insulator and the metal electrodes must be optimized. But more importantly, we will try to elucidate how impurities (like contamination from precursors used for the deposition process) and defects (O vacancies) can be intentionally added to improve the device properties. Ultimately, optimization of device performance is paramount for adoption of these devices for advanced, highly efficient computing hardware.

2:00pm **C2-1-ThA-3 Optoelectronic and Thermoelectric Properties of New Heterobilayers of Janus-Type Noble-Metal Chalcogenides Materials*, Mourad Boujnah,*** CINVESTAV-Unidad Queretaro, Mexico

Janus and non-Janus monolayers are one of the transformations of the 2D materials viz present an exceptional opportunity to control and manipulate their physical properties. Herein, we predict the two-dimensional of noble-Metal Chalcogenides (NMCs) materials A_2B (A = Ag, Au and B = S, Se) heterobilayes (HtBLs) through first-principles calculations. The Ab initio molecular dynamics simulations demonstrate that these monolayers possess excellent dynamic and mechanical stabilities. According to that, a combination of Janus and non-Janus of NMCs monolayers (MLs) and HtBLs. High optical absorption of around 4.5×10^5 cm^{-1} and high anisotropic carrier mobility of ~10^5 cm^2 $V^{-1}s^{-1}$ is observed, which indicates that they may shine in the next generation of electronic and optoelectronic devices. All of these explorations not only enhance the types of 2D materials but also provide a structural reference for designing new MLs on the molecular level. The band gap values of αand βphases calculated at the HSE06 level are between 1.35 and 3.70 eV.The calculated lattice thermal conductivity of Ag_2S (about 0.85 W $m^{-1}K^{-1}$) is low while the electrical conductivities and Seebeck coefficients are high at room temperature. Thus, the properties of these combinations show a high potential for thermoelectric applications.

2:20pm **C2-1-ThA-4 High-Entropy Ba(Ti,Zr,Ta,Hf,Mo)(on)$_3$ Gate Dielectric Films for Zno-Channel Thin Film Transistors*, Van Dung Nguyen,*** Department of Materials Science and Engineering, National Cheng Kung University (NCKU), Taiwan, Viet Nam*; K. Chang,* Department of Materials Science and Engineering, National Cheng Kung University (NCKU), Taiwan

In this study, high entropy Ba(Ti,Zr,Ta,Hf,Mo)(ON)$_3$dielectric films were fabricated on an ITO/glass substrate via a combinatorial sputtering technique. Favorable compositions were efficiently determined from a wide range of the Ba(Ti,Zr,Ta,Hf,Mo)(ON)$_3$ space. The high entropy oxynitride (HEON) was then incorporated in a metal-insulator-metal (MIM) stack and thin film transistor to investigate dielectric and electrical performance. HEON exhibits high dielectric constant and low dielectric loss, which is promising for MIM and TFT applications. HEON-based TFTs show excellent performance with a high on/off current ratio of 10^8, low threshold voltage (V_T) of 0.14 V, a low subthreshold swing of 0.08 V×dec^{-1} and interfacial defect (D_{it}) of 7 × 10^{10} eV×cm^{-2}. Moreover, the devices exhibited stable performance with small V_T shifts and negligible changes in the maximum drain current under gate bias stress (GBS). HEON-based TFTs outperformed various reported thin film transistors, indicating the great promise of Ba(Ti,Zr,Ta,Hf,Mo)(ON)$_3$ as a dielectric layer in thin film transistors.

2:40pm **C2-1-ThA-5 Hydrothermal Fabrication of The Heterojunction of $BaTiO_3$ Nanorod Arrays with Ag_2O and their Applications*, Yen-Lun Chiu,*** *K. Chang,* National Cheng Kung University (NCKU), Taiwan

$BaTiO_3$ (BTO) is an attractive material because of its excellent piezoelectric characteristics. The property can be tailored through morphology control, specifically in the form of nanoparticles or one-dimensional nanorod and nanowire arrays. However, studies on this topic directly through hydrothermal processes for the fabrication of three-element compounds are still lacking. In this study, the nanocomposite, which combined well-aligned BTO nanorod arrays and Ag_2O nanoparticles, were synthesized through a single or two-step hydrothermal reaction by the addition of various surfactants e.g., polyethylene glycol-400 (PEG-400). To study the morphology effect on the junction, hydrothermal parameters, including concentrations of precursor solutions, reaction time, temperatures, different surfactants, and substrate positions in an autoclave, were manipulated. X-ray diffraction and scanning electron microscopy were employed to determine the phase and morphology of the resultant composite samples. In addition, an atomic force microscope was employed to determine the topography of the samples, and the amplitude of the piezoresponse (d_{33}) was measured through a piezoresponse force microscope. The morphology effect on the piezoelectricity and the optoelectronics of the samples was systemically studied and optimized for related applications.

3:00pm **C2-1-ThA-6 Toughening Mechanisms of Al Nanoparticles in Flexible Mo Thin Films Revealed by in-Situ Synchrotron Diffraction Experiments*, Barbara Putz,*** *T. Edwards,* Empa, Swiss Federal Laboratories for Materials Science and Technology, Thun, Switzerland*; P. Kreiml,* Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria*; E. Huszar, L. Pethö,* Empa, Swiss Federal Laboratories for Materials Science and Technology, Thun, Switzerland*; D. Többens,* Helmholtz Zentrum Berlin, Germany*; J. Michler,* Empa, Swiss Federal Laboratories for Materials Science and Technology, Thun, Switzerland

The combination of a nanoparticle gas phase condensation source with physical vapour deposition opens up plentiful potential for the fabrication of unique nanocomposite thin films, as it allows incorporation of nanoparticles with tailored size, shape, distribution and volume density without precipitation-related restrictions concerning phase diagrams and solubility. In this work, we use combined magnetron sputtering and nanoparticle (NP) deposition to fabricate Mo thin films (200 nm thickness) with and without incorporated Al NPs (diameter 50 nm) on flexible polymer substrates. Microstructure, NP size and concentrations of our nanocomposites were characterized by cross-sectional scanning (SEM) and transmission electron microscopy (TEM). Pure Mo layers are frequently used as part of the metallization of flexible thin film transistors; however they suffer from inherently brittle electro-mechanical behaviour, with through-thickness cracks forming at very low applied strains. To study deformation mechanisms as a function of Al nanoparticle concentration and test the hypothesis that ductile nanoparticles incorporated into the brittle matrix can introduce toughening effects such as crack deflection, arrest or bridging, the electro-mechanical behaviour of the nanocomposites and pure Mo reference films was studied with X-ray diffraction and four point probe resistance measurements during polymer-supported in-situ tensile experiments. Results indicate a clear toughening of Mo thin films with increasing amounts of incorporated Al nanoparticles, as revealed by the shape of the film stress curves recorded parallel and perpendicular to the loading direction. The less severe degradation of electrical conductivity during straining indicates that the nanoparticles limit the extend of mechanical failure of the Mo matrix. Combined with post-mortem focused ion beam (FIB) and SEM analyses of tensile induced cracks, this shed further light on the role of Al nanoparticles during crack initiation and propagation. In summary, the novel manufacturing approach and resulting nanocomposites are promising candidates for multifunctional thin films in next-generation electronic devices.

3:20pm **C2-1-ThA-7 Fabrication of 5g sub-6 Ghz Antennas on Polyimide Substrates Using Laser Thermo-Responsive Polymer Silver Nanocatalysts***, Y. Chen, J. You,* National Defense University, Republic of China*; M. Youh,* Ming Chi University of Technology, Taiwan, Republic of China*; C. Lee, T. Chiang,* ***Chang-Pin Chang****, M. Ger,* National Defense University, Republic of China

In the study, laser-activated nanosilver catalyst inks were used to fabricate copper-selective metal patterns for sub-5G-6 GHz antennas. The activity of the catalyst ink can be performed by laser activation treatment. Electroless plating was performed on catalytically active polyimide substrates used to form metallic antenna patterns. PEI-GA was synthesized from polyethyleneimine (PEI) and Glutaraldehyde (GA), followed by a heat-curable Ag composite ink composed of Ag salt and tert-butyl peroxybenzoate (TBPB) to enhance the adhesion between the Cu coating and the PI substrate. After laser activation of the lacquer ink and continuous copper chemical deposition on PI, a layer of copper with good adhesion will be formed on the PI substrate. Copper patterns can be easily prepared by combining laser direct patterning of lacquer inks and electroless copper deposition. This is a way to quickly obtain the best metallic wire patterns on polyimide substrates for fabricating sub-6 GHz antennas for 5G. FTIR-ATR analysis and characterization of monomer and polymer functional group changes before and after cross-linking, and verification of substrate metallization by SEM, EDS, and Cross-cut tester were performed. The laser direct writing process is fast and easy to apply and is expected to replace the existing printed circuit process in the future. The produced metallic wires can also be used in 5G antennas. There is great potential for development in the market. A convincing method and potential solution can be given in this study.

3:40pm **C2-1-ThA-8 Metal-Semiconductor Amorphous Boron Carbide Contacts***,* ***Vojislav Medic****, N. Ianno,* University of Nebraska - Lincoln, USA

The development of amorphous hydrogenated boron carbide (BC) devices is an increasingly important research topic due to its application in radiation safety and deep space exploration. To improve the device performance research has been conducted in optimization of BC, its fabrication and through it, its electronic properties. However, to our knowledge, a study of metal-semiconductor amorphous boron carbide contacts has not been performed. In addition to understanding and quantifying the effect of contact resistance on device performance, it is important to differentiate metals that form Schottky or Ohmic contacts with BC. The spreading resistance model is used to quantify BC resistivity and metal-BC contact resistance. As the thickness of the deposited BC film is much smaller than the radius of the metal contact area, spreading resistance is linearly dependent on film thickness.

$R_s=\rho*b/(\pi a^2)$

b – film thickness, a – contact radius, ρ – resistivity of BC

Since the total resistance can be calculated from Ohmic measurements, the equation below shows the linear dependence of total resistance on BC thickness.

$R=\rho*b/(\pi a^2)+2*Rc$

R_c – contact resistance on each side of BC films

The linear equation for total resistance can be extrapolated to b=0 from the respective I-V curves of various thickness BC films with identical metal contacts, yielding twice the contact resistance. Once R_c is determined ρ can be calculated from any I-V curve.The I-V curves are collected from varying thickness BC films deposited via PECVD from orthocarborane/Ar or metacarborane/Ar gas mixtures, on a plane of metal with the constant size metal dot top contact deposited in a subsequent step. This effectively forms a BC resistor (Figure 1). Specific metals can be categorized as Schottky or Ohmic type contacts by observing the I-V curve measurements. Figure 2 shows the data collected for Cr contacts and Ti contacts on n-type BC. Both of those metals form a Schottky contact, which results in two diodes in series when a completed device is made. However, in Figure 3 Cr contacts on p-type BC structures show an Ohmic contact, and the resistance of this structure can be analyzed using the spreading resistance model previously discussed.As BC deposited from orthocarborane or metacarobrane polymeric precursors is p-type or n-type respectively, we plan to study how different metals from the same groups in the periodic table interact with either p-type or n-type BC, whether they produce Schottky contacts or Ohmic contacts, with the goal of quantifying losses that occur at the metal-BC junction due to contact resistance.

4:00pm **C2-1-ThA-9 Modifying Oxidation State Distribution in Interfacial Layer of Ge Nmosfet with Pre- or Post- Remote Plasma Oxidation Treatment***,* ***Pei-Hsiu Hsu****,* National Tsing Hua University, Taiwan*; D. Ruan,* Fuzhou University, China*; K. Chang-Liao,* National Tsing Hua University, Taiwan

In this research, the effect of pre- or post- remote plasma oxidation treatment on interfacial layer (IL) of germanium (Ge) n-type metal oxide semiconductor field effect transistor (nMOSFET) has been discussed in detail. The pre-remote plasma oxidation treatment, which is similar with traditional post IL oxidation annealing, might reduce the unstable oxidation state in the IL. However, the remaining plasma damage may still enlarge surface roughness and induce high gate leakage current. On the other hand, the post-remote plasma oxidation treatment can effectively passivate the oxygen vacancy with well-bonded oxygen atom, instead of a post high-k deposition annealing process. Nevertheless, it seems that IL quality might not be further improved by the post high-k oxidation treatment. After analyzing X-ray photoelectron spectroscopy and electrical characteristics, it is found that the Ge nMOSFETS with pre-remote plasma oxidation treatment exhibits low subthreshold swing and high on-off current ratio. It may provide an important reference for high performance Ge device fabrication.

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