Electronic Materials and Processing
Room: 314 - Session EM+MI+NS-MoM

Complex Oxides and Their Interfaces
Moderator: Jessica Hilton, Mantis Deposition, Lisa M. Porter, Carnegie Mellon University

8:20am **EM+MI+NS-MoM1 Emergent Phenomena at Complex Oxide Interfaces**, ***Susanne Stemmer***, University of California at Santa Barbara **INVITED**

Two-dimensional electron gases (2DEGs) at interfaces between two insulating oxides have attracted significant attention because they can exhibit unique properties, such as strong electron correlations, superconductivity, and magnetism. In this presentation, we will discuss properties arising from strong electron correlations in narrow quantum wells of the band insulator $SrTiO_3$, sandwiched between Mott insulating rare earth titanates, $SmTiO_3$ and $GdTiO_3$, respectively. These quantum wells exhibit very high sheet electron high-densities, of approximately 1 electron per planar unit cell of the quantum well. We demonstrate electron correlation effects due to short-range Coulomb interactions, including mass enhancement, interface-induced magnetism in the electron gas, and a transition to a correlated insulator at the lowest thickness in quantum wells bound by ferrimagnetic $GdTiO_3$. We show that the metal-insulator transition is coupled with the sudden onset of structural distortions in the quantum well. In contrast, quantum wells bound by antiferromagnetic $SmTiO_3$ exhibit almost no structural distortions, incipient antiferromagnetism, no metal-insulator transition, and non-Fermi liquid behavior. We will discuss the implications of the results in the context of two-dimensional electron correlation physics.

This work was performed in collaboration with Clayton Jackson, Pouya Moetakef, Jack Zhang, Jinwoo Hwang, Leon Balents, and Jim Allen.

9:00am **EM+MI+NS-MoM3 Atomic and Electronic Structure of the Ferroelectric $BaTiO_3$-Ge (001) Interface**, ***Kurt Fredrickson***, The University of Texas at Austin, *P. Ponath, A.B. Posadas,* University of Texas at Austin, *M.R. McCartney, T. Aoki, D.J. Smith,* Arizona State University, *A.A. Demkov*, University of Texas at Austin

In this study, we demonstrate the epitaxial growth of $BaTiO_3$ on Ge(001) by molecular beam epitaxy using a thin Zintl template buffer layer. A combination of density functional theory, atomic-resolution electron microscopy and *in situ* photoemission spectroscopy is used to investigate the electronic properties and atomic structure of the $BaTiO_3$/Ge interface. Aberration-corrected scanning transmission electron micrographs reveal that the Ge(001) 2x1 surface reconstruction remains intact during the subsequent $BaTiO_3$ growth, thereby enabling a choice to be made between several theoretically predicted interface structures. The measured valence band offset of 2.7 eV matches well with the theoretical value of 2.5 eV based on the model structure for an in-plane-polarized interface. The agreement between the calculated and measured band offsets, which is highly sensitive to the detailed atomic arrangement, indicates that the most likely $BaTiO_3$/Ge(001) interface structure has been identified.

9:20am **EM+MI+NS-MoM4 Strain-Controlled Stochiometry Variations in $CaMnO_3$ Epitaxial Thin Films**, ***Rajeswari Kolagani***, *G. Yong, Z. Warecki, C. Stumpf, D. Schaefer, P. Sharma, C. Hart, A. Burger*, Towson University

$CaMnO_3$ is a material of interest for application in novel energy technologies such as thermoelectric power generation, and as a photo catalyst for hydrogen energy storage. We are currently investigating the properties of epitaxial thin films of $CaMnO_3$ (CMO) and its electron doped derivatives towards tuning material properties that enable these applications. Oxygen stoichiometry and its effect on structural and electronic properties are key variables in optimizing thin films of these materials. We will present our studies of CMO thin films grown epitaxially by Pulsed Laser Deposition on several compatible oxide substrates with varying degrees of tensile and compressive lattice mismatch. Lattice mismatch results in the distortion of the unit cell symmetry from cubic to tetragonal. In hole-doped rare earth manganites such as $La_{0.7}CaMnO_3$, tensile as well as compressive lattice mismatch strain is known to cause a suppression of the insulator-metal transition, leading to an increase in electrical resistivity. In contrast, our studies of the structural and electrical properties of CMO thin films indicate that tensile strain causes a pronounced decrease in the electrical resistivity. The strained films have an expanded out of plane lattice parameter which is consistent with reduced oxygen stoichiometry. These results indicate that the tensile strain causes CMO thin films to be more susceptible to the formation of oxygen vacancies, thus reducing electrical resistivity. This is in agreement with recent theoretical predictions correlating strain and oxygen vacancies, where tensile strain induced in-plane expansion of the unit cell is shown to favor oxygen deficiency. The potential for employing lattice mismatch strain for tuning film composition has important implications for technological applications. We will present our detailed investigations of the correlation of strain and oxygen stoichiometry in $CaMnO_{3-d}$ andrelated manganite compositions, employing high resolution X-ray diffraction, temperature dependent resistivity measurements, and characterization of the film surface morphology using atomic force microscopy.

9:40am **EM+MI+NS-MoM5 Controlling Complex Oxide Chemistry to Enable Advanced Dielectric, Ferroelectric, and Electronic Applications**, ***Lane Martin***, University of California, Berkeley **INVITED**

Current and next-generation advanced functional materials are testing our ability to produce high-quality, complex materials with ever increasing precision. Particular interest has been given to candidate complex oxide materials which present a diverse range of material properties and functionality not easily produced in other classes of materials. The ultimate integration and utilization of these materials, however, will require that we can carefully and deterministically balance the intrinsic phenomena of interest in these materials with a knowledge of the potential extrinsic effects that can arise form defects which result from our inability to produce these complex materials with the precision we desire. This is made more challenging by the fact that these complex oxide systems are prone to and can accommodate large densities of point defects through a range of internal compensation mechanisms. In this presentation, we will explore the interrelationship between the complex oxide growth process, the chemical nature of these complex materials, the resulting structure and strain evolution, and the ultimate effect on properties in a range of prototypical complex oxide materials. We will explore these interrelationships in model systems including the classic dielectric materials $SrTiO_3$ and $LaAlO_3$, highly-controlled heterointerfaces that exhibit exotic physics including the $LaAlO_3/SrTiO_3$ system, and ferroic systems such as $BaTiO_3$ and others. In this context, we will demonstrate routes by which we can deterministically utilize the tendency for these materials to form point defects to enhance epitaxial thin film strain, developing new modalities of strain control of thin-film materials that go beyond traditional lattice mismatch effects, and how the combination of epitaxial strain and defects in materials can be used to enhance performance, independently tune susceptibilities, and provide new insights into the nature of these complex materials. For instance, in $BaTiO_3$ we will illustrate how one can couple epitaxial strain to defect structures to provide an additional out-of-plane strain component that can dramatically enhance ordering temperatures and will explore the use of compositionally-graded heterostructures to further extend what can be done with epitaxial strain to manipulate dielectric, ferroelectric, and electronic properties of materials.

10:40am **EM+MI+NS-MoM8 Monolithic Integration of Epitaxial $BaTiO_3$ on Si and SiGe for Ferroelectric Devices**, *L. Mazet, R. Bachelet, G. Saint-Girons,* Institut des Nanotechnologies de Lyon (INL) - CNRS - ECL, France, *D. Albertini, B. Gautier,* Institut des Nanotechnologies de Lyon (INL) - CNRS - INSA de Lyon, France, *M.M. Frank, J. Jordan-Sweet, I. Lauer, V. Narayanan,* IBM T.J. Watson Research Center, *M. Hytch, S. Schamm-Chardon,* CEMES - CNRS - Université de Toulouse, France, ***Catherine Dubourdieu***, Institut des Nanotechnologies de Lyon (INL) - CNRS - ECL, France **INVITED**

Ferroelectric oxides integrated on a semiconductor substrate are of particular interest for various applications such as memory or logic devices, electro-optic devices or as piezoelectric materials for sensors and actuators. Among the ferroelectric compounds, $BaTiO_3$ is an attractive candidate for large-scale applications compared to Pb- or Bi-based oxides. It is a well-known perovskite largely studied for its dielectric, piezoelectric and ferroelectric properties.

In this talk, I will briefly review the challenges associated with the monolithic integration of crystalline complex oxides on a semiconductor and more particularly with the integration of ferroelectrics. Molecular Beam Epitaxy (MBE) provides unique advantages to precisely construct, almost atom by atom, the oxide/semiconductor interface.

I will then present an experimental work on the epitaxy of $BaTiO_3$ thin films (1.2 - 20 nm) on silicon and $Si_{1-x}Ge_x$ substrates. Films are grown by MBE, in the thickness range of 1.2-20 nm. Different growth conditions such as temperature and oxygen pressure are explored to optimize the $BaTiO_3$ film quality and to minimize the SiO_2 interfacial layer regrowth between Si and the $SrTiO_3$ buffer layer. The surface quality is monitored *in-situ* by reflection high-energy electron diffraction (RHEED) and *ex-situ* by X-ray

reflectometry (XRR) and atomic force microscopy (AFM). The crystalline structure is studied by conventional and synchrotron X-ray diffraction. It is also investigated at the nanoscale using advanced transmission electron microscopy techniques. Strain maps determined with high precision (0.05%), 5 nm spatial resolution and with a large field of view (1 μm) using dark field electron holography will be discussed for selected samples. The crystalline domain orientations (*c*- versus *a*-domains) will be discussed with respect to the growth conditions and thickness. The ferroelectric properties are investigated by piezoresponse force microscopy (PFM). Ferroelectric films are obtained in optimized conditions that will be discussed. Ultrathin films of few monolayers are investigated to determine the onset of ferroelectricity.

I will conclude with ongoing perspectives on the integration of such heterostructures in new field-effect devices for low power logic applications.

11:20am **EM+MI+NS-MoM10 The Surface Study of Hexagonal $LuFeO_3$ Multiferroic Thin Films**, ***Shi Cao***, *X.S. Xu, T. Paudel, E.Y. Tsymbal, P.A. Dowben*, University of Nebraska-Lincoln

The surface properties of hexagonal $LuFeO_3$ thin film have been studied by ultra-high vacuum based characterization technologies such as X-ray/ultra-violet photoemission spectroscopy (XPS/UPS), inverse photoemission spectroscopy (IPES) and XMCD-PEEM. Hexagonal $LuFeO_3$ is a stable multiferroic at room temperature with potential magneto-electric properties. The application of this material in voltage controlled magnetic devices depends very significantly on the interface composition and interface magnetism. The angle resolved XPS shows the possible iron-rich termination and the oxygen deficiency due to the sensitivity of the surface to the of sample preparation methods. The combined UPS and IPES allow us to infer that this multiferroic oxide, $LuFeO_3$, has a band gap about 2.35eV. All these characterizations are consistent with the density function theory calculations of the surface and bulk band structure.

11:40am **EM+MI+NS-MoM11 Integration of Ferroelectric Perovskites on Ge(001) by ALD: A Case Study of $BaTiO_3$**, ***Thong Ngo***, *M.D. McDaniel, S.N. Chopra, J.G. Ekerdt, A.B. Posadas, A.A. Demkov*, The University of Texas at Austin

Gemanium, which exhibits higher hole and electron mobilities than silicon, might become a candidate to replace silicon as a channel material in a field effect transistor (FET) beyond the 3D FET generation. Unlike Si, when the high-κ dielectrics are integrated on Ge, the chemical instability of GeO_2 is an advantage. Moreover, the instability of GeO_2 also enables epitaxial functional oxides on Ge. Crystalline perovskites can be high-κ insulating, with many also being ferromagnetic, ferroelectric, multiferroic, or superconducting. This wide range of properties, combined with possibilities for lattice match to Ge(001), allows for multi-functional oxides to be engineered on Ge(001).

Epitaxial integration of ferroelectric barium titanate, $BaTiO_3$ (BTO), on Ge has attracted much attention due to the low lattice mismatch between Ge(001) and BTO (0.25% above Curie temperature, T_c = 120 °C). The efforts to epitaxially integrate ferroelectric BTO on Ge(001) have been demonstrated using molecular beam epitaxy (MBE) by several groups. However, for device manufacturing applications, atomic layer deposition (ALD) has advantages over MBE due to its high step coverage, significantly low thermal budget, scalability, and low cost.

We demonstrate an all-chemical route to epitaxially integrate BTO directly on Ge(001). Amorphous BTO films were grown on the 2×1 reconstructed, clean Ge(001) surface at 225 °C using ALD. Barium bis(triisopropylcyclopentadienyl), titanium tetraisopropoxide, and water were employed as co-reactants. The films become highly crystalline after a vacuum anneal at 600–700 °C. In-situ x-ray photoelectron spectroscopy confirms the stoichiometry of the BTO films with no detectable GeOx formation or carbon incorporation. In-situ reflection high energy electron diffraction (RHEED) shows high order of BTO film crystallinity after vacuum annealing. X-ray diffraction (XRD) is used to determine the crystallinity and the orientation of BTO films. Electrical characterization, including capacitance-voltage, leakage current, interface trap density, and piezoresponse force microscopy measurements will also be performed to explore the high-κ insulating and ferroelectric properties of BTO films on Ge(001). The integration of BTO films on Ge(001) by ALD is a promising method for fabricating a ferroelectric FET at production scale.

Authors Index

Bold page numbers indicate the presenter