Electronic Materials and Devices
Room 321/322 - Session EM-WeM

Multifunctional Electronic Materials
Moderator: C.J. Palmstrom, University of Minnesota

8:20am **EM-WeM1 Peter Mark Memorial Award Address: Epitaxial Complex Oxide Heterostructures: Electrostatic Modulation of Correlated Electron Behavior**, *C.H. Ahn*[1], Yale University **INVITED**
Complex oxide materials exhibit a tremendous diversity of behavior, including phenomena that have only been observed in oxides, such as high temperature superconductivity. An even richer spectrum of possibilities becomes available if one combines different complex oxides in epitaxial thin film form to create artificially structured, heterogeneous systems. One can use such materials to electrostatically modulate correlated electron behavior, including superconductivity and magnetism, without introducing chemical or structural disorder. It is also possible to combine complex oxides, such as ferroelectrics, with semiconductors to explore new functionality in semiconducting systems.

9:00am **EM-WeM3 MBE Growth and Properties of Fe-, Cr- and Mn-doped TiO2 Rutile and Anatase**, *S.A. Chambers*, S. Thevuthasan, T. Droubay, S.M. Heald, C.M. Wang, A.S. Lea, V. Shutthanandan, Pacific Northwest National Laboratory; *J. Osterwalder*, University of Zurich, Switzerland; *Y.J. Kim*, Hanbat National University, Korea; *R.P. Sears, B. Taylor, B.S. Sinkovic*, University of Connecticut
Room temperature ferromagnetism in Co-doped anatase TiO_2 has inspired a number of experimental and theoretical efforts. A high Curie point, good electron mobility, and optical transparency are attractive for use in spin electronics and optoelectronics. A natural question concerns the use of other magnetic dopants. Combinatorial doping of anatase and rutile with Sc, V, Cr, Mn, Fe, Ni, Cu using laser ablation by Matsumoto et al. reveal that only Co-doped anatase is ferromagnetic. However, DFT calculations by van Schilfgaarde for Cr, Mn, Fe and Co in anatase predict that Co, Cr and Fe make the material ferromagnetic, whereas Mn is antiferromagnetic. We are currently exploring Fe and Cr as dopants in MBE-grown TiO_2 rutile and anatase, and plan to investigate Mn in the near future. The substrates for rutile and anatase films are rutile $TiO_2(110)$ and $LaAlO_3(001)$, respectively. Films were characterized with RHEED, XPS, XPD, XAS, EXAFS, XMCD, AFM, SAM, TEM and MOKE. Cr and Mn are more likely to substitute for Ti in rutile than Fe because CrO_2 and MnO_2 exhibit rutile structures that are reasonably well lattice matched to TiO_2. No such phase exists for Fe. Moreover, CrO_2 is a half-metallic ferromagnet in the bulk. Cr indeed substitutes for Ti in the rutile lattice, and assumes a +3 formal oxidation state for doping levels of a few atomic percent. The first films have been found to be antiferromagnetic. In contrast, attempting to dope rutile with Fe leads to secondary phase Fe_3O_4. Fe (II) and Fe(III) are present, as expected if Fe_3O_4 is present. In addition, these films exhibit magnetic hysteresis and circular dichroism, but these signals are presumably due to the presence of minority phase Fe_3O_4. Cr exhibits a +3 oxidation state and substitutes for Ti for doping levels of a few atomic percent in anatase. Magnetic measurements of these films are pending at the time of writing of the abstract.

9:20am **EM-WeM4 Unusual Behavior of Electrical Conductivity and Thermopower Found in $Mn_{1.68-X}Cu_{.6+X+Y+Z}Co_{.24-Y}Ni_{.48-Z}O_4$ Thin Films**, *F.S. Ohuchi*, J.G. Moyer, D.A. Kukuruznyak, M.S. Prowse, University of Washington
The thermopower, S, and electrical conductivity, σ, are measured on variations of a reference composition, $Mn_{1.68-X}Cu_{.6+X+Y+Z}Co_{.24-Y}Ni_{.48-Z}O_4$. Doped compositions show parallel increases or decreases in conductivity and thermopower magnitude unlike typical band-gap conducting materials. This is desirable for increasing the efficiency parameter called the power factor, $S^2\sigma$, for thermoelectric applications. While thermopower varies by as much as 30%, the conductivity changes by up to a factor of four in the compositions explored. Conduction is attributed to small polaron hopping between neighboring Mn ions. Thin films are obtained through Metal Organic Decomposition processing. This is a low-temperature fabrication route that allows for the retention of meta-stable

Mn^{4+} and Cu^{1+} ions that are essential to favorable electronic behavior. Compositional variations modify the Mn^{3+}, Mn^{4+}, Cu^{1+}, and Cu^{2+} concentrations, and in turn change the conductivity and thermopower. Supplemental XPS work defines changes in Cu oxidation states and oxygen content, and thermopower data provides Mn oxidation state information. Using the Heikes and Nernst-Einstein transport models we explain the seemingly incongruent behavior in thermopower and conductivity and identify that the discrepancy occurs in the conductivity factor. The nature of the unusual conduction behavior will be discussed.

9:40am **EM-WeM5 Using Strain to Control Microwave Tunability and Loss in Barium Strontium Titanate Thin Films**, *S.W. Kirchoefer*, W. Chang, J.A. Bellotti, J.M. Pond, Naval Research Laboratory; *D.G. Schlom*, Pennsylvania State University **INVITED**
Barium strontium titanate thin films exhibit an electric field dependent dielectric constant which can be exploited for tunable microwave devices. This technology has been of limited applicability due to the relatively high dielectric losses that typically accompany high tuning. The control of dielectric loss is of critical technological importance. Manipulation of deposition conditions and film impurities have been investigated widely as means for achieving improved films. Engineered film strain is an additional material parameter that can be controlled toward these ends, and this talk will report on experiments that demonstrate the advantages of both strain minimization and strain enhancement on the microwave properties of barium strontium titanate and strontium titanate thin films. It will be shown that the structural distortion caused by film strain results in decreased dielectric constant and tuning for compressive strain and increased corresponding values for tensional strain at room temperature. These results can be understood by examining the effects of lattice distortion on Curie temperature. A model based on thermodynamics and strain-induced polarization will be presented. The effects of strain on dielectric losses and device quality factor will also be discussed. Results from substrate mismatch strain and film annealing studies will be presented. Ongoing efforts to measure effects of extrinsic strain induced by externally-applied pressure will be discussed.

10:20am **EM-WeM7 Displacive Phase Transition in $SrTiO_3$ Thin Films Grown on Si(001)**, *F.S. Aguirre-Tostado*, CINVESTAV-Querétaro, México, Mexico; *A. Herrera-Gómez*, CINVESTAV-Querétaro, México; *J.C. Woicik*, National Institute of Standards and Technology; *R. Droopad, Z. Yu*, Motorola; *D.G. Schlom*, Pennsylvania State University; *J. Karapetrova, P. Zschack*, University of Illinois and Argonne National Lab; *P. Pianetta*, Stanford Synchrotron Radiation Laboratory
Polarization dependent x-ray absorption fine structure and x-ray diffraction have been used to study the local structure in $SrTiO_3$ thin films grown epitaxially on Si(001). For films less than a critical thickness of ~ 80 Å, a splitting of the Ti-O distance perpendicular to the interface is observed: $r_{Ti-O} = 1.87 \pm 0.02$ Å and $r_{Ti-O} = 2.09 \pm 0.06$ Å, whereas only a single Ti-O distance is observed within the plane of the interface: $r_{Ti-O} = 1.95 \pm 0.01$ Å. These findings indicate that the in-plane compressive strain imposed on the $SrTiO_3$ layer by the Si substrate results in a tetragonal plus displacive ferroelectric distortion of the $SrTiO_3$ cubic unit cell. This study therefore suggests the existence of a Curie "thickness" for strained-layer, epitaxial perovskite growth.

10:40am **EM-WeM8 Dielectric Response of Asymmetric $KNbO_3/KTaO_3$ Superlattices**, *J. Sigman*, H.J. Bae, D.P. Norton, University of Florida; *J.D. Budai, P.H. Fleming, L.A. Boatner*, Oak Ridge National Laboratory
The $K(Ta,Nb)O_3$ perovskite is an interesting paraelectric/ferroelectric system with tunability of the dielectric response with applied electric field. Pulsed laser deposition (PLD) has been used to achieve atomic layer-by-layer growth in $KTaO_3/KNbO_3$ superlattices. Previously, a symmetric 1 unit cell x 1 unit cell $KTaO_3/KNbO_3$ was grown on $KTaO_3(100)$ and its dielectric response and structural properties were studied. Increasing capacitance with increasing applied dc bias for temperatures just below the structural transition was observed and suggested an anitiferroelectric response. We have investigated several asymmetric $KTaO_3/KNbO_3$ superlattices to provide further elucidation on this anomalous dielectric response. This positive tunability appears to be a function on the thickness the $KNbO_3$ layer. Above three unit cells of $KNbO_3$, the positive tunability disappears. Below three unit cells of $KNbO_3$, the

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[1] **Peter Mark Memorial Award Winner**

positive tunability is seen in the same temperature region as the 1 x 1 superlattice, regardless of the Nb:Ta thickness ratio.

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