Monday Morning, November 9, 2009

Thin Film

Room: B3 - Session TF1-MoM

Thin Films: Growth and Characterization I

Moderator: S. Gupta, University of Alabama

8:40am TF1-MoM2 Photoluminescence Properties of SrAl₂O₄:Eu²⁺,Dy³⁺ Thin Phosphor Films Grown by Pulsed Laser Deposition, *O.M. Ntwaeaborwa*, *P.D. Nsimama*, *H.C. Swart*, University of the Free State, South Africa

Thin films of SrAl₂O₄:Eu²⁺,Dy³⁺ phosphor were grown on silicon substrates using a 248 nm KrF pulsed laser to evaluate the effects of different processing parameters on photoluminescence properties of the phosphor. The processing parameters which were varied during the films growth include temperature, pressure, and the number of pulses. X-ray diffraction (XRD), scanning electron microscopy (SEM) and atomic force microscopy (AFM) were used to examine the structure, particle morphology and surface topography of the films. The chemical composition and thicknesses of the films were determined by Rutherford backscattering spectroscopy (RBS). Photoluminescence spectra of the films recorded by the Cary Eclipse spectrophotometer were characterized by major green phosphorescent emission with a maximum at ~520 nm and minor red emission with a maximum at 630 nm. The green and red photoluminescence at 520 and 630 nm are associated with the $4f^65d \rightarrow 4f^7(^8S_{7/2})$ and $^5D_0-^7F_2$ transitions of Eu²⁴ and residual Eu³⁺ ions respectively. The effects of processing parameters on the PL intensity and the possible mechanism of the green phosphorescence were discussed

9:00am TF1-MoM3 Multifunctional Double Perovskite Thin Films and Heterostructures, A. Gupta, The University of Alabama INVITED A double perovskite is a perovskite with the general formula of $A_2BB'O_{6}$, where A is a divalent alkaline earth cation and B and B' are transition-metal ions. Depending on the relative size and oxidation state, the B and B' ions can be crystallographically completely ordered, making up a rocksalt-type lattice. La₂NiMnO₆ is an ordered double perovskite that is a ferromagnetic semiconductor with a $T_{\rm CM}$ of 280 K. Recent studies of La₂NiMnO₆ in the bulk have revealed large magnetic-field induced changes in the resistivity and dielectric properties at temperatures as high as 280 K [1,2]. This is a much higher temperature than previously observed for such a coupling between the magnetic, electric, and dielectric properties in a ferromagnetic semiconductor. Substitution at the A site can also lead to multiferroic behavior in the double perovskites. Azuma et al. have succeeded in synthesizing the 'designed' compound Bi₂NiMnO₆ in the bulk under high pressure and established its multiferroic properties, with ferroelectric and ferromagnetic transition temperatures of 485 K and 140 K, respectively [3]. We have synthesized epitaxial thin films of La₂NiMnO₆ [4], Bi₂NiMnO₆ [5], and their heterostructures using the pulsed laser deposition (PLD) technique. A related ferromagnetic semiconductor, La₂CoMnO₆, has also been epitaxially stabilized [6]. High quality epitaxial films of these double perovskites are grown on lattice-matched substrates such as SrTiO₃, NdGaO₃ and LaAlO₃. We have structurally characterized the double perovskite films using a variety of techniques. Additionally, the magnetic, electrical and magnetodielectric properties of the thin films and heterostructures have been studied in detail.

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[2] H. Das, U. V. Waghmare, T. Saha-Dasgupta, and D. D. Sarma, Phys. Rev. Lett. 100, 186402 (2008).

[3] M. Azuma, K. Tanaka, T. Saito, S. Ishiwata, Y. Shimakawa, and M. Takano, J. Am. Chem. Soc. **127**, 8889 (2005).

[4] H. Guo, J. Burgess, S. Street, A. Gupta, T. G. Calvarese, and M. A. Subramanian, Appl. Phys. Lett. 89, 022509 (2006).

[5] P. Padhan, P. LeClair, A. Gupta, and G. Srinivasan, J. Phys.: Condens. Matter 20, 355003 (2008).

[6] H. Z. Guo, A. Gupta, T. G. Calvarese, and M. A. Subramanian, Appl. Phys. Lett. **89**, 262503 (2006).

9:40am TF1-MoM5 Influence of Nanostructure on Charge Transport in RuO₂ Thin Films, *M.M. Steeves*, *R.J. Lad*, University of Maine

Ruthenium dioxide exhibits metallic electrical conductivity, and may have both electron and hole contributions to its charge transport. In this study, polycrystalline thin films of RuO₂ were grown on fused quartz substrates by RF reactive magnetron sputtering, and a parametric study was carried out to probe the influence of film nanostructure on the four-point Van der Pauw resistivity and Hall coefficient. The films were grown via reactive RF magnetron sputtering of a Ru target in an Ar/O₂ plasma using a range of deposition rates and with substrate temperatures ranging from 20-500°C. A wide variety of nanostructures and film textures were obtained as determined by high resolution x-ray diffraction for film thicknesses ranging from 40-180 nm as measured by x-ray reflectivity and profilometry. The films exhibited strains of the order of 0.5% and average crystallite sizes ranging from 20-70 nm. Room temperature resistivities varied between 200-400 $\mu\Omega$ cm and showed a relatively weak dependence on temperature. Hall coefficients ranged from +200 to -200 x10⁻⁵ cm³/C as a function of temperature, depending on exact nanostructure as well as the heating environment. The observation of both positive and negative Hall coefficients for different RuO₂ films is in contrast to the reported single crystal value of $-11 \times 10^{-5} \text{ cm}^3/\text{C}$ for which electrons are the majority carrier. Correlations between nanostructure and transport properties are given in terms of grain size, strain, film defects, and mobility of the majority carriers.

10:00am TF1-MoM6 Electrical and Structural Properties of Ultrathin Polycrystalline and Epitaxial TiN Films Grown by Reactive dc Magnetron Sputtering, F. Magnus, A.S. Ingason, S. Olafsson, J.T. Gudmundsson, University of Iceland

Ultrathin TiN films were grown by reactive dc magnetron sputtering on amorphous SiO₂ substrates and single-crystalline MgO substrates at various growth temperatures. The resistance of the films was monitored in-situ during growth to determine the coalescence and continuity thicknesses. TiN films grown on SiO₂ at 600°C are polycrystalline and have nominal coalescence and continuity thicknesses of 8 Å and 19 Å, respectively. TiN films grow epitaxially on the MgO substrates at 600°C. The nominal coalescence thickness is 2 Å and the thickness where the film becomes continuous cannot be resolved from the coalescence thickness. X-ray reflection measurements indicate a significantly higher density and lower roughness of the epitaxial TiN films.

10:40am **TF1-MoM8** Cubic and Wurtzite Sc_{1-x}Al_xN Solid Solutions Grown by Reactive Magnetron Sputter Epitaxy onto ScN (111) and AlN(0001) Seed Layers, C. Höglund, Linköping University, Sweden, J. Bareño, Argonne National Laboratory, J. Birch, B. Alling, Linköping University, Sweden, Z. Czigány, Hungarian Academy of Sciences, Hungary, L. Hultman, Linköping University, Sweden

Reactive magnetron sputter epitaxy was used to grow thin solid films of Sc1. $_{x}Al_{x}N$ ($0 \le x \le 1$) onto ScN(111) and AlN(0001) seed layers at substrate temperatures of 600°C and 800°C, respectively. The films were analyzed by Rutherford backscattering spectroscopy (RBS), elastic recoil detection analysis (ERDA), x-ray diffraction (XRD) and transmission electron microscopy (TEM). RBS and ERDA showed that stoichiometric films were obtained in the entire composition range (molar fractions x = 0, 0.14, 0.29, 0.51, 0.73, 0.90, 1.0) using elemental Sc and Al targets and N₂ as the reactive gas. TEM and XRD show that rocksalt structure (c) Sc_{1-x}Al_xN(111) solid solutions can be epitaxially grown onto the isostructural c-ScN(111) seed layers with AlN molar fractions up to $x \sim 0.6$, whereafter the system phase separates into c- and wurtzite structure (w) Sc1-xAlxN. Upon phase separation, the w-domains are present in three different orientations relative to the seed layer, namely $Sc_{1-x}Al_xN(0001) \parallel ScN(111)$ with $Sc_{1-x}Al_xN[-12-$ 10] \parallel ScN[1-10], Sc_{1-x}Al_xN(10-11) \parallel ScN(111) with Sc_{1-x}Al_xN[-12-10] \parallel ScN[1-10], and Sc_{1-x}Al_xN(10-11) || ScN(113). When growth was performed onto w-AlN(0001) seed layers, epitaxial w-Sc1-xAlxN(0001) with AlN molar fractions x in the range ~0.50 to 1.00 were obtained. For AlN molar fractions of 0.28 and less, the film formed an epitaxial c-Sc_{1-x}Al_xN(111) phase with double position domains.

The lattice parameter for the c-Sc_{1-x}Al_xN films closely followed the values predicted by first principles density functional theory calculations, only slightly deviating from Vegard's law. On the contrary, the lattice parameters of the w-Sc_{1-x}Al_xN varied considerably less than predicted. Our calculated mixing enthalpies of c-, w-, and zinc blende Sc_{0.50}Al_{0.50}N solid solutions predict that the alloy is metastable with respect to phase separation for all temperatures below the melting points of AlN and ScN.

11:00am **TF1-MoM9** Process Control of Vanadium Oxide Thin Films Grown by Pulsed-dc Reactive Sputtering for Microbolometer Applications, C. Venkatasubramanian, W.R. Drawl, S.S.N. Bharadwaja, M.W. Horn, S. Ashok, The Pennsylvania State University

Low resistivity thin films of vanadium oxide with high temperature coefficient of resistance (TCR) are currently used as the imaging layer in uncooled infrared imaging. However, process control remains an issue because the films are formed under oxygen-starved conditions. In this

paper, the influence of cathode current (target current) hysteresis on the properties of pulsed-dc reactive sputtered vanadium oxide thin films is investigated. VO_x thin films were sputter deposited from a vanadium metal target under different Ar/O ratios. The gas flow rates and oxygen partial pressures were varied systematically, and the corresponding changes in the cathode current were monitored. Increasing the gas flow rate from 10 sccm to 100 sccm caused the cathode current to decrease by ~25%, but on reversing the flow rate, the cathode current did not go back up along the same curve, instead exhibiting a hysteretic behavior. A similar trend was observed for the change in oxygen partial pressure between 0 and 20% as well. The width and position of the hysteresis curve depends on the relative values of the gas flow rates and the oxygen partial pressures. VO_x thin films deposited at various points along the hysteresis curve were evaluated using four-probe resistivity measurements over a wide temperature range. The room temperature resistivity of the films varied by more than six orders of magnitude and was found to have a progressive dependence on the cathode current. Structural characterizations such as X-ray diffraction and transmission electron microscopy studies indicated that the microstructure changes gradually from nano-crystallite to amorphous nature with the increase in total gas flow rate and/or oxygen partial pressure.

11:20am **TF1-MoM10** Compositional and Structural Evolution of Sputtered Ti-Al-N, *P.H. Mayrhofer*, *L. Chen*, *M. Moser*, Montanuniversitaet Leoben, Austria, *Y. Du*, Central South University, China

The compositional and structural evolution of Ti-Al-N thin films as a function of the total working gas pressure (p_T) , the N₂-to-total pressure ratio (p_{N2}/p_T) , the substrate-to-target distance (ST), the substrate position, the magnetron power current (I_m) , the externally applied magnetic field, and the energy and the ion-to-metal flux ratio of the ion bombardment during reactive sputtering of a Ti0.5Al0.5 target is investigated in detail. Based on this variation we propose that the different poisoning state of the Ti and Al particles of the powder-metallurgically prepared Ti0.5Al0.5 target in addition to scattering and angular losses of the sputter flux cause a significant modification in the Al/Ti ratio of the deposited thin films ranging from ~ 1.05 to 2.15. The compositional variation induces a corresponding structural modification between single-phase cubic, mixed cubic-hexagonal and single-phase hexagonal. However, the maximum Al content for singlephase cubic Ti1-xAlxN strongly depends on the deposition conditions and was obtained with x = 0.66, for the coating deposited at 500 °C, $p_T = 0.4$ Pa, ST = 85 mm, and $p_{\rm N2}/p_{\rm T}$ = 17%. Our results show, that in particular, the N₂to-total pressure ratio in combination with the sputtering power density of the Ti_{0.5}Al_{0.5} compound target has a pronounced effect on the Al/Ti ratio and the structure development of the coatings prepared.

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