Tuesday Morning, November 5, 2002

Magnetic Interfaces and Nanostructures
Room: C-205 - Session MI+EL+SC-TuM

Ferromagnetic Semiconductors
Moderator: B.T. Jonker, Naval Research Laboratory

8:20am **MI+EL+SC-TuM1 ab initio Magnetic Exchange Interactions in DMS and TiO_2**, ***M. van Schilfgaarde***, Arizona State University **INVITED**

The electronic structure of TM-doped TiO2 is studied within the ab initio local spin-density approximation and compared to more traditional TM-doped III-V DMS semiconductors. The conduction band of TiO2 consists mainly of Ti d character. Substituting a 3d TM for Ti, localized levels split off the conduction band; they are spin-split by an on-site exchange interaction and are responsible for the magnetism. The deepest level is of t2 symmetry and sweeps deeper in the gap in the series TM=V,Cr,Mn,Fe,Co. In the dilute alloy, the impurity level broadens into a narrow band. Thus the conductivity is expected to occur through a hopping mechanism, increasing with decreasing temperature as is observed in Co:TiO2. The character of this level is compared to TM d levels in the III-V DMS alloys (Cr,Mn,Fe):(Al,Ga,In)(N,P,As). Using a linear-response technique, the LSDA is mapped analytically onto a magnetic hamiltonian, which was used to investigate exchange interactions in random TM:TiO2 and (Cr,Mn):(Al,Ga,In)(N,P,As) alloys. Several novel phenomena will be described in the DMS case; for example Tc is predicted to increase monotonically with concentration for Cr:III-V, while for Mn:III-V Tc reaches a maximum at about 10% Mn concentration. The exchange interactions are found to have elements in common with both the carrier-mediated model and the double exchange/superexchange model, but also show important differences. For (V,Cr,Mn,Fe,Co):TiO2, the filling, magnetic moment and exchange interactions change systematically and are well described by a double exchange/superexchange model. However, for Tc to reach the observed RT in Co:TiO2, a source of holes is needed.

9:00am **MI+EL+SC-TuM3 $Co_xTi_{1-x}O_2$ Anatase Heteroepitaxy on Si(001)**, ***T. Droubay***, Pacific Northwest National Laboratory, *A.C. Tuan*, University of Washington, *S.A. Chambers*, Pacific Northwest National Laboratory

With a Curie temperature above 700K, high remanence, and respectable coercivity, Co-doped TiO_2 anatase ($Co_xTi_{1-x}O_2$) is one of the more magnetically robust dilute magnetic semiconductor (DMS) materials currently under investigation. The future of this material for near-term device use as a spin injector requires deposition on and compatibility with traditional semiconductors such as silicon. Successful growth of crystalline oxides on silicon without oxidizing the underlying substrate is a formidable challenge. Our goal in this work is to grow epitaxial $Co_xTi_{1-x}O_2$ on Si(001) by using a suitable template layer, and then determine the resulting magnetic and electronic properties. We have previously shown that polycrystalline $Co_xTi_{1-x}O_2$ grown on Si(001) with its native oxide is ferromagnetic at room temperature. We are now working on $Co_xTi_{1-x}O_2$ heteroepitaxy on Si(001) using an ultrathin epitaxial $SrTiO_3$ buffer layer to prevent formation of titanium silicide and SiO_2 at the interface that result from a thermodynamic instability. An added benefit of the $SrTiO_3$ buffer layer is to generate a nearly zero conduction band offset to Si, which is essential for efficient n-type spin injection. A detailed analysis of the growth and properties of this heteroepitaxial system will be presented.

9:20am **MI+EL+SC-TuM4 Epitaxial Growth and Properties of Co-doped TiO_2 Anatase on $LaAlO_3$(001)**, ***S.A. Chambers***, *T. Droubay, C.M. Wang, S.M. Heald, S. Thevuthasan, A.S. Lea, C.F. Windisch, Jr.*, Pacific Northwest National Laboratory, *R.F.C. Farrow, L. Folks, J.-U. Thiele, M.G. Samant, R.F. Marks*, IBM Almaden Research Center

We are investigating Co-doped TiO_2 anatase heteroepitaxy on $LaAlO_3$(001) by oxygen plasma assisted molecular beam epitaxy. This material is of considerable interest because it is ferromagnetic well above room temperature. Thus, it may be a useful DMS for spintronics. The use of a higher growth rate (0.04 nm/sec) results in the nucleation of nanocrystals of rutile, the more stable form of TiO_2, within the continuous anatase film. The density of rutile nanocrytals increases as the quality of the substrate surface decreases. A lower growth rate (0.01 nm/sec) results in a much better film morphology, although a low density of smaller nanocrystals remains. Unlike the fast-grown films, these films show no evidence for any phase other than anatase. A number of techniques reveal that Co substitutes for Ti in the lattice and exhibits a +2 oxidation state; there is no evidence for elemental Co in any form. Each Co(II) substitution for Ti(IV) requires an O^{2-} anion vacancy in order to maintain charge neutrality, and evidence for such a vacancy is forthcoming from preliminary Co K-shell EXAFS. Such vacancies do not generate free carriers because they are uncharged. Hall effect and XPS measurements show that the films are n-type, the most likely cause being the presence of O atom vacancies that form during growth. These vacancies are independent of the presence of Co, and are negatively charged, thereby providing a source of free electrons from shallow donor states. The magnetization depends critically on free carrier concentration, as expected for a DMS. The exact Curie temperature is currently being determined, but appears to be in excess of 700K.

9:40am **MI+EL+SC-TuM5 Ferromagnetism in Mn-implanted Single Crystal Oxides**, ***D.P. Norton***, *S.J. Pearton, B.S. Jeong, Y.W. Heo, A.F. Hebard, N.A. Theodoropoulou*, University of Florida, *L.A. Boatner*, Oak Ridge National Laboratory, *Y.D. Park*, Seoul National University, Korea, *R.G. Wilson*, Consultant

Several semiconducting oxides, including ZnO, offer significant potential in providing spin-based functionality. Theoretical predictions suggest that room-temperature carrier-mediated ferromagnetism should be possible in Mn-doped p-type ZnO. In this paper, we report on the synthesis and properties of magnetically-doped semiconducting oxides, including ZnO. While previous efforts report no ferromagnetism in Mn-doped ZnO that is n-type due to group III impurities (consistent with theory), we find ferromagnetism in n-type ZnO that is co-doped with Mn and Sn. Hysteresis was observed in magnetization versus field curves for Mn-implanted n-type ZnO:Sn. Differences in zero field-cooled and field-cooled magnetizations persists up to ~ 150 K for Sn-doped ZnO crystals implanted with 3 at % Mn. These results indicate that ZnO doped with Mn and Sn may prove promising as a ferromagnetic semiconductor for spintronics.

10:00am **MI+EL+SC-TuM6 Self-compensation in Manganese-doped Ferromagnetic Semiconductors**, ***S.C. Erwin***, *A.G. Petukhov*, Naval Research Laboratory

We present theoretical evidence that the observed hole compensation in manganese-doped ferromagnetic semiconductors is due to interstitial manganese. We show that under the non-equilibrium conditions used during growth, interstitial Mn is readily formed near the surface by a simple low-energy adsorption pathway. In GaAs, isolated interstitial Mn impurities are electron donors, each compensating two substitutional Mn acceptors under p-type conditions. We show that partial compensation is a prerequisite for ferromagnetic order below the metal-insulator transition, and that the Curie temperature is highest when 1/6 of the Mn is interstitial.

10:20am **MI+EL+SC-TuM7 Ferromagnetic Semiconductor Heterostructures[1]**, ***N. Samarth***, Penn State University **INVITED**

The molecular beam epitaxy (MBE) of ferromagnetic semiconductor heterostructures provides model systems for exploring fundamental issues in semiconductor spintronics. We provide an overview of heterostructures that combine the ferromagnetic semiconductor (Ga,Mn)As with conventional III-V and II-VI semiconductors, as well as with the metallic ferromagnet MnAs. After an introduction to the properties of MBE-grown (Ga,Mn)As, we discuss two classes of heterostructures: (a) hybrid ferromagnetic metal/semiconductor tunnel junctions that allow us to unambiguously probe spin injection into semiconductors using all-electrical techniques and (b) hybrid ferromagnetic/semiconductor photodiodes that serve as toy spintronic "devices" whose photo-response is magnetically controlled.

[1] This work is carried out in collaboration with S. H. Chun, K. C. Ku, S. J. Potashnik, and P. Schiffer, and is supported by grants from NSF, ONR and DARPA

11:00am **MI+EL+SC-TuM9 Epitaxial Growth of the Diluted Magnetic Semiconductor Cr_xGe_{1-x}**, ***G. Kioseoglou***, *A.T. Hanbicki*, Naval Research Laboratory, *Y.D. Park*, Seoul National University, Korea, *S.C. Erwin, B.T. Jonker*, Naval Research Laboratory

Ferromagnetic semiconductors (FMS) provide an opportunity to control spin-dependent behavior in semiconductor device heterostructures. Although much effort has focused on III-Mn-V materials such as GaMnAs , the mechanism of ferromagnetic order remains unclear; in particular the precise roles played by the dopant and the semiconductor host. We have explored this issue recently by developing a new Group-IV FMS, MnGe.[1] Here we report our work to develop an elemental FMS using a different dopant, Cr-doped Ge. This choice was motivated partly by our density-functional theory (DFT) calculations, which indicate that CrGe and MnGe should have comparable Curie temperatures. We report the epitaxial growth of Cr_xGe_{1-x} and describe the structural, magnetic and transport properties. The samples were grown on GaAs(001) substrates by molecular beam epitaxy at substrate temperatures of 40-500°C and the crystallinity was confirmed by the RHEED pattern. The Cr concentration used was 2-3% as determined from X-ray fluorescence. The RHEED pattern indicates single crystal growth for substrate temperatures above 200°C, with sharp 1x1 streaks. Growth at 40-70°C is initially single crystal, but the pattern becomes increasingly diffuse with film thickness. The samples are strongly p-type, and the hole density varies with the Cr concentration. SQUID measurements were performed on all samples to investigate the magnetic character of the Cr:Ge system. Samples grown at the higher growth temperatures exhibit only paramagnetic order. Co-doping with both Mn and Cr is also investigated. This work was supported by the DARPA SpinS program and ONR.

[1]Y.D. Park, et al., Science 295, 651 (2002).

11:20am **MI+EL+SC-TuM10 Cr-Doped III-V Ferromagnetic Semiconductors**, ***M.E. Overberg***, *G.T. Thaler, R.M. Frazier, C.R. Abernathy, S.J. Pearton, N.A. Theodoropoulou, A.F. Hebard,* University of Florida, *R.G. Wilson,* Private Consultant, *J.M. Zavada*, U.S. Army Research Office

Ferromagnetic semiconductors, consisting of a semiconductor host material doped with transition metal ions, are becoming increasingly prevalent in the literature as a candidate for incorporating the spin degree of freedom into device structures. To date, the vast majority of work in this area has centered on the incorporation of Mn into both II-VI and III-V materials by a variety of techniques. However, recent theoretical work has indicated that Cr may be a more suitable dopant for achieving room-temperature ferromagnetism within these materials.[1] In this paper, we will report on the preparation of GaCrN, GaCrP, and AlGaCrP by the direct implantation of Cr. The magnetic and magneto-transport (anomolous Hall Effect) properties of these films will be quantified both versus implantation dose (x=0.04, 0.06, 0.10) and versus post-implantation annealing, to identify an optimum combination of dose and annealing conditions. Analysis by SQUID magnetometry of the GaCrN with 6% Cr indicates the presence of a strong ferromagnetic phase with a Curie temperature above the 350 K limit of the magnetometer. High resolution x-ray diffraction (HRXRD) and transmission electron microscopy (TEM) results from the implanted films will also be presented to address the issue of the formation of second phases within these materials. HRXRD rocking curves of the implanted materials will also be used to trace the evolution of the implantation-induced lattice damage with annealing as well as strain-related effects due to the incorporation of Cr into substitutional lattice sites.

[1] K. Sato, and H. Katayama-Yoshida, Jap. J. Appl. Phys., Pt. 2, 40 (5B), p. L485 (2001).

11:40am **MI+EL+SC-TuM11 Suppression of Phase Segregation during MBE Growth of GaMnN Using Nitrogen-Hydrogen Plasma**, *Y. Cui*, ***L. Li***, University of Wisconsin-Milwaukee

Epitaxial growth of GaMnN by electron-cyclotron-resonance plasma-assisted molecular beam epitaxy using nitrogen-hydrogen plasma was studied by reflection high-energy electron diffraction, scanning electron microscopy, energy dispersive spectroscopy, and x-ray diffraction. The electron diffraction pattern changed from streaky to spotty when hydrogen was added to the nitrogen plasma, indicating that the effective N/Ga ratio was increased. Films grown with nitrogen plasma are phase segregated into GaN and manganese nitrides. In contrast, when nitrogen-hydrogen plasma was used, the films are single phase Ga1-xMnxN, with x can be as high as 0.06. These results indicate that phase segregation can be suppressed by adding hydrogen to the nitrogen plasma during growth.

Authors Index

Bold page numbers indicate the presenter