Thursday Afternoon, November 6, 2003

Semiconductors
Room 321/322 - Session SC+MI-ThA

Ferromagnetic and Dilute Magnetic Semiconductors

Moderator: S.C. Erwin, Naval Research Laboratory

2:00pm **SC+MI-ThA1 Electronic Structure Theory of Mn-doped GaAs***, A. Zunger,* National Renewable Energy Laboratory*; **P. Mahadevan,*** National Renewable Energy Laboratory, India **INVITED**

(1) Orientation dependent ferromagnetism: Models involving the interaction between the transition metal spin and free carriers have conventionally been used to describe ferromagnetism in dilute magnetic semiconductors. In contrast to the expectations of such a model, we find that the GGA calculated energy of the ferromagnetic state for two 3d transition metal (TM) impurities in GaAs show a strong dependence on the crystallographic orientation of the TM pairs. For Mn in GaAs, the ferromagnetic state is strongly stabilized for pairs in the direction. The stabilization is greatest along the directions for which the p-d hybridization matrix elements coupling the Mn atoms are the largest. (2) Interstitial-substitutional complexes: Examining the formation energy of Mn at various lattice sites, we find that Mn at an interstitial (Mn(i)) site could have comparable energy to Mn at a Ga site (Mn(Ga)). Under epitaxial growth conditions, the solubility of both substitutional and interstitial Mn is strongly enhanced over what is possible under bulk growth conditions. The high solubility opens the possibility of Mn atoms forming small clusters. While isolated Mn(i) are hole killers (donors), and should therefore destroy ferromagnetism, complexes such as Mn(Ga)-Mn(i)-Mn(Ga) are found to be more stable than complexes involving Mn(Ga)-Mn(Ga)-Mn(Ga). The former complexes exhibit partial or total quenching of holes, yet Mn(i) in these complexes provides a channel for a ferromagnetic arrangement of the spins on the two Mn(Ga). This suggests that ferromagnetism in Mn doped GaAs arises both from holes due to isolated Mn(Ga)as well as from strongly Coulomb stabilized Mn(Ga)-Mn(i)-Mn(Ga) clusters.

2:40pm **SC+MI-ThA3 Microscopic Valence Band Structure Near Mn and Local Magnetism in Ga@sub 1-x@Mn@sub x@As***, **J. Tang**, M.E. Flatté,* University of Iowa

The microscopic spin-dependent disturbances to the valence band near Mn atoms in Ga@sub 1-x@Mn@sub x@As and the indirect Mn-Mn interaction are studied. The GaAs host is described by a multiband tight-binding Hamiltonian that incorporates spin-orbit interaction, and the Mn impurity is described by a local p-d hybridization and on-site potential. Local spin-polarized resonances within the valence band that significantly enhance the LDOS near the band edge. The quantitative enhancement we calculate is consistent with angle-resolved photoemission and interband magnetoabsorption measurements. We present the hybridization energy for two parallel Mn magnetic moments. The splitting of the acceptor level is highly anisotropic and exceeds 10 meV even if the Mn impurities are separated by as many as 20 Å. This suggests that scanning tunneling spectroscopy can probe the Mn spin orientation and measure the Mn-Mn interaction energy as a function of distance. This work was supported by the ARO MURI DAAD19-01-1-0541.

3:00pm **SC+MI-ThA4 Cross-sectional STM Study of Mn-doped GaAs****, J.M. Sullivan,*** Naval Research Laboratory*; G.I. Boishin,* Naval Research Laboratory and Nova Research Inc.*; S.C. Erwin, L.J. Whitman, A.T. Hanbicki, B.T. Jonker,* Naval Research Laboratory

When doped with Mn, GaAs exhibits long-range ferromagnetic order at temperatures up to ~150K. It is generally believed that ferromagnetism in GaMnAs is mediated by holes created by the substitution of Mn for Ga. Recent studies have suggested that a substantial amount of Mn is also present at interstitial sites, where Mn acts as a donor, partially compensating the holes and reducing the Curie temperature. To characterize the location and electronic configuration of Mn in device-quality Mn-doped GaAs, we have combined the complementary techniques of cross-sectional scanning tunneling microscopy (XSTM) and density functional theory (DFT). XSTM was used to atomically characterize a GaMnAs film across a single {110} cleavage plane. We used DFT to help interpret our images by theoretically simulating the XSTM image of Mn near the GaAs(110) surface. We considered Mn occurring as substitutionals, interstitials, and substitutional-interstitial complexes; a range of physically plausible charge states was considered for each. Defects in the first four layers near the surface were studied. STM filled-state images were simulated at the level of Tersoff-Hamann theory by integrating the local density of states over an energy window given by the experimental bias voltage. Thus, these complementary techniques allow us to identify Mn-related defects in the GaAs zinc-blende structure. *Supported by the US Office of Naval Research and the Defense Advanced Research Projects Agency.

3:20pm **SC+MI-ThA5 Thin Film Mn/GaAs(100) Interfacial Reactions***, **J.L. Hilton**, B.D. Schultz, C.J. Palmstrom,* University of Minnesota

Although a number of ferromagnetic Mn-based compounds have been epitaxially grown on GaAs, there is a lack of detailed understanding of the interfacial interactions and their effects on spin transport. To date, no detailed Mn/GaAs interfacial reaction studies have been reported. In this study, the interfacial reactions of Mn thin films deposited in-situ on molecular beam epitaxy (MBE)-grown GaAs(100) epilayers are studied. Initial studies involved characterization of ex-situ post-growth anneals of Al(50Å)/Mn(2000Å)/GaAs(100) structures at temperatures of 200, 300, 350, 400, and 500°C for times ranging from 1-30 hours. Prior to annealing, the Mn films on GaAs appear from reflection high-energy electron diffraction and x-ray diffraction (XRD) to be polycrystalline, and Rutherford backscattering (RBS) indicates that no extensive interfacial reactions occur during growth. After annealing at temperatures higher than 200°C, XRD diffraction peaks corresponding to a tetragonal Mn@sub 2@As-like phase and a tetragonal MnGa-like phase are observed. RBS data at both normal and grazing geometries indicate significant Mn-Ga-As reactions occur during anneals in excess of 200°C with the formation of a region with Mn@sub 0.6@Ga@sub 0.2@As@sub 0.2@ composition. Higher temperature anneals result in the dissociation of this region into a MnGa-like region near the sample surface and a Mn@sub 2@As-like region near the GaAs substrate. RBS measurements of the reaction layer thickness for various annealing times at 300°C indicate the interfacial reactions are diffusion controlled. Results from RBS, XRD, and transmission electron microscopy of Al/Mn/GaAs structures will be combined with results from in-situ scanning tunneling microscopy and x-ray photoelectron spectroscopy of 0-20 monolayer Mn coverage studies to determine the nature and behavior of the reactions between Mn, Ga, and As at the metal-semiconductor interface. Supported by ONR, DARPA, and NSF.

3:40pm **SC+MI-ThA6 Cross Sectional Scanning Tunneling Microscopy Studies of Mn Segregation in Ga1-xMnxAs Films***, **J.N. Gleason**, M.E. Hjelmstad, R.S. Goldman, S. Fathpour, S. Ghosh, P.K. Bhattacharya,* University of Michigan

Ga@sub 1-X@Mn@sub X@As is a promising candidate for spintronic applications compatible with conventional GaAs technologies. Theoretical studies have predicted that an increase in disorder of Mn atom positions will lead to a significant increase in the Curie Temperature.@footnote 1@ Therefore, we have investigated the effects of Mn segregation in Ga@sub 1-X@Mn@sub X@As grown by low temperature molecular beam epitaxy using ultra high vacuum cross-sectional scanning tunneling microscopy (XSTM). The heterostructures consist of 10-period superlattices of alternating Ga@sub 1-X@Mn@sub X@As (x=0.5, 2.5 and 5.0%) and Al@sub 0.20@Ga@sub 0.80@As layers, sandwiched between thick p+ GaAs layers. Constant current XSTM images reveal nanometer-sized regions with higher apparent tip height, presumably related to a local increase in the density of states associated with the presence of Mn atoms in Ga@sub 1-X@Mn@sub X@As. In the x=0.5% films, the nanometer-sized bright regions appear relatively dispersed, with ~ 5nm separation. For the x=2.5% and 5% films, agglomeration of the nanometer-sized bright regions is observed, and apparently increases with increasing Mn composition. The apparent Mn clustering does not appear to be affected by the presence of adjacent Al@sub 0.20@Ga@sub 0.80@As superlattices, indicating that any local misfit stress does not act as a sink for Mn accumulation. The apparent Mn clustering is likely due to a long-range attractive potential between Mn atoms, and may be associated with charge carrier screening, similar to earlier GaAs:Zn studies.@footnote 2@ As the Mn composition increases, the free carrier concentration increases, and the screening length decreases. This would in turn lead to a lower self-repulsion of Mn atoms, and an increase in Mn clustering. We will also discuss the effects of annealing on Mn segregation in Ga@sub 1-X@Mn@sub X@As. @FootnoteText@ @footnote 1@M.Berciu et al., Phys. Rev. Lett. 87, 107203 (2001).@footnote 2@P. Ebert et al., Phys. Rev. Lett. 83, 757 (1999).

4:00pm **SC+MI-ThA7 Manipulation of Ferromagnetism by Light in III-V-based Magnetic Alloy Semiconductors and Related Nanostructures***, **H. Munekata,*** Tokyo Institute of Technology, Japan **INVITED**

Because of moderate carrier concentrations (10@super 15@ - 10@super 20@ cm@super -3@), semiconductors and associated hetero- and nanostructures are suitable electronic systems to control both charges and spins by electromagnetic means. Particularly in magnetic semiconductors, manipulation of carrier spins can result in the cooperative and amplified effects through the spin exchange interaction between carrier spin s and local spin S. Those effects would open ways to develop multi-functional devices with low power consumption. One of such precursory demonstrations is the manipulation of magnetism with light in ferromagnetic III-V alloy semiconductors (In,Mn)As and (Ga,Mn)As. In this paper, we discuss the experimental results on (1) photo-generated carrier-induced ferromagnetism in p-(In,Mn)As/GaSb heterostructures, including ultrafast magnetic softening achieved in collaboration with Kono's group in Rice University, (2) collective rotation of ferromagnetically coupled Mn spins and its picosecond spin dynamics in ferromagnetic p-(Ga,Mn)As caused by the illumination with circularly polarized light without a magnetic field (optical spin injection), and (3) light-induced change in magnetic susceptibility at room temperature in GaAs-Fe composite structures, added with the demonstration of optically-controlled micro-cantilevers by Shinji's group of Tokyo Institute of Technology. Works towards room temperature ferromagnetism by other groups will also be reviewed. This work is supported in part by "Semiconductor Nanospintronics (02-)" of the Ministry of Education, Culture, Sports, Science and Technology, Japan.

4:40pm **SC+MI-ThA9 Growth of (Ga,Mn)N: a Diluted Magnetic Semiconductor by Chemical Beam Epitaxy (CBE)**, ***A. Carreno**, C. Boney, A. Bensaoula,* The University of Houston

The GaN material system is a very promising candidate for the realization of electronic devices based on dilute magnetic semiconductor (DMS) films. The incentive behind DMS materials is the potential to form high-density magnetic memory integrated ICs, semiconductor-based magnetic sensors, magneto-optical devices for communications systems, and other spin-based and photonic-based applications. Many reports have indicated that high doping levels of Mn in GaN lead to ferromagnetic materials with Curie temperatures at or above room temperature. To date (Ga,Mn)N has been fabricated by several epitaxial and non-epitaxial techniques. However, to our knowledge, we are the first to report the epitaxial growth of (Ga,Mn)N by CBE. (Ga,Mn)N has been grown on sapphire substrates using TEG, NH3, and solid Mn as precursors. Very smooth GaMnN films exhibiting bright 2D RHEED patterns have been obtained with Mn concentrations between 0.5-2.0% as determined by EPMA and XPS. XPS depth profiling verifies that the Mn is of uniform concentration throughout the films. In addition to RHEED, the CBE chamber employs two Time of Flight Ion Scattering Spectroscopy techniques, Direct Recoil Spectroscopy (DRS) and Mass Spectroscopy of Recoiled Ions (MSRI). These TOF techniques are used as an in-situ, real time analytical process which allows the surface composition information of film components and impurities to be determined as well as analyzing the structural characteristics based on changes in the relative signal levels with azimuthal rotation of the sample. In these ways DRS/MSRI has been used to detect the incorporation of Mn into the GaN matrix during film growth and from azimuthal data extract the surface periodicity which allows construction of surface structure models for GaN and (Ga,Mn)N surfaces. In addition to available Raman and photoluminescence data, characterization of magnetic properties of the (Ga,Mn)N films is currently under way and will be reported.

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