Monday Morning, November 4, 2002

Electronic Materials and Devices
Room: C-107 - Session EL+SC+MI-MoM

Semiconductors
Moderator: A. Rockett, University of Illinois

9:00am **EL+SC+MI-MoM3 Low-temperature Epitaxial Growth of the Wide Bandgap Semiconductor SiCAlN**, ***I.S.T. Tsong***, Arizona State University **INVITED**

Two compounds, SiC and AlN, normally insoluble in each other below 2000C, are synthesized as a single-phase solid solution thin film by molecular beam epitaxy (MBE) at 750C using a unimolecular precursor H3SiCN and Al atoms. The growth of epitaxial SiCAlN films with hexagonal structure takes place on 6H-SiC(0001) and Si(111) substrates. The surface morphology, microstructure, and composition of the films are analyzed by atomic force microscopy (AFM), cross-sectional transmission electron microscopy (XTEM), Rutherford backscattering spectrometry (RBS) and high-resolution electron energy loss spectroscopy (EELS). Two structural models for the hexagonal SiCAlN films are constructed based on first-principles total-energy density functional theory calculations, each showing agreement with experimental XTEM observations. The predicted fundamental bandgap is 3.2 eV for the stoichiometric SiCAlN, in good agreement with photoluminescence (PL) measurements. Bandgap engineering is a distinct possibility by varying the composition of the pseudo-binary (SiC)-(AlN) film.

9:40am **EL+SC+MI-MoM5 Evolution of Structure and Optical Properties of GaAsN Films Grown by Reactive Molecular Beam Epitaxy**, ***M.J. Reason***, *W. Ye, X. Weng, V. Rotberg, R.S. Goldman*, University of Michigan

Narrow gap nitride semiconductor alloys have shown significant promise for a wide range of electronic, optoelectronic and photovoltaic applications. At present, the ultimate limit of nitrogen solubility in GaAs, as well as the effects of growth conditions on stress relaxation and optical properties of narrow gap nitride films are not well understood. In this work, we have examined the evolution of nitrogen incorporation, strain relaxation, and optical properties of GaAsN films grown by solid-source molecular beam epitaxy using an N2-rf plasma source. The samples consisted of 500 nm buffer layers of GaAs grown at 580C and 20 nm layers of GaAs grown at 500C, both using a high arsenic flux; followed by 100-500 nm thick layers of GaAsN grown at 400C using a 10% N2/Ar gas mixture at a 0.15 sccm flow rate, with a variety of arsenic beam equivalent pressures (BEP). The structure and properties of the samples were investigated by reflection high energy electron diffraction (RHEED), multi-beam optical stress sensing (MOSS), high resolution x-ray rocking curves (XRC), nuclear reaction analysis (NRA), atomic force microscopy, and photoluminescence. For all of the arsenic fluxes studied, in-situ RHEED during the GaAsN layer growth reveals a pattern similar to that observed during the growth of the GaAs layers. As the arsenic BEP is increased, MOSS shows that the film stress decreases, indicating a lowering of the apparent nitrogen incorporation into GaAsN. Interestingly, variations in the absolute nitrogen concentrations determined from NRA analysis and a Vegard's law interpretation of XRC suggest significant nitrogen incorporation into interstitial sites. We will discuss the effects of arsenic flux on the stress relaxation and optical properties of a variety of GaAsN and InGaAsN films and heterostructures.

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10:00am **EL+SC+MI-MoM6 Effects of LED Processing Steps on the Surface of Doped GaN Epilayers**, ***K.H.A. Bogart***, *D.D. Koleske, A.A. Allerman, A.J. Fischer, K.W. Fullmer, K.C. Cross, C.C. Mitchell*, Sandia National Laboratories

Gallium nitride (GaN)-based materials are critical for the creation of UV optoelectronic devices such as light-emitting diodes (LEDs). Ohmic contacts with low contact resistivities to p-type ($<1x10^{-3}\Omega cm^2$) and n-type ($<1x10^{-5}\Omega cm^2$) GaN are essential for improving optical device performance. Understanding the characteristics of p- and n-type GaN epitaxial layer surfaces and the interfaces formed with the contact metals is vital for optimization. Fabrication of an LED requires several processing steps including dicing, annealing, surface cleans (to remove native oxides), lithography, metal deposition, and plasma etching. The effects of processing steps on the surface morphology and electrical characteristics of the epitaxial materials and metal contacts have been investigated using scanning probe microscopies and the circular transmission line method (CTLM). One of the first LED processing steps is dicing a 50 mm wafer using photoresist for surface protection, which is later removed with solvents. For p-type GaN ($5x10^{17}cm^3$), AFM analysis showed that the surface roughness nearly doubled after photoresist exposure from an average of 0.24±0.05 nm to 0.50±0.10 nm. The source of the roughness increase was the formation of pits into the surface, ~1 nm in depth. In another LED processing step, n-type GaN is exposed by plasma etching a mesa structure into the p-type GaN overlayer. One half of a wafer with a 1.2µm n-type GaN ($1.7x10^{18}cm^3$) epitaxial film was plasma etched with chlorine-based chemistry. AFM analysis showed that the etched n-type GaN film (RMS=1.11±0.23nm) was not significantly more rough than non-etched n-type GaN film (RMS=1.70±0.59nm). However, after annealing ($500°C/N^2$), the plasma etched film had more Ohmic behavior by (CTLM) than did the non-etched film. More extensive experiments following the GaN epitaxial layers in processing will be presented and effects on contacts discussed.

10:20am **EL+SC+MI-MoM7 Hydrogen Removal Mechanisms from Gallium Nitride**, ***B.D. Thoms***, *Y. Yang, J. Lee*, Georgia State University **INVITED**

The reaction between hydrogen and GaN is important since hydrogen is often present (sometimes in abundance) during growth and processing and since it produces significant effects. For instance, the effect of hydrogen on the efficacy of Mg dopants has been widely reported and both annealing and electron exposures have been used to remove hydrogen. In addition, recombinative desorption of hydrogen is an important part of many dry etching processes. Removal of hydrogen requires both the transport of hydrogen to the surface and desorption from the surface. In this talk, the authors will discuss characterization of surface and subsurface hydrogen on GaN(0001) and its removal by annealing and by electron exposure.

11:00am **EL+SC+MI-MoM9 N-type Diamond Electronics With Nitrogen Doped Ultrananocrystalline Diamond**, ***J.E. Gerbi***, Argonne National Laboratory, *B.W. Alphenaar*, University of Louisville, *O. Auciello*, Argonne National Laboratory, *J. Birrell*, University of Illinois at Urbana-Champaign, *J.A. Carlisle, D.M. Gruen*, Argonne National Laboratory

Thin diamond films have extremely attractive properties for electronic device applications: high thermal conductivity, carrier mobility, and breakdown fields. However, efforts to create diamond based electronic devices have been hampered by the difficulty in incorporating dopants. Attempts to dope diamond films have resulted in low p-type carrier concentrations or unstable p-type surface layers. N-type doping has been even less successful, and it has not yet been possible to synthesize n-type diamond films with sufficiently high room-temperature conductivities. Ultra-nanocrystalline diamond (UNCD) is a fine-grained (3-5nm), phase-pure diamond material with atomically abrupt grain boundaries. Synthesized by microwave CVD using Ar-rich Ar/CH_4 plasmas, both the structure and electronic properties of UNCD can be tailored by doping with a controlled amount of N_2 in the plasma. As the N_2 content in the plasma increases to 20% , the grain size and grain boundary width of the UNCD films increase. This microstructural change correlates with a striking increase in room-temperature conductivity . Most importantly, nitrogen doped UNCD films are n-type with activation energies as low as 0.05 eV. This is striking, as traditional nitrogen substitutional doping of diamond produces a very deep state of 1.7eV, rendering the material useless for room-temperature applications. We use this material to demonstrate the first n-type diamond MESFET that can be operated at room temperature. We have characterized the films using Raman spectroscopy, NEXAFS, SIMS, Hall mobility measurements, and HRTEM, and measure device properties such as I-V curves and transconductance. The ohmic vs. Schottky behavior of various contacts to nitrogen doped UNCD as a function of growth chemistry has also been studied. A discussion of the microstructure-property relationship of nitrogen-doped UNCD films will be presented in the context of the UNCD-based MESFET performance.

11:20am **EL+SC+MI-MoM10 Electronic Structure and Spin-Polarization of Mn-containing Dilute Magnetic III-V Semiconductors**, ***L. Kronik***, *M. Jain, J.R. Chelikowsky*, University of Minnesota **INVITED**

The systematic use of electron spin, in addition to its charge, holds great promise for a new class of semiconductor devices with unprecedented functionality. Recently, Mn-containing, "dilute magnetic", III-V semiconductors have emerged as candidate materials for such a technology. They can potentially produce charge carriers with well-defined spin, yet are compatible with already existing semiconductor technologies. In order to assess the performance limits of such materials theoretically, we present first principles pseudopotential - density functional calculations for the

electronic structure of the dilute magnetic semiconductors $Mn_xGa_{1-x}As$ and and $Mn_xGa_{1-x}N$, with an experimentally relevant realistic x=0.063, in their ordered ferromagnetic phase. We predict that both materials allow, in principle, for a theoretical limit of 100% spin-injection, and that spin-polarized transport can be attained in both materials in the context of a simple band picture. This is because in MnGaAs, hybridization of As 4p and Mn 3d orbitals splits the valence band, resulting in a ~0.5 eV energy range where holes have a well-defined spin and an effective mass comparable to that of GaAs. In MnGaN, the situation is even more favorable: hybridization of Mn 3d and N 2p orbitals results in the formation of a ~1.5 eV wide impurity band, which supports effective mass transport. We will discuss the technological impact of these findings and compare our results to pertinent experimental data.

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