Thursday Afternoon, October 5, 2000

Semiconductors
Room 306 - Session SC+SS+EL-ThA
III-Nitride Growth and Nucleation

Moderator: V.M. Bermudez, Naval Research Laboratory

2:00pm **SC+SS+EL-ThA1 Kinetics of GaN Growth and Decomposition*, D.D. Koleske*,** *A.E. Wickenden, R.L. Henry, M.E. Twigg, J.C. Culbertson,* Naval Research Laboratory **INVITED**

While many devices have been demonstrated in the group III nitrides, details of the chemical reaction mechanisms for producing high quality GaN using metallorganic vapor phase epitaxy (MOVPE) continues to be an active area of research. In this presentation, I will highlight the results from several kinetic studies of GaN growth. This will include investigations of GaN decomposition in a commercial MOVPE reactor at temperatures and pressures typically used for growth. The GaN decomposition rates were measured in H@sub 2@, N@sub 2@, mixed H@sub 2@ and N@sub 2@, and mixed H@sub 2@ and NH@sub 3@. From these studies an enhancement in the GaN decomposition rate is observed in pure H@sub 2@ and mixed H@sub 2@ and NH@sub 3@ flows as the reactor pressure is increased above 100 torr. @footnote 1@ The mechanism for enhanced GaN decomposition will be presented. Measurements of GaN growth (with trimethylgallium) and decomposition (without trimethylgallium) rates under otherwise identical conditions indicate the extent of decomposition and incorporation during growth. GaN decomposition also accounts for a decrease in the GaN nucleation at higher pressures during the initial high temperature growth. This decrease in the nucleation density leads to increased grain size and higher quality GaN films.@footnote 2@ Kinetic issues relating to incorporation of defects will also be presented. These issues include a growth model for stoichiometric GaN growth,@footnote 3@ and the kinetics of surface carbon removal. All work sponsored by the Office of Naval Research. @FootnoteText@ @footnote 1@ D.D. Koleske, et al., Appl. Phys. Lett. 73, 2018 (1998); ibid. 75, 1646 (1999). @footnote 2@ A.E. Wickenden, et al., J. Electron. Mat. 29, 21 (2000). @footnote 3@ D.D. Koleske, et al., J. Appl. Phys. 84, 1998 (1998).

2:40pm **SC+SS+EL-ThA3 Carbonization of Si (111) by Gas Source Molecular Beam Epitaxy using Triethyl Gallium and Subsequent GaN Growth*, E. Kim,*** *A. Tempez, A. Bensaoula,* University of Houston

Next to sapphire, SiC is the most commonly utilized substrate for GaN heteroepitaxy. In addition to a better lattice match it has the advantage of being available in either conducting or insulating form. The most desirable substrate from both processing and cost point of view is Si since it will allow direct integration of GaN-based devices with conventional Si technology. To that end many approaches have been attempted to overcome the lattice mismatch and nucleation issues for GaN deposition on Si. We have already reported on RF-MBE and chemical beam epitaxy (CBE) of GaN on Si(111) using AlN buffer layers and demonstrated LEDs from our materials. To further improve on our previous results we explored the use of SiC as a buffer layer for the growth of GaN on Si. In this paper we demonstrate deposition of GaN on a SiC buffer layer formed by in situ carbonization of Si using a metalorganic precursor (triethylgallium: TEG) as the carbon source. The carbonization of the Si (111) surface is identified using in-situ time of flight low energy ion scattering, ex-situ XPS and XRD. The thickness, the crystalline quality and the surface morphology of the carbonized layer are found to be very temperature dependent. A 6H-SiC polycrystalline thin film is formed above 780°C. Layers formed at 800°C are thicker and rougher than those formed at 780°C. In either case, Ga is not incorporated into the SiC layer. The SiC layer is shown to efficiently block the formation of SiO@subx@N@suby@ surface species which hinders the GaN nucleation and makes GaN/Si heteroepitaxy non-reproducible. GaN layers deposited in the same reactor by CBE using TEG and ammonia were analyzed as a function of the SiC layer thickness and annealing temperature. Data from these layers as well as from RF-MBE GaN deposited on these SiC buffer layers will also be presented. This project was funded by a NASA cooperative grant #NCC8-127 to the Space Vacuum Epitaxy Center.

3:00pm **SC+SS+EL-ThA4 Epitaxial III-V Nitride Growth on SiC(0001) by Means of A@super 3@@Sigma@@sub u@@super +@ Metastable Molecular Nitrogen*, D.C. Jordan,*** *D.J. Smith, I.S.T. Tsong, R.B. Doak,* Arizona State University

High quality epitaxial III-N semiconductor films, ranging in thickness from 300 to 900 Å, have been grown using A@super 3@@Sigma@@sub u@@super +@ metastable nitrogen molecules. The work employed a corona discharge supersonic free-jet (CD-SFJ) to generate a molecular beam containing exclusively the A@super 3@@Sigma@@sub u@@super +@ activation state in an otherwise ground state N@sub 2@ beam. AlN films were grown on 6H-SiC(0001) and Si(001) substrates. GaN films were grown on the same substrates and on buffer layers of AlN deposited in situ on 6H-SiC(0001). The N-atom incorporation efficiency (defined as the number of N-atoms attaching to a III-N surface per incident metastable A@super 3@@Sigma@@sub u@@super +@ molecule) approached 100% in most instances and was found to be independent of substrate temperature from 600 to 900 Â°C, implying direct molecular chemisorption as the underlying reaction mechanism. These measurements support theoretical predictions that A@super 3@@Sigma@@sub u@@super +@ is an ideal precursor for III-N growth.

3:20pm **SC+SS+EL-ThA5 Crystal Growth Kinetics and Transport in GaN Epitaxial Lateral Overgrowth*, M.E. Coltrin,*** *C.C. Willan, M.E. Bartram,* Sandia National Laboratories **INVITED**

Epitaxial Lateral Overgrowth (ELO) is a useful technique to improve material quality and reduce defects in GaN. In ELO, a mask pattern of dielectric material, usually either silicon nitride or silicon dioxide, is deposited on top of a GaN buffer layer. Further growth of GaN occurs selectively on exposed areas of the underlying buffer layer, and not on the dielectric material. Typically, ELO conditions are optimized for a maximum lateral - to - vertical growth rate ratio. Growth kinetics of GaN crystal faces and transport effects will be discussed in this paper. Dimensions of the exposed and masked areas in line and dot patterns, pattern orientation with respect to the underlying substrate, and growth time were systematically varied. Growth rate information was obtained from scanning electron microscope (SEM) measurements. The coupling between transport and kinetic effects was examined by means of 2-D and 3-D numerical simulations. In general, transport of material from the masked to the unmasked regions is quite efficient. However, ELO deposition growth efficiency is shown to decrease dramatically when the ratio of exposed to masked areas becomes very small. ELO experiments incorporating deep trenches will be described, which are designed to distinguish between lateral transport of material via gas-phase vs. surface diffusion. Gas-phase transport of material appears to dominate. We have found a quantitative way to translate results from different pattern dimensions into a pseudo time basis by scaling growth features by a length scale W, the size of the exposed deposition window.

4:00pm **SC+SS+EL-ThA7 Thick GaN on Si Substrate by Hydride Vapor Phase Epitaxy using Epitaxial Lateral Overgrowth Technique*, J.W. Lee,*** *J.B. Yoo,* Sungkyunkwan University, Korea

The thick GaN growth is a very essential issue for the fabrication of GaN substrate. Epitaxial lateral overgrowth (ELOG) is one of the promising techniques for the high quality GaN epilayer as a fabrication of optical and electronic devices. In this study, two-step growth of GaN was optimized to grow high-quality GaN. First, we attempt ELOG technique for growth of GaN on a Si(111) substrate by MOCVD. Then the thick GaN film was overgrown on ELOG GaN by HVPE. Because of their large lattice mismatch between GaN and Si, the use of an intermediate layer or buffer layer is essential. For the growth of GaN on Si substrate the AlN layer was used to buffer layer. The AlN buffer layer was deposited by RF sputtering. The LT-GaN by was induced another buffer layer on Si substrate. The ELOG GaN on Si substrate was grown by MOCVD. The TMGa and ammonia were used as source gases. The growth temperature of ELOG GaN was changed range in 500°C to 1100°C. The thick GaN was grown by conventional HVPE. The chlorinated gallium and ammonia were used as source gas for Ga and N, respectively. The growth temperature of thick GaN was varied from 800°C to 1100°C. The SiO@sub 2@ was grown by PECVD for the use of ELOG mask on buffer layers. The stripe pattern was developed along and crystal axis of GaN. The various stripe windows with a different spacing between stripes were developed on the SiO@sub 2@ mask by conventional photolithography and wet chemical etching. The effect of growth parameters such as AlN, LT-GaN, growth temperature, stripe patterned direction were investigated. Surface roughness and morphologies of ELOG GaN film were analyzed by atomic force microscopy (AFM) and scanning electron microscope (SEM). The effect of ELOG on thick GaN-film was characterized by double crystal x-ray diffractometer (DCXRD), low temperature photoluminescence (PL) and transmission electron microscope (TEM).

4:20pm **SC+SS+EL-ThA8 Growth and Electronic Structure of ScN, a New Refractory III-V Semiconductor***, **D. Gall**, I. Petrov, J.E. Greene,* University of Illinois, Urbana

ScN layers, 40 to 345 nm thick, were grown on MgO(001) substrates at 750 °C by ultra-high-vacuum reactive unbalanced magnetron sputter deposition in pure N@sub 2@ discharges at 5 mTorr. All films were stoichiometric with N/Sc ratios of 1.00±0.02. Microstructural and surface morphological evolution were found to depend strongly on the energy E@sub i@ of N@sub 2@@super +@ ions incident at the film surface during deposition. Nucleation and the initial growth of ScN layers deposited with E@sub i@ = 13 eV are dominated by the formation of 111 and 002-oriented islands which exhibit local epitaxy. However, preferred orientation rapidly evolves toward a purely 111 texture by a film thickness of ~50 nm as 002 grains grow out of existence in a kinetically-limited competitive growth mode. In distinct contrast, ScN layers deposited with E@sub i@ = 20 eV are single crystals which grow in a cube-on-cube epitaxial relationship with MgO(001). ScN optical properties were determined by transmission, reflection, and spectroscopic ellipsometry while in-situ x-ray and UV valence-band photoelectron spectroscopy were used to determine the density of states (DOS) below the Fermi level. The measured DOS exhibits peaks at 3.8 and 5.2 eV stemming from the N 2p bands and at 15.3 eV due to the N 2s bands. The imaginary part of the measured dielectric function @epsilon@@sub 2@ consists of two primary features due to direct X- and @GAMMA@-point transitions at photon energies of 2.7 and 3.8 eV, respectively. The ScN band structure was calculated using an ab initio Kohn-Sham approach which treats the exchange interactions exactly within density-functional theory. Combining experimental and computational results, we show that ScN is a semiconductor with an indirect @GAMMA@-X bandgap of 1.3±0.3 eV and a direct X-point gap of 2.4±0.3 eV.

4:40pm **SC+SS+EL-ThA9 Structure and Optical Properties of ScN(001) Grown by Molecular Beam Epitaxy***, **H. Al-Brithen**, A.R. Smith, W.M. Jadwisienczak, H.J. Lozykowski,* Ohio University

Scandium nitride is grown by molecular beam epitaxy on MgO(001) substrates. Reflection high energy electron diffraction and x-ray diffraction both confirm the (001)-orientation of the ScN layer. The measured lattice constant is in close agreement with the expected lattice constant a = 4.501 Å, and there is no sign of strain aside from that due to differential thermal contraction between film and substrate during cooling. As measured by atomic force microscopy and scanning tunneling microscopy (STM), these films are found to be smooth, with terraces separated by steps of height a/2. As the Sc flux is varied, the growth morphology also varies - from that of plateaus and pyramids (for lower Sc flux) to that of spiral mounds (for higher Sc flux). We associate the transition with a particular ratio of Sc flux to N flux. Films grown with a lower Sc/N flux ratio have a distinct reddish appearance, and a turn-on feature at 570 nm in the cathodoluminescence (CL) spectrum is measured, consistent with a band gap energy of about 2.2 eV. Films grown with higher Sc/N flux ratio are dark in appearance, and no turn-on feature at 570 nm is observed in the CL spectrum. STM images atomically resolve the rock-salt surface lattice for films grown with lower Sc/N flux ratios; however, for films of higher Sc/N flux ratio, small protrusions are observed on the terraces, which are most likely excess Sc atoms. The effect of the Sc/N flux ratio on the stoichiometry of the films will also be discussed.

5:00pm **SC+SS+EL-ThA10 ScN Thin Films and Thin Film Devices***, **X. Bai**, M.E. Kordesch,* Ohio University

ScN films have been grown by plasma assisted physical vapor deposition (PAPVD) and reactive sputtering on quartz, sapphire, silicon and MgO. Growth temperature ranges from 300K to 1100K, thickness ranges from 50nm to 800nm. For PAPVD films, the XRD results show that ScN grows with (111) texture on quartz, both ScN (111) and (200) textures are observed on sapphire (0001), and (200) textured growth on Si (100). ScN films grown at 300 K are amorphous. Sputtered films show both (111) and (200) texture under various conditions. ScN grows epitaxially on MgO (100). Measurement of the lattice constant ranges from 0.442 nm on quartz to 0.458 nm on silicon. Temperature dependent condcutivity measurements show that ScN is a semiconductor. Intrinsic, p type and n type ScN can be synthesized, with carrier concentrations between 10@super12@ cm@super-3@ to 10@super22@cm@super-3@. The index of refraction is determined from IR measurements to be 2.46 ± 5%. The best optical bandgap result from our measurements is 2.26 eV. There are theoretical predictions of an indirect gap at about 1 eV, outside of our measurement range. ScN films have been used to fabricate p-n junctions, junctions with p and n type Si, and lattice mismatched isotype n-n junction with GaN. Functional ohmic contacts to ScN have been fabricated using Ti, Pd and Ni.

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