Monday Morning, October 2, 2000

Semiconductors
Room 306 - Session SC1+EL+SS-MoM
Chemistry of Silicon Oxides and Nitrides

Moderator: E. Cartier, IBM

8:20am **SC1+EL+SS-MoM1 Atomic-Order Thermal Nitridation of Si(100) and Subsequent Epitaxial Growth of Si***, **T. Watanabe**, M. Sakuraba, T. Matsuura, J. Murota,* Tohoku University, Japan

Atomic-order nitridation by NH@sub 3@ on Si(100) and subsequent Si growth by SiH@sub 4@ were investigated using an ultraclean low-pressure CVD system with a Xe flash lamp. Thermal nitridation on Si(100) at 400°C in an NH@sub 3@ environment with and without the flash lamp light irradiation is explained by Langmuir-type physical adsorption of NH@sub 3@ and nitridation by the adsorbed NH@sub 3@. The nitridation can be enhanced by Xe flash lamp light irradiation, and the N atom concentration tends to saturate to about 2.7x10@super 15@ cm@super -2@. In the Si deposition on the ultrathin silicon nitride, it is found that N desorption from the Si nitride films hardly occurs, and Si grew on silicon nitride, whose N atom concentrations are from about 2x10@super 14@ cm@super -2@ to about 2.7x10@super 15@ cm@super -2@, at 385°C in an SiH@sub 4@ environment with and without the flash lamp light irradiation. The incubation period of Si growth is observed and increases with increasing N atom concentration of the silicon nitride film. On the silicon nitride of N atom concentration of about 2x10@super 14@ cm@super -2@, the incubation period is hardly observed and it is found by RHEED measurements that Si epitaxially grew. Layer-by-layer growth control of silicon nitride is proposed by combining atomic-order nitridation on Si and atomic-layer growth of Si on the silicon nitride.

8:40am **SC1+EL+SS-MoM2 The Role of Inter-dimer Interactions in NH@sub 3@ Dissociation on Si(100) - (2 x 1)***, K.T. Queeney,* Smith College*; K. Raghavachari,* ***Y.J. Chabal,*** Bell Laboratories, Lucent Technologies

The chemistry of gas-phase precursors to film growth on the Si(100) surface in ultrahigh vacuum is often well-described by localized interaction of the adsorbate with a single Si-Si dimer.@footnote 1@ However, our combined experimental and theoretical studies of the dissociation of NH@sub 3@ to form NH@sub 2@-Si-Si-H on this surface reveal that this reaction is in fact governed by a complex set of inter-dimer interactions involving both bare and adsorbate-covered Si dimers. External transmission FTIR spectroscopy allows us to probe both the lower-frequency @delta@(NH@sub 3@) modes of metastable, undissociated NH@sub 3@ and the higher-frequency @nu@(SiH) modes resulting from dissociation. By comparing our experimental results with density functional calculations describing two-dimer clusters, we find that the vibrational spectra can only be interpreted when inter-dimer effects are considered. Specifically, while hydrogen bonding between undissociated NH@sub 3@ and dissociated NH@sub 2@ species renders coupling of adjacent nitrogen-containing groups thermodynamically favorable, kinetic control of the dissociation process yields a predominance of the opposite configuration, resulting from the influence of dissociated species on the buckling of neighboring bare dimers during adsorption. We propose that such adsorbate-induced effects on the electronic structure of neighboring dimers may have general implications for controlling the two-dimensional ordering of reactions on the dimerized Si(100) surface. @FootnoteText@ @footnote 1@ See for example: R. Konecny and D. J. Doren, J. Chem. Phys. 1997, 106 (2426); B. B. Stefanov and K. Raghavachari, App. Phys. Lett. 1998, 73 (824).

9:00am **SC1+EL+SS-MoM3 Quantum Chemical Study of Silicon Nitride Deposition Using Ammonia***, **Y. Widjaja**, C.B. Musgrave,* Stanford University

Density functional theory is used to examine the reaction mechanisms of nitridation of the Si(100)-2x1 surface by NH@sub 3@. The surface is modeled using the cluster approximation. A detailed reaction mechanism is investigated including ammonia adsorption and decomposition, insertion of N into Si-Si bonds, and H@sub 2@ desorption. We find that nitrogen prefers to be in the subsurface layer, bonded to three Si atoms. The energy barriers leading to the nitridation of the Si(100) surface are also calculated. The activation barrier of the rate limiting step is found to be higher than the activation barrier for NH@sub 3@ desorption. This confirms the experimental observation that a large fraction of the NH@sub 3@ that dissociates on adsorption will recombine and desorb. Furthermore, we have also calculated the vibrational frequencies of various surface nitride structures. The computed frequencies are then compared with the experimental HREELS spectra. The comparison further allows the unambiguous characterization of the surface species. Using the calculated barriers and frequencies we use transition state theory to estimate a rate for nitridation of the (100) silicon surface. We investigate the validity of the cluster approximation and find that bigger cluster models are necessary to describe the nonlocal electronic effects.

9:20am **SC1+EL+SS-MoM4 Thermal Nitridation of Ultrathin Silicon Dioxide Films Using NH@sub 3@ Gas***, **O. Jintsugawa**, M. Sakuraba, T. Matsuura, J. Murota,* Tohoku University, Japan

Nitrided ultrathin SiO@sub 2@ film is attractive as the gate insulator of future MOS devices. In this work, thermal nitridation of thin SiO@sub 2@ films and transport of nitrogen species into SiO@sub 2@ films were investigated. A 30Å-thick SiO@sub 2@ film on Si(100) was formed by wet oxidation at 700°C , and was thermally nitrided for 90min at 750-850°C in NH@sub 3@ gas at 100Pa using an ultraclean low-pressure CVD system. The depth profile of N atom was obtained by the repetition of etching by a 1%-diluted HF solution and XPS measurements. By the thermal nitridation, most of the N atoms were present near the SiO@sub 2@ surface and the N atom concentration was remarkably lower (1/2 and 1/10 at 850 and 750°C, respectively) than that of the nitrided Si surface without the SiO@sub 2@ film. By 850°C nitridation, N atom diffused into the SiO@sub 2@ film and Si substrate nitridation were observed. The N atom concentration was estimated to be 4x 10@super 15@cm@super -2@ on the SiO@sub 2@ surface, 1x10@super 21@cm@super -3@ in the SiO@sub 2@ film, and 8x10@super 13@cm@super -2@ at the SiO@sub 2@/Si interface. Binding energy of N 1s at the SiO@sub 2@ surface and in the SiO@sub 2@ film was shifted 2eV-higher than that at the SiO@sub 2@/Si interface. By 750°C nitridation, the N atom concentration on the SiO@sub 2@ surface was 3x10@super 14@ cm@super -2@ and, in the SiO@sub 2@ film and at the SiO@sub 2@/Si interface, the N atom concentration was less than the detection limit (about 3x10@super 20@cm@super -3@ and 4x10@super 12@cm@super -2@, respectively). This result indicates that the existence of surface oxygen more greatly suppresses the reaction of NH@sub 3@ at the lower temperature. Pressure and time dependence of nitridation on the SiO@sub 2@ surface, in the SiO@sub 2@ and at the SiO@sub 2@/Si interface will be also presented.

9:40am **SC1+EL+SS-MoM5 Probing the Chemistry of Dielectric Thin Film Growth on Si Surfaces***, L.D. Flores,* ***J.E. Crowell,*** University of California, San Diego **INVITED**

The surface and gas phase chemistry involved during dielectric thin film growth of doped and undoped silicon dioxide has been studied using the atmospheric pressure reaction between tetraethoxysilane (TEOS) and ozone. The studies involve low temperature deposition of dielectric thin films using a new atmospheric-pressure chemical vapor deposition (APCVD) reactor utilizing a commercial injector / vent assembly. The APCVD reactor is coupled to a N@sub 2@-purged glovebox and a UHV surface analysis facility equipped with XPS, AES, TPD, and IR spectroscopy capabilities. Gas-phase transmission FTIR spectroscopy measurements were performed in-situ during deposition at 400°C by probing the variable gap region between the 400°C heated Si wafer and the injector. The primary products produced upon reaction of TEOS and ozone are acetic acid, formic acid, formaldehyde, carbon monoxide, carbon dioxide, and water. Reaction of TEOS and oxygen in the gas phase is negligible compared to reactions involving ozone at identical temperatures under these conditions. Potential TEOS / O@sub 3@ reaction products and their reaction with boron and phosphorus containing dopant sources has been investigated in order to clarify their role in the oxidation process and to clarify the chemical mechanism. This was accomplished by following the reaction with ozone of some possible and observed ozonation products in a flow reactor / gas cell using transmission FTIR spectroscopy. The products of acetaldehyde ozonation are shown to be different from pathways leading to acetic acid production during TEOS ozonation. Mechanistic pathways unique to Si-O-C containing species will be presented. The products formed upon introduction of boron and/or phosphorus containing precursors to the process flow will also be discussed.

10:20am **SC1+EL+SS-MoM7 Thickness Control of an Ultrathin Oxide Film on Si(100)2x1 Synthesized by Ozone: A Kinetic Study on Initial Oxidation***, **K. Nakamura**, A. Kurokawa, H. Itoh, S. Ichimura,* Electrotechnical Laboratory, Japan

One of the alternative oxidants for the fabrication of an ultrathin silicon oxide film is ozone. Using highly concentrated ozone, we have succeeded so far in synthesizing an oxide film of 2nm on Si(100) at lower substrate temperature (for example, at 350°C). This oxide film has high density equivalent to that of a thermally grown oxide, much smaller thickness of structural transition layers, and can be obtained also by modifying and upgrading an already existing native oxide film.@footnote 1,2@ Moreover, the oxide thickness must be precisely and accurately controlled because of its practical use as a gate oxide film in MOSFET. In this paper, therefore, we will study growth kinetics of initial oxidation by ozone on silicon surfaces in detail. To fabricate an ultrathin silicon oxide film by ozone, clean Si(100)2x1 surfaces at between room temperature and 700°C were exposed to highly concentrated (>80%) ozone. Initial oxide growth was mainly monitored by x-ray photoelectron spectroscopy (XPS). The results indicate different kinetics on each oxide layer. Following to an adsorption on the surface investigated also by second harmonic generation (SHG), oxide growth on each of the first three oxide layers proceeded in accordance with Langmuir kinetics, indicating random adsorption on the active sites on each layer. Within this thickness, oxidation rates on the second and third layers possessed positive values of activation energy, while the growth rate on the first layer showed no activation barrier. Above this thickness, an oxide film by ozone grew in proportion to exposure time instead above the critical substrate temperature of 550°C. These suggest that control of film thickness should be optimized in the first three layers and above the fourth, respectively, due to different growth mechanisms. @FootnoteText@ @footnote 1@ K. Nakamura, S. Ichimura, A. Kurokawa, K. Koike, G. Inoue, and T. Fukuda, J. Vac. Sci. Technol. A 17 (1999) 1275. @footnote 2@ A. Kurokawa, K. Nakamura, S. Ichimura, and D. W. Moon, Appl. Phys. Lett. 76 (2000) 493.

10:40am **SC1+EL+SS-MoM8 FTIR at Liquid/Solid Interfaces: In-situ Studies of HF Etching of SiO@sub 2@ on Si(100)*, **K.T. Queeney,*** Smith College Department of Chemistry*; E.E. Chaban, Y.J. Chabal,* Bell Laboratories, Lucent Technologies

While much important semiconductor surface chemistry--cleaning, passivating and etching--takes place at the liquid/solid interface, the inherent difficulty of probing such interfaces has limited mechanistic understanding of these processes. We have developed a novel experimental setup that allows us to probe semiconductor/liquid interfaces with FTIR spectroscopy, circumventing the limitations of conventional multiple internal reflection spectroscopy to access the full frequency range of interest (850-4000 cm@super -1@), in particular the Si-O vibrational modes between 900 and 1250 cm@super -1@. We have used this capability to study in detail the etching in dilute hydrofluoric acid of SiO@sub 2@ on Si(100), lending new and valuable insight into the details not only of the chemical nature of the Si/SiO@sub 2@ interface, but also of structural aspects of the remainder of the film, including the SiO@sub 2@/air (water) interface. By analyzing spectra acquired sequentially during the etching process, we derive a layer-by-layer picture of the oxide spectral response; correlation of those spectra with changes in film structure are made via optical modeling. Varying the dielectric constant of the overlying medium (i.e. air versus water) allows quantification of spectral sensitivity to effects such as surface roughness. In addition, the in-situ nature of these studies allows us to evaluate the kinetics of the etching process and provides strong evidence for a structurally distinct layer near the Si(100) substrate, characterized by a marked change in vibrational signature, that is resistant to etching.

Semiconductors
Room 312 - Session SC2+EL+SS-MoM
Dissimilar Materials

Moderator: H.A. Atwater, California Institute of Technology

8:20am **SC2+EL+SS-MoM1 Integration of Epitaxial Oxide and Nitride Heterostructures with Dissimilar Substrates by Pd-In Wafer Bonding and Laser Lift-off*, **T. Sands**, W.S. Wong, L Tsakalakos, N.W. Cheung,* University of California, Berkeley **INVITED**

The functionality of integrated microsystems can be enhanced through intimate integration of disparate classes of materials. Combining the best materials for their respective functions (e.g., information processing, light emission/detection, and piezoelectric actuation) without sacrificing materials properties is often only possible if the materials are synthesized and processed separately, and subsequently combined. In this talk, a fast, simple and robust "paste-and-cut" method for accomplishing this integration step is described. The process combines low-temperature transient-liquid-phase (TLP) metal bonding with excimer laser lift-off (LLO) to integrate epitaxial group-III nitride (e.g., AlN and InGaN) and perovskite oxide (e.g., PZT and PMN-PT) heterostructures with virtually any substrate, including polymers, stainless steel, and CMOS silicon. Both the TLP and LLO steps are characterized by minimal heating of the receptor substrate, thus maximizing the range of materials classes that may be intimately combined. In our TLP metal bonding process, donor and receptor substrates are coated with Pd/In bilayers and pressure-bonded at 200°C to achieve a high-contact-area PdIn@sub 3@ intermetallic bond with a melting point above 600°C. The L LO process uses a single pulse from a uv laser (e.g., KrF excimer at 248 nm with a pulse length of 38 nsec), irradiating the film/substrate interface through the transparent substrate (sapphire or MgO), to decompose the film at the interface with the substrate. The short pulse duration enables thermal decomposition of the film interface without significant heating of the receptor substrate. Examples of TLP/LLO paste-and-cut integration, including vertical (In,Ga)N light-emitting diodes on Si, and epitaxial ferroelectric (PZT) films on stainless steel, will illustrate the potential of this integration method for the functional enhancement of microsystems. @FootnoteText@ W.S. Wong is now at Xerox PARC, Palo Alto, CA.

9:00am **SC2+EL+SS-MoM3 Growth of SiGe Alloys on Strain-Engineered Si on Insulator (SOI) Substrates***, **P. Rugheimer**, C.H. Lee, D.E. Savage,* University of Wisconsin, Madison*; E. Mateeva,* Colorado School of Mines*; P. Moran, A. Lal, T.F. Kuech, M.G. Lagally,* University of Wisconsin, Madison

Self-organized 3D islands and misfit dislocations form in order to relieve strain during heteroepitaxial growth of SiGe on Si(001). In this work, we use patterned SOI substrates to mediate strain and influence film morphology. Films are grown, using both MBE and CVD, on lithographically defined mesas with lateral dimensions ranging from 2 to 20 microns patterned onto both 10nm Si on SiO2 bonded-wafer substrates and Si(001) control substrates. We have also grown epitaxial films on SOI substrates with MEMs type cantilevers etched on the surface. These cantilevers create regions of either tensile or compressive stress where epitaxial film growth takes place. Film morphology for the samples is followed in-situ during growth with RHEED and ex-situ post growth with X-ray diffraction, Atomic Force Microscopy (AFM) and Cross-sectional Transmission Electron Microscopy (CTEM). We find that growth on patterned mesas as well as cantilevers results in some elastic strain relaxation. Possible mechanisms, such as short-range viscous compliance, anisotropic strain relief, or mediation of dislocations, will be discussed. Supported by NSF-MRSEC and by ONR.

9:20am **SC2+EL+SS-MoM4 Techniques and Interface Effects in Creating Alternative Substrates using GaAs Wafer Bonding***, **A.M. Cain**, P.J. Hesse, D.R. Thomas, K.G. Eyink, D.H. Tomich, M. Ruddell, T.W. Haas, M.L. Seaford,* Air Force Research Laboratory

Compliant substrate technology offers the promise of allowing epitaxial growth of lattice mismatched semiconductors suitable for use in heterogeneous integration. An essential step in realizing a compliant technology is the adequate bonding of the compliant layer to a suitable handle wafer. This work will describe a new wafer bonding facility that allows for precise control of the bonding parameters such as temperature, pressure, atmosphere, and bond processing conditions. The equipment is built around a vacuum furnace fitted with a controllable piston to apply pressure to the bonding wafers. Bonding can be carried out in vacuum or in a variety of inert or reducing atmospheres. The bond furnace is enclosed in a dry box to reduce particle contamination and to reduce atmospheric interactions with bonding surfaces. The equipment is fully computerized to allow for complex bond processing steps. This equipment has been utilized to investigate the effects of various surface chemical treatments of GaAs wafers prior to the bonding process. The technique of arsenic capping of MBE grown buffer layers has been utilized to bond wafers at temperatures as low as 250 °C. Bonding did not occur at 200 °C in agreement with line of sight RGA data that was used to determine the temperatures at which the arsenic was desorbed from the interfaces of the bonding wafers. The conditions used for bonding will be described and characterizations of the interface quality using transmission infrared microscopy and acoustic wave microscopy will be given. Except for occasional particles in the bond interfaces it is possible with this approach to obtain consistently bonded wafers. Comparisons with other surface treatments such as use of epitaxial ready wafers and wafers prepared using conventional etching techniques known to have approximately 2.5nm of oxide present will also be given.

9:40am **SC2+EL+SS-MoM5 Relaxation of SiGe Films on Silicon-on-Insulator Substrates Utilizing Borosilicate Glass***, **E.M. Rehder**, D.E. Savage, P. Moran,* University of Wisconsin, Madison*; T.S. Kuan,* SUNY at Albany*; M.G. Lagally, T.F. Kuech,* University of Wisconsin, Madison

We have grown epitaxial silicon germanium (SiGe) alloy films and studied the relaxation effects of thin silicon-on-insulator (SOI) substrates. Bond and etchback SOI (BESOI) wafers having a top Si layer of 15nm were fabricated. The insulators in these structures were either SiO@sub 2@, using commercial wafers, or chemical vapor deposited borosilicate glass as the insulator. Si@sub 0.82@Ge@sub 0.18@ films were grown on these substrates by ultra high vacuum chemical vapor deposition at temperatures of 550, 630, and 670°C. Films were grown up to 175nm in thickness, which is beyond the equilibrium critical thickness. The low growth temperatures nonetheless result in metastable strained films. Any observed relaxation during growth was then enabled by the SOI. The relaxation following growth was studied by high-resolution double and triple crystal x-ray diffraction and cross sectional transmission electron microscopy. The growth layers on substrates using the SiO@sub 2@ insulator as well as those grown directly on Si substrates are identical and fully strained. However, SOI substrates utilizing a borosilicate glass with 50% B@sub 2@O@sub 3@ content yielded films in which the film strain was reduced by 30%. Post-growth annealing at temperatures from 700 to 1050°C were employed to promote relaxation. When annealed at 950°C the film on the Si substrate remained largely unrelaxed, while the film on the SiO@sub 2@-SOI substrate relaxed to 50%. Lower temperatures resulted in no relaxation, while annealing at 1050°C allows interdiffusion to occur resulting in additional relaxation. Cross-sectional TEM images of these samples reveal a complex dislocation structure in both the film and substrate. The relationship between the oxide viscosities at these temperatures and the image forces affecting dislocation formation and motion will be discussed.

10:00am **SC2+EL+SS-MoM6 Growth of Single Crystalline AlN on Si(111) using Surface Reconstruction Induced Epitaxy***, **M. Jenkins**, A. Faik,* University of North Carolina*; M.R. Sardela Jr,* University of Illinois*; M.-A. Hasan,* University of North Carolina

AlN is a direct wide bandgap (6.2 eV) material suitable for applications in UV emission and detection. In addition, it has a close lattice constant to GaInN, which provides a tunable band gap for emission in the blue to red region. Moreover, integration of group III-nitrides with Si would enable optical interconnects and high power device fabrication on Si. In this work, we have demonstrated growth of hexagonal single crystalline AlN(001) on Si(111) using surface reconstruction induced epitaxy. The Si(111)7x7 surface was first passivated by deposition of ~0.3 monolayer (ML) of Al at 650-700 °C. Each Al atom bonds to 3 Si atoms on the surface, which give rise to the well-known Si(111)@sr@3x@sr@3 surface. The well ordered, Al-passivated Si(111)@sr@3x@sr@3 surface was then used as a template to initiate epitaxial growth of AlN on Si. Without Al passivation, N would react with the clean Si surface forming amorphous Si@sub 3@N@sub 4@, which provides a disordered template and prevents epitaxial growth of AlN. The growth was conducted by using an atomic N flux from a RF atomic source and thermal deposition of Al from an effusion cell. Reflection of high-energy electron diffraction (RHEED), high-resolution X-ray diffraction and transmission electron microscopy results confirmed the formation of single crystalline AlN. The results showed that epitaxial growth of AlN depends strongly on the Al/N flux ratio, growth temperature, and the RF power.

10:20am **SC2+EL+SS-MoM7 Enhanced Thermal Stability of Au Film on GaN by Thin Cr Interfacial Layer***, **J.H. Kim**, H.J. Kang,* Chungbuk National University, Korea*; C.Y. Kim,* LG CIT, Korea*; J.M. Seo,* Chonbuk National University, Korea

In order to enhance the thermal stability of Au film on GaN, 4 ML of thin Cr layer had been deposited prior to Au evaporation. The AFM image shows that, upon postannealing at 650C, Au overlayer with Cr interlayer still keeps its uniformity without forming either pits or islands, while the same amount of Au without Cr interlayer is agglomerated. The corresponding results of scanning Auger microscopy combined with the high resolution x-ray photoelectron spectroscopy indicate that the interfacial Cr partially mixes with GaN and partially mixes with Au overlayer, and reduces the Schottky barrier height of p-type GaN by 0.4 eV. The core level analyses of Cr 2p, Au 4f and Ga 2p indicate a small portion of Ga species also segregates to the top side of this AuCr alloy overlayer. It has been concluded that the role of Cr interlayer for enhancing thermal stability of Au overlayer is in the gradual relaxation of the strain originating from thermal-expansion-coefficient-difference through diffusing into both sides without losing N species.

10:40am **SC2+EL+SS-MoM8 Effects of Hydrogen on the Properties of Cu(TMVS)(hfac) Sourced CVD Copper Films***, **J. Hong**, D. Yang, S. Shetty, T.S. Cale,* Rensselaer Polytechnic Institute

We describe a study of the effects of hydrogen pre- and post-treatment on films grown by Cu(TMVS)(hfac) sourced Cu CVD on TaN substrates using an LPCVD system. Our previous work@footnote 1,2@ showed that the use of water vapor as a co-reactant during Cu CVD can improve the adhesion between the copper film and the substrate. However, the resistivity and surface roughness of the deposited film were degraded when too much water vapor was introduced, probably due to the formation of Cu oxide. The hydrogen pretreatment is an attempt to reduce the native oxide layer on the TaN barrier layer. Films deposited on pretreated substrates have lower resistivity than those on untreated substrates. We have also studied the effects of hydrogen post-treatment on films grown with various amounts of water vapor as a co-reactant. Film properties depend on the duration of the water vapor flow, and the hydrogen post-treatment baking time and temperature. In all cases, resistivity was decreased after treatment compared to untreated films--an effect that we attribute to the reduction of Cu oxides formed in the film. The effect of hydrogen on the surface roughness depends on the amount of water vapor present during deposition and the length of the hydrogen treatment. We conclude that the resistivity of the Cu films is improved and surface roughness is changed with the use of hydrogen as pre- and post-treatment in Cu CVD process protocols. @FootnoteText@ @footnote 1@ D. Yang, J. Hong and T. S. Cale, in Proceedings of the Advanced Metallization Conference in 1999 (AMC 1999), "Effects of Process Variables on Cu(TMVS)(hfac) Sourced copper CVD films". @footnote 2@ D. Yang, J. Hong, and T. S. Cale, in MRS Symposium Proceedings of the MRS Spring 2000 Meeting, "Evolution of Surface Morphology During Cu(TMVS)(hfac) Sourced copper CVD films".

Monday Afternoon, October 2, 2000

Semiconductors
Room 306 - Session SC+EL+SS-MoA
Reactions on Semiconductors

Moderator: R.A. Wolkow, National Research Council of Canada

2:00pm **SC+EL+SS-MoA1 Adsorption of SiH@sub 4@ on Si(001)(2x1) Investigated by Infrared Spectroscopy***, **M. Shinohara**, A. Seyama, Y. Kimura, M. Niwano,* Tohoku University, Japan

Adsorption of silane molecules, SiH@sub 4@ and Si@sub 2@H@sub 6@, onto Si(001) has so far been investigated extensively, because of the potential of using the silane molecules as the source gas for gas source molecular beam epitaxy (GS-MBE) for the growth of Si. Previous studies on Si deposition using silanes have suggested that during the course of Si crystal growth, silanes dissociatively adsorb on Si surface dangling bonds as trihydride (SiH@sub 3@) and dihydride (SiH@sub 2@) species and then decomposes to surface monohydride species, SiH. However, there has been only a little amount of information about the type of hydride species that are generated during the adsorption of silane on Si surfaces. In this study, we used infrared absorption spectroscopy (IRAS) in the multiple internal reflection geometry (MIR) to investigate the adsorption of SiH4 on the Si(001)(2x1) surface. IRAS-MIR provides us with valuable information about the hydrogen bonding configurations on semiconductor surfaces. Comparing infrared data with the density functional cluster calculation, we show that the silane molecule dissociatively adsorbs on Si(001)(2x1) to populate a dihydride (SiH@sub 2@) at the bridge site between two adjacent dimers and a monohydride species; the latter is formed by terminating the unsaturated dangling bonds of dimers by hydrogen atoms that are released from the silane molecule. We found that at high surface hydrogen coverage, surface silyl (-SiH@sub 3@) group and monohydride (SiH) species are generated. We interpret that at high hydrogen coverage, silane adsorbs onto a single dimer that has two unsaturated dangling bonds on which a hydrogen atom and a sylil group (-SiH@sub 3@) stick. We also show that a dihydride species that was initially generated by silane adsorption, dissociates even at room temperature and the released hydrogen atoms migrate on the surface to produce more monohydride species.

2:20pm **SC+EL+SS-MoA2 Si(001):As Gas-source Molecular Beam Epitaxy: As Incorporation and Film Growth Kinetics***, **H. Kim**,* University of Illinois*; G. Glass,* PTD, Intel Corp.*; J.A.N.T. Soares,* University of Illinois*; P. Desjardins,* Ecole Polytechnique de Montreal*; J.E. Greene,* University of Illinois

Arsenic-doped Si(001) layers with concentrations C@sub As@ up to 5x10@super 18@ cm@super -3@ were grown on Si(001)2x1 at temperatures T@sub s@ = 575 - 900 °C by GS-MBE using Si@sub 2@H@sub 6@ and AsH@sub 3@. At constant flux ratio, C@sub As@ decreases, while the film growth rate R@sub Si:As@ increases, with T@sub s@. TPD measurements show that As segregates strongly to the growth surface and that the observed decrease in C@sub As@ at high T@sub s@ is primarily due to increasingly rapid arsenic desorption from the segregated layer. Decreasing T@sub s@ enhances As incorporation. However, it also results in lower R@sub Si:As@ due to higher steady-state As surface coverages which decrease the total dangling bond coverage and, hence, the Si@sub 2@H@sub 6@ adsorption rate. At constant T@sub s@, C@sub As@ increases, while R@sub Si:As@ decreases, with increasing AsH@sub 3@ flux. All incorporated As resides at substitutional electrically active sites for concentrations up to 3x10@super 18@ cm@super -3@, the highest value yet reported for Si(001):As growth from hydride source gases. D@sub 2@ TPD spectra exhibit @beta@@sub 1@ and @beta@@sub 2@ peaks associated with Si monodeuteride and dideuteride desorption as well as a new peak @beta@@sub 3@ attributed to desorption from Si-As mixed dimers. Steady-state arsenic surface coverages during film growth, and the As segregation enthalphy, were quantitatively determined as a function of C@sub As@ by comparison with As-adsorbed Si(001) reference samples with known As coverages. From AsH@sub 3@ adsorption kinetics and incorporation data, the AsH@sub 3@ reactive sticking probability on Si(001) was determined and As incorporation kinetics were quantitatively modeled. Initial experiments have demonstrated that temperature-modulated growth can be used to increase both R@sub Si:As@ and C@sub As@ while providing layers which are atomically flat.

2:40pm **SC+EL+SS-MoA3 Scanning Tunneling Microscopy of Impurity Dimers on Hydrogen-Terminated Si(100)-2x1 Surface***, **S. Matsuura**,* University of Tokyo, Japan*; M. Fujimori, S. Heike, Y. Suwa, H. Kajiyama, T. Onogi,* Hitachi, Ltd., Japan*; K. Kitazawa,* University of Tokyo, Japan*; T. Hashizume,* Hitachi, Ltd., Japan

We report a new dimer structure on a hydrogen-terminated n-type Si(100)-2x1-H surface found by a scanning tunneling microscopy (STM). The dimer structure is observed almost same as regular surface Si dimers at filled state, at empty state, however, is observed as different structure showing spatial variation of electronic density of states. Similar results were obtained in the case of As-doped surface. The surface density of the structures derived from measurement of the samples with different dopant concentrations was found to be proportional to the dopant density. Electronic structures calculated by first-principles calculations for a phosphorous dimer or an arsenic dimer on the Si(100)-2x1-H surface are in good agreement with the bias dependent STM images of the newly-found structure on the P-doped or As-doped Si(100) surface, respectively. We concluded that the dimer structure represents dopant atoms incorporated on the Si surface and forming a dimer. The calculation also revealed that the surface phosphorous and arsenic atoms are more stable forming dimers than being isolated on the hydrogen-terminated Si surface.

3:00pm **SC+EL+SS-MoA4 Adsorption and Reaction of Fluorinated Fullerenes on Silicon***, **Y. Fujikawa**, J.T. Sadowski,* Tohoku University, Japan*; K.F. Kelly,* Pennsylvania State University*; K.S. Nakayama, T. Sakurai,* Tohoku University, Japan

The adsorption structure of fluorinated fullerene molecules deposited on silicon was studied using scanning tunneling microscopy (STM) and high-resolution electron energy loss spectroscopy (HREELS). The results of HREELS indicated that the fluorine atoms around the molecules were detached from the molecules and chemisorbed to the surface. These fluorine adsorption sites were directly observed around the adsorbed molecules in the STM images. Some of the fluorine-adsorbed sites were found to form thread-like structures, suggesting that the molecules print the fluorine atoms on the terrace due to the rolling movement of the molecules. Annealing produced different degrees of defluorination of the fullerenes and etching of the silicon surface depending on the temperature. By imaging the intermolecular structure of the molecules with the STM, we can directly observe the loss of the fluorine atoms.

3:20pm **SC+EL+SS-MoA5 STM Study of Self-Assembled Quantum-Dot Arrays of Sn on Si(111)-(7x7) Surface***, **M. Yoon**, R.F. Willis,* The Pennsylvania State University

The adsorption and diffusion mechanisms of Sn on the Si(111)-(7x7) at sub-monolayer coverages have been studied by scanning tunneling microscopy (STM). It is found that the preference of Sn adsorbates on the faulted-halves of the 7x7 unit cell is dependent on adsorbate coverage up to @THETA@ ~ 0.3 monolayer (ML). At higher coverages (~0.3 - 0.5 ML), the tin atoms cluster together on both halves of the 7x7 unit cell, forming a two-dimensional array of self-assembled quantum dots. This is in contrast to the behavior recently reported@footnote 1@ for Tl condensation on Si(111)-(7x7). In this latter case, the element occupies faulted half-cells preferentially and the surface remains metallic. In the present case, the Sn clusters are semiconducting, the surface showing an energy bandgap which increases with increasing coverage. The surface returns to metallic behavior as the number of Sn atoms approaches that of one monolayer of Si. @FootnoteText@ @footnote 1@L. Vitali, M. G. Ramsey, and F. P. Netzer, Phys. Rev. Lett. 83, 316 (1999).

3:40pm **SC+EL+SS-MoA6 Evolution of Surface Morphology During Sb Growth on Ge(100)***, **L.H. Chan**, E.I. Altman,* Yale University

Surfactants such as Sb have been found to promote layer-by-layer growth on metal and semiconductor surfaces. It is known that Sb and Ge intermix only at elevated temperature past 630K. Temperature programmed desorption was performed to study the energetics of Sb adsorption on Ge(100). The results demonstrated a typical high temperature peak that saturated at 1020 K before the appearance of a low temperature sublimation peak below 650 K with increasing Sb exposure. An additional high temperature peak at 1070 K was attributed to bulk incorporation of Sb. On a nominal 1 ML Sb covered Ge(100) surface prepared by deposition at 300K and annealing above the multiplayer desorption peak, scanning tunneling microscopy studies showed three surface layers were exposed. The images displayed bias dependent contrast suggesting the layers were not chemically uniform. To address the reasons for the morphology changes and to identify different components on the surface, a systematic study of Sb growth as a function of coverage and temperature was conducted. At room temperature, Sb adsorbs as tetramers and pairs of dimers. Several Sb@sub 4@ adsorption states are identified. Subsequent island growth leads to a poorly ordered surface with short strands of Sb dimer rows. The growth of longer dimer rows was interrupted by the growth of other nearby dimer rows randomly distributed on the Ge surface. Antimony incorporated into the top layer on either annealing or deposition at 600 K. Annealing gave well-structured dimer rows across the surface in all layers. However, intermixing of Sb and Ge at elevated temperature created ad-dimer clusters, vacancy islands, and reattachment of Sb and Ge ad-dimers on the top layer to the step edges. The implications of these results on surfactant-mediated growth will be discussed.

4:00pm **SC+EL+SS-MoA7 Effects of Exposure on GaSe Passivated Si(111)**, ***J.A. Adams***, *A. Bostwick, S. Meng, B.R. Schroeder, M.A. Olmstead, F.S. Ohuchi,* University of Washington

GaSe growth on Si(111) 7x7 between 500°C and 550°C results in the formation of a bilayer, which passivates the substrate dangling bonds and serves as the interface for further film growth. Ga sits directly atop surface Si, and the resultant interface bonding leaves Se lone-pair states on the surface, similar to Si(111):As. This makes the Si(111):GaSe surface resistant to contamination, and additional GaSe does not stick for T@sub substrate@@>=@500°C. We have studied the effects of exp osure to various atmospheric constituents on the electronic states and surface structure of the bilayer-passivated silicon surface using x-ray photoelectron spectroscopy and diffraction (XPS/XPD), low-energy electron diffraction (LEED) and ultraviolet photoelectron spectroscopy (UPS). We find that exposure to N@sub 2@ at atmospheric pressure has no apparent effect on the atomic or electronic structure and no N@sub 2@ is found to stick on the surface. However, we find that exposure to atmosphere for 5 minutes does change the surface states as observed from UPS, although LEED shows that the atomic structure of the GaSe bilayer does not change. The surface states can be almost completely recovered upon annealing at 500°C for 1 minute. Exposure to other atmospheric constituents such as O@sub 2@ and H@sub 2@O were also studied.

4:20pm **SC+EL+SS-MoA8 Temporal Changes of Photoemission Spectra of the Alkali-metal-induced Ge(111) 3x1 Surface**, ***G. Lee,*** Korea Research Institute of Standards and Science, Korea; *C. Hwang,* Korea Research Institute of Standards and Science; *Y. Park, S. Cho,* Korea Research Institute of Standards and Science, Korea; *H. Lee,* Korea Research Institute of Standards and Science; *E. Cho,* Chonnam National University, Korea

We investigated the temporal changes of the core-level photoemission spectra of the Ge(111)3x1 reconstructed surface induced by alkali metals (Li and Na) in UHV chamber. It is found that while the spectra from the Ge(111)3x1-Na surface is hardly affected, those from the Ge(111)3x1-Li surface change significantly in time. We identify that the changes of the core-level spectra from the Ge(111)3x1-Li surface are due to the contamination by residual oxygen gas in the chamber. The contamination rate of the Ge(111)3x1-Li surface is even higher than that of the clean surface, contradicting the expectation that alkali-metal-induced 3x1 reconstruction passivates the surface against oxidation. We discuss the difference in the contamination rate between the Ge(111)3x1 surfaces induced by different alkali-metal adsorbates.

4:40pm **SC+EL+SS-MoA9 Role of Excited Electronic States in Reactions on Si(100)**, ***J.S. Hess***, *D.J. Doren,* University of Delaware

Low-lying excited electronic states of the Si(100) surface can play a role in activated adsorption reactions. The nature of the lowest surface excited state and its coupling to the surface ground state will be described. Density functional theory calculations on cluster models of Si(100) have been used to predict the minimum energy difference between the optimized ground state and first excited state levels. The minimum energy crossing point between the two states was explicitly calculated, as was the spin-orbit coupling between them. The energy needed to reach the excited state surface is low enough, and the coupling between the states is strong enough, that crossing between the two states will be facile. The two states will be in thermal equilibrium and a significant population of the excited state is expected at typical reaction temperatures. The role of the excited state in selected reactions will also be discussed.

5:00pm **SC+EL+SS-MoA10 Dynamics of Photo-induced Reaction on a Chlorinated Si(111) Surface**, ***S. Haraichi,*** *F. Sasaki,* Electrotechnical Laboratory, Japan

In order to study photo-induced reaction of Si/Cl in the low fluence region, which is an influential candidate for low-damage manufacturing at the atomic level, the reaction mechanism was examined in terms of the photo-excitation dynamics using femtosecond second-harmonic generation (SHG). SH signals on a clean 7x7 surface show a rapid dip induced by the pump beam, which is finished within several 100 fs. It is ascribed to charge transfer from the bulk Si to the 7x7 surface and subsequent surface recombination of photo-produced carriers through surface dangling bond states. The rapid dip is not seen on the chlorinated surface, because the surface dangling bond states are disappeared. With the increase of the pump beam power the decay profile of SH signals drastically changes and an upward peak clearly appears on the chlorinated surface. The upward peak is due to the precursor of surface reaction on the Si/Cl system. Though we observed both of photo-excitation SH dynamics on an n-type and a p-type Si surface, the difference was not found. The band bending near the chlorinated surface does not contribute to the reaction dynamics, because it is most likely that the photo-produced carriers immediately flatten the bands. We also observed the reaction dynamics dependence on the pump photon energy. The threshold pump power of the reaction induced by a 1.55 eV pump peam and a 3.1 eV pump beam were 45 mW and 4 mW, respectively. This difference is not only due to an absorption coefficient but also the excitation levels and the relaxation paths, because the upward peak position of SH dynamics was different in two pump photon energy.

Semiconductors
Room 306 - Session SC+EL+SS-TuM
Compound Semiconductors

Moderator: J.W. Rogers, Pacific Northwest National Laboratory

8:20am **SC+EL+SS-TuM1 Reconstructions and Steady-state Surface Structures on InAs(001)-(2x4): Implications for Atomistic Modeling of Growth***, **W. Barvosa-Carter**, F. Grosse,* HRL Laboratories and University of California, Los Angeles*; M. Gyure,* HRL Laboratories*; J.H.G. Owen, C. Ratsch,* HRL Laboratories and University of California, Los Angeles*; R.S. Ross, J.J. Zinck,* HRL Laboratories

Heterostructures involving InAs, GaSb, and AlSb are increasingly finding applications in high-frequency, infrared, and 'spin-tronic' devices. Interface structure in these devices can be critical in determining device performance. The robustness of any model that seeks to relate process parameters and in-situ sensor signals to the surface chemistry or roughness of the growing film ultimately depends on our understanding of the relevant surface reconstructions and epitaxial growth mechanisms. Using MBE, RHEED, and atomic-resolution STM, we have studied the reconstructions and 'steady-state' surface structures present on MBE-grown InAs homoepitaxial surfaces in the (2x4) growth regime. On InAs we find two reconstructions that are relevant for growth: the familiar @beta@2(2x4) (as on GaAs) and the less familiar @alpha@2(2x4). We find excellent agreement between detailed atomic-resolution STM and first-principles simulated images of these structures. Upon quenching, we find that "steady-state" InAs surfaces exhibit small islands and adatom-like structures residing on a disordered mixture of the @beta@2 and @alpha@2 reconstructions, and that the proportions of these structures vary as a function of As pressure and temperature. Hence, the growth surface structure for InAs is remarkably different than for GaAs, where only the @beta@2 reconstruction is present with relatively few defects under device growth conditions. These results are in excellent qualitative agreement with an ab initio-based Monte Carlo model that is being developed in parallel with the experimental effort to describe reconstructions and growth on this surface.

8:40am **SC+EL+SS-TuM2 Oscillations of Local Density of States at the Epitaxially Grown InAs(111)A Surfaces Characterized by Low-temperature Scanning Tunneling Microscopy***, **K. Kanisawa**, M.J. Butcher, H. Yamaguchi, Y. Hirayama,* NTT Basic Research Laboratories, Japan

The characterization of semiconductor surface electrons is very important for understanding microscopic electron behavior. Though the local density of states (LDOS) has been studied at metal surfaces by using low-temperature scanning tunneling microscopy (LT-STM), the only studies that have been reported for semiconductors are on cleaved (110) surfaces. A LT-STM study of an epitaxial semiconductor surface makes it possible to compare the electron behavior directly with nanometer-scale morphology. We have performed a LT-STM study of the epitaxially grown InAs(111)A surface on the GaAs(111)A substrate in layer-by-layer growth mode at 5 K. Topographic and dI/dV images were obtained simultaneously by using a lock-in technique. In the dI/dV images, LDOS oscillation patterns were clearly imaged at surface defect sites, which were identified in the corresponding STM images. At an isolated defect, clear LDOS Friedel oscillations made of concentric circles were observed. From the dependence of the oscillation period, the effective mass was calculated to be 0.043m@sub 0@, which is consistent with that of InAs with a relatively high electron concentration. In the case of steps with a height difference of integral monolayers, the oscillation patterns showed dark bands along the steps. In contrast the Frank partial dislocations, with height differences of fractional monolayers, showed bright bands. This implies that there are large differences between the electron scattering phases at the steps and at the dislocations. During the InAs growth, triangular regions are formed on the surface by three {111} stacking fault planes. Such boundaries showed symmetric and regular patterns inside. Our detailed analysis suggests that these patterns are related to zero-dimensional electron systems confined within the InAs nanostructures.

9:00am **SC+EL+SS-TuM3 Something Old, Something New, Something Borrowed, Something BLUE - Fifty Years of III-V Compound Semiconductors!***, **R.D. Dupuis**[1],* University of Texas, Austin **INVITED**

III-V compound semiconductors, first identified in 1950, have become critically important for the commercial development of advanced semiconductor devices and systems. In the past fifty-some years, many workers from all over the world have contributed to this outstanding success. The epitaxial growth of III-V films began in 1960 with the early work of Holonyak who used iodine transport in a closed tube to produce epitaxial layers of GaAs/GaAs, GaAs/Ge, and various GaAsP alloys. Open-tube VPE and LPE for III-Vs were developed soon after this work. In 1967, Manasevit, et al., demonstrated the metalorganic chemical vapor deposition (MOCVD) epitaxial growth process and in 1970 Cho, et al. reported the first molecular beam epitaxy (MBE) growth of GaAs. Thus, twenty years after the first identification of III-Vs as semiconductors, all of the epitaxial growth processes we use today had been developed. It has taken 30 more years of technological and scientific advances to arrive at the understanding of these materials that we take for granted today. In fact, much of the new advanced communications systems that will be employed in the next 10 years depend fundamentally upon III-V epitaxial growth. In this talk, I will briefly review some aspects of the history of the development of these material systems and growth processes and I will discuss some of the recent results as well as speculate on the future development of III-V compound semiconductor materials.

9:40am **SC+EL+SS-TuM5 Strain-Induced Anisotropy of Gallium Phosphide Islands on Gallium Arsenide***, **C.H. Li**,* University of California, Los Angeles*; L. Li,* University of Wisconsin, Milwaukee*; Q. Fu, M.J. Begarney, R.F. Hicks,* University of California, Los Angeles

We have undertaken a study to produce ordered nanostructures on compound semiconductor surfaces by the heteroepitaxial growth of highly strained island structures. Phosphorous-rich (2x4) islands are produced by decomposing phosphine on gallium arsenide (001)-(4x2) surfaces in ultrahigh vacuum. These islands exhibit anisotropy of approximately 10 to 1 with the (2x4) domains dramatically elongated along the [110] direction. The island width increases with the phosphorous coverage from 24 @Ao@ at 0.1 ML to 48 @Ao@) at 0.75 ML. This is attributed to strain induced by the lattice mismatch of phosphorous dimers on gallium arsenide. The implication of this finding to the epitaxial growth of GaP/GaAs heterostructure will be discussed at the meeting.

10:00am **SC+EL+SS-TuM6 Relative Reactivity of Arsenic and Gallium Dimers and Backbonds during the Adsorption of Molecular Oxygen on GaAs(100)(6x6)**, ***P. Kruse**, J.G. McLean, A.C. Kummel,* University of California, San Diego

The semiconductor industry has a strong interest in understanding and employing the reactions of oxygen with III-V materials for fabrication of GaAs CMOS devices. We have monitored the initial stages of the chemisorption of molecular oxygen on the GaAs(100)(6x6) reconstructed surface by means of room temperature scanning tunneling microscopy. This surface is terminated by both gallium dimers and arsenic dimers, allowing for a direct comparison of their reactivity. Neither the As nor Ga dimer bonds react with thermal molecular oxygen. Likewise, the Ga-As back bonds of the Ga dimers do not exhibit any reactivity. Instead, the chemisorption proceeds with 100% chemical selectivity via the reaction of molecular oxygen with the As-Ga back bonds of the As dimers. The interaction between the highly electronegative oxygen atoms and the surface is initiated through the high electron density at the arsenic atoms. One oxygen atom displaces the attacked arsenic atom while the other oxygen atom bonds to two neighboring gallium atoms, resulting in the thermodynamically most stable reaction products: metallic arsenic clusters and gallium oxide.

10:20am **SC+EL+SS-TuM7 Role of Ligand Termination in Atomic-Layer-Controlled Growth***, **R.M. Osgood**, N. Camillone III, Y. Luo, M. Han,* Columbia University **INVITED**

We describe employment of a series of in situ UHV diagnostics to study the surface chemistry of ligand capping in limiting reactions for atomic-layer-defined growth of semiconductor thin films. In the study, molecular precursors were on surfaces held at temperatures from 180-300K in a UHV chamber. The terminating groups, formed by the dosing, were identified and their chemistry investigated using thermal desorption spectroscopy, NEXAFS, Auger, spectroscopy, and LEED. Using CdS growth on ZnSe(100) as the model system, we have found that CH@sub 3@ and H terminal groups

---

[1] **Featured Speaker - Science and Technology in the 21st Century**

deposited by reactions with Cd(CH@sub 3@)@sub 2@ and H@sub 2@ S, respectively, effectively limit growth precisely on all except the first monolayer. A study of intermixing in the first layer shows clearly the role of surface temperature in controlling the reaction chemistry and coverage of terminating species. The implications with regard to atomic-layer-controlled growth of other systems will also be discussed.

11:00am **SC+EL+SS-TuM9 Two-step MOCVD Growth of Piezoelectric ZnO Thin Film on SiO@sub 2@/Si Substrates***, **S. Muthukumar**, N.W. Emanetoglu, G. Patounakis, C.R. Gorla, S. Liang, Y. Lu,* Rutgers University

ZnO is a wide bandgap semiconductor with a direct bandgap of 3.3eV. Piezoelectric ZnO has high electro-mechanical coupling coefficient. Thin film piezoelectric ZnO deposited on semiconductor substrates is used for surface and bulk acoustic wave (SAW & BAW) devices, which offer advantages such as low power consumption, circuit miniaturization and cost reduction by integration with main stream MMIC technology. Furthermore, temperature compensation may be achieved in the ZnO/SiO2/Si system as ZnO and Si have positive temperature coefficient of delay (TCD), while SiO2 has negative TCD. Temperature compensated SAW devices are attractive for both communication and sensor technologies. In the present work, ZnO thin films were grown on SiO2/Si substrates by MOCVD. The structural properties of the films were investigated using XRD, SEM, and scanning probe microscopy. The films grown at 300°C were dense and had a smooth surface morphology, but poor crystallinity. In contrast, the films grown at 500°C were predominantly c-oriented, but had a rough surface. A two-step growth process was developed to obtain films with both good crystallinity and smooth surface. A high temperature (450-500°C) buffer layer was initially deposited, to provide a highly crystalline template for the subsequent low temperature (300-330°C) growth. Annealing was done on the thin films in N2 and O2 ambient for different durations to improve film resistivity, essential for fabricating low-loss SAW devices. The SAW velocity, coupling coefficient and TCD of the ZnO/SiO2/Si system were investigated through modeling and computer simulation based on Adler's transfer matrix method and Green's function analysis. The test devices with the proper ZnO and SiO2 thickness exhibited multiple temperature compensated frequency points in the 1.42 GHz to 2.15 GHz range. These results show that temperature compensated ZnO/SiO2/Si system is promising for fabricating low-loss SAW devices.

11:20am **SC+EL+SS-TuM10 Spontaneous Island Formation Caused by Reconstruction Changes During III-Sb Homoepitaxy@footnote 1@***, **A.S. Bracker**, B.Z. Nosho, B.R. Bennett, J.C. Culbertson, B.V. Shanabrook, L.J. Whitman,* Naval Research Laboratory

Most III-V semiconductor surfaces exhibit reconstructions with compositions that differ from the bulk material. These nonunity III:V stoichiometries constitute an inherent source of interfacial roughness during molecular beam epitaxy when the reconstruction changes during growth. This issue is especially important for the AlSb and GaSb(001) surfaces, because several reconstructions exist over the range of substrate temperatures and beam fluxes typically used for growth. For AlSb, the relevant reconstructions include @alpha@(4x3), @beta@(4x3), @gamma@(4x3), and c(4x4), in order of increasing Sb:Al coverage.@footnote 2@ We have used scanning tunneling microscopy (STM) and reflection high-energy electron diffraction (RHEED) to characterize how the initial stages of homoepitaxy depend on the surface reconstruction and growth conditions. When the growth conditions cause a transition between reconstructions, islands spontaneously form on the surface. In addition to roughening an otherwise flat surface, these islands change the island size distribution during subsequent growth. Unfortunately, the RHEED patterns for the three (4x3) surfaces all have a similar streaky (1x3) symmetry during growth, making it difficult to optimize growth conditions based on this diagnostic alone. However, because of its sensitivity to surface roughness, RHEED intensity oscillations may be used to monitor the reconstruction-mediated roughening. We will discuss the realistic growth situations where this type of roughening should be important. @FootnoteText@ @footnote 1@This work was supported by ONR and DARPA. @footnote 2@Barvosa-Carter et al., Phys. Rev. Lett. 84, 4649 (2000).

11:40am **SC+EL+SS-TuM11 Photon-activated Electron-Transfer-Reaction Surface Modification of GaAs(001)***, **N. Camillone III**, K.A. Khan,* Columbia University*; J.A. Yarmoff,* University of California, Riverside and Lawrence Berkeley National Laboratory*; R.M. Osgood, Jr.,* Columbia University

UHV methods for adjusting the reconstruction and composition of the top layer of atoms on a semiconductor surface are expected to have important implications for precise control of growth surfaces and surface reactions. In this talk we will describe a transformation of the surface reconstruction resulting from a photoinduced electron transfer reaction occurring thereupon. We have carried out preliminary studies which demonstrate that variation in photon exposure and thermal treatment allows the surface reconstruction to be controllably adjusted from the Ga-rich c(8x2) to the (4x6), (3x1) and As-rich c(2x8) terminations. The modification of the reconstruction is the result of a modification of the surface stoichiometry due to the extraction of surface Ga atoms as a result of reaction with bromine. The bromine is produced at the surface by photoinitiated dissociative electron attachment to methyl bromide molecules physisorbed in a single monolayer at ~ 90 K. Subsequent to the photoinduced surface reaction, the gallium is removed by annealing to desorb a gallium bromide product. A comparison of the results obtained with low energy electron diffraction, temperature programmed desorption and energy-resolved photofragment angular distribution measurements shows that the most As-rich surface obtained by our technique is identical in structure to that of a control surface prepared using the standard iodine thermal reaction method. In principle, the use of this photon-activated reaction, and others like it, could allow for precise patterning of the surface structure based on control of photon or electron exposure, molecular coverage, thermal treatment and lateral patterning of the incident photon or electron beam.

Tuesday Afternoon, October 3, 2000

Semiconductors
Room 306 - Session SC+EL+OF-TuA
Organic Chemistry on Semiconductor Surfaces

Moderator: J.E. Crowell, University of California, San Diego

2:00pm **SC+EL+OF-TuA1 Novel Reactions of Organic Molecules for Controlled Modification of Semiconductor Surfaces***, **D.J. Doren**,* University of Delaware **INVITED**

Recent theoretical work on reactions of organic molecules with semiconductor surfaces will be described. The focus will be on several mechanisms that allow molecules to react with low activation barriers on (100) surfaces of Si, Ge and diamond. Cycloaddition reactions are the most thoroughly understood reactions of organic molecules on these surfaces, having been studied extensively by both theory and experiment. This work has established several families of molecules that readily chemisorb. However, in several cases, there are competing side reactions. The origins of this competition, and some approaches to controlling selectivity tbrough the choice of precursor molecule, will be discussed. Finally, a reaction that attaches an organic molecule to the surface by dissociation (as opposed to cycloaddition) will be described.

2:40pm **SC+EL+OF-TuA3 Peter Mark Memorial Award Address***, **S.F. Bent**[1],* Stanford University **INVITED**

Tailoring the surface properties of semiconductor materials through organic modification is one means of providing new functionality to the semiconductor surface, incorporating properties such as passivation, lubrication, optical response, molecular recognition, or biocompatibility. Chemical modification also has tremendous utility for the controlled synthesis of organic/semiconductor interfaces for numerous electronic and optical applications, including the coupling of organic-based devices to silicon-based microchip technology. In this presentation, I will discuss different organic attachment strategies used to functionalize semiconductor surfaces in a dry processing environment. Unsaturated molecules, such as alkenes or dienes, can be attached by cycloaddition reaction across the Si-Si dimer at the Si(100)-2x1 surface; the reaction occurs at the surfaces of Ge and diamond, as well. Amine groups provide another reactive functionality for surface attachment. The relative reactivities of cycloaddition, N-H bond dissociation, and nitrogen lone pair interactions at the Si(100)-2x1 surface will be described using a series of pyrrole compounds. The use of protecting groups to manipulate the surface reaction pathway will be demonstrated. The potential for these different classes of attachment reactions to impact future applications will also be discussed.

3:20pm **SC+EL+OF-TuA5 Structure of Cyclopentene Adsorbed on InP (001)-(2x1) Surface***, **Q. Fu**, C.H. Li, D.C. Law, M.J. Begarney, R.F. Hicks,* University of California, Los Angeles

It has been a growing interest in engineering ordered, defect free organic thin films on semiconductor substrates for the next generation miniature electronic devices. Using metalorganic vapor phase epitaxy, we have successfully grown indium phosphide (2x1) surface terminated with a complete layer of phosphorous dimers. On InP (2x1) surface, a dangling bond on each phosphorous dimer is filled with a single electron, which makes it an ideal substrate for growing organic films through reactions with @pi@-bond of unsaturated molecules. Here, we have characterized the molecular structure of cyclopentene adsorbed on the InP (2x1) surface by scanning tunneling microscopy, internal-reflectance infrared spectroscopy, reflectance difference spectroscopy, and molecular cluster calculations. It is found that the exposed phosphorous dimers are the adsorption sites for the unsaturated organic molecule. Two adsorption configurations were identified: one with the C@sub 5@H@sub 8@ molecule sitting on top of a P dimer, and another one with the C@sub 5@H@sub 8@ molecule bridging across two neighboring P dimers. At the meeting, we will present a comparison of cyclopentene adsorption characteristics on InP (001)-(2x1) versus Si (100)-(2x1).

3:40pm **SC+EL+OF-TuA6 Formation and Reaction of Organic Layers on Germanium: Reaction of 1,5-cyclooctadiene with the Ge(100) Surface***, P. Prayongpan, D.S. Stripe, **C.M. Greenlief**,* University of Missouri, Columbia

Organic alkenes can bond to Ge(100) surfaces to produce monolayer organic films that are chemically homogeneous and structurally ordered. The bonding of these molecules to the Ge(100)-(2x1) reconstructed surface is analogous to a class of ring-forming reactions known in organic chemistry as [2+2] cycloaddition reactions. While the bulk reactions involve the reaction of two alkene groups to form a four-member ring, the analogous surface reaction involves two electrons from the organic alkene and two electrons from the surface Ge=Ge dimers. Here, the formation of ordered organic layers on Ge(100) substrates is examined by the reaction of 1,5-cycloocatadiene with Ge(100). This molecule reacts with the Ge dimers leading to a [2+2] cycloaddition reaction product. A combination of ab initio calculations and surface sensitive experimental techniques are used to probe the interactions. Surface modification of the organic layers is also explored. The reaction of the organic layers with atomic hydrogen and a series of alcohols will be discussed.

4:00pm **SC+EL+OF-TuA7 A Comparative Study of the Bonding of N-Containing Heterocyclic Molecules to the Si(001) Surface***, **X. Cao**, S.K. Coulter, H. Liu, J. Liu, R.J. Hamers,* University of Wisconsin, Madison

Recent studies of a variety of unsaturated hydrocarbons has lead to increased interest in understanding the factors controlling bonding of more complex organic molecules to silicon surfaces. By understanding the propensity for heterocyclic molecules to bond into various possible configurations, we are able to gain insight into the factors controlling selectivity in molecule-surface bonding. We have studied the adsorption of pyrrole and its partially-unsaturated analog, 3-pyrroline, onto the Si(001)-(2x1) surface using Fourier-transform infrared spectroscopy, X-ray photoelectron spectroscopy, and scanning tunneling microscopy (STM). At 300 K, XPS spectra of pyrrole show a single, sharp N(1s) level, while FTIR spectra show that the molecule retains the high-frequency peaks that are characteristic of aromatic molecules; isotropic labeling studies show that attachment occurs through the N atom via cleavage of the N-H bond. These results show that pyrrole retains its aromatic character after bonding to the surface. In contrast, XPS and FTIR data for 3-pyrolline shows that it can bond through the N atoms or through its C=C bond via the surface equivalent of a [2+2] cycloaddition reaction. This study shows that molecules with aromatic rings show a strong preference for retention of this aromaticity, while molecules without aromaticity have more diverse chemical bonding configurations. Implications for understanding the attachment of other N-containing molecules to surfaces will be discussed.

4:20pm **SC+EL+OF-TuA8 Reaction of Pyrrole and Pyrrole Derivatives on Si(100)-2x1***, **G.T. Wang**, C. Mui, C.B. Musgrave, S.F. Bent,* Stanford University

The ability to covalently bond to semiconductor surfaces organic layers with custom-tailored functionality could have applications in a number of areas, including lithography, molecular electronics, sensors, and low k dielectric materials. Previous studies have shown that the Si(100)-2x1 surface dimer can react with unsaturated hydrocarbons, forming covalently bound [4+2] Diels-Alder and [2+2] cycloaddition products at the surface. Amines have shown promise as alternative candidates for layer-by-layer growth and the model amine ammonia is known to react with silicon via N-H dissociation across the surface dimer. The use of more complex amines for surface modification requires an understanding of how various functional groups in the amine affect its reactivity and bonding configuration with the surface. In this study, the interaction of pyrrole and pyrrole derivatives, including saturated and unsaturated secondary and tertiary amines, with the Si(100)-2x1 surface under ultra-high vacuum is investigated via multiple internal reflection infrared spectroscopy, Auger electron spectroscopy, temperature programmed desorption studies, and ab initio quantum chemistry calculations. The results show that the nitrogen lone pair plays an important role in the reaction of amines with the Si(100) surface. In particular, the stable room temperature molecular adsorption of methylpyrrolidine through its lone pair is permitted due to the presence of a protecting methyl group, while its unprotected analogue, pyrrolidine, proceeds to covalently bond to the surface through N-H dissociation. Additionally, results examining the reaction of the Si(100) surface with a model amide (N-methylacetamide), which contains both carbonyl and amine functionalities through a peptide unit and hence could serve as a bifunctional unit for layer-by-layer growth, are presented.

4:40pm **SC+EL+OF-TuA9 Attaching Aromatic Molecules to the Si(001) Surface via Oxygen and Sulfur Tethers***, **S.K. Coulter**, M.P. Schwartz, J. Liu, R.J. Hamers,* University of Wisconsin, Madison

Phenol, benzenethiol and phenyl disulfide have been used as model systems to compare the bonding of chemically-similar aromatic molecules to the Si(001)-2x1 surface through different Group VI tethers. The behavior of these substituted aromatic hydrocarbons on the Si(001) surface has

---

[1] **Peter Mark Memorial Award Winner**

been investigated using Fourier transform Infrared Spectroscopy (FTIR), X-ray Photoelectron Spectroscopy (XPS) and Scanning Tunneling Microscopy (STM). Both FTIR and XPS indicate that phenyl disulfide bonds exclusively through the sulfur substituent groups. Phenol and benzenethiol molecules bond predominately through their oxygen/sulfur substituent groups, although a small minority may chemisorb on the surface via ring attachment. Thermal studies indicate that the molecules attached to the surface via sulfur or oxygen tethers are stable to temperatures above 550 K. STM studies show that these molecules attach directly to the silicon dimer and, in the case of phenyl disulfide, form ordered rows of aromatic rings.

5:00pm **SC+EL+OF-TuA10 Chemical Reactions on the Diamond(100) Surface: First-principles Theory and Comparisons to Experiment***, **D.R. Fitzgerald**, D.J. Doren,* University of Delaware

Density functional theory calculations have been used to investigate the structures, energetics, and reaction pathways of the [4+2] and [2+2] cycloaddition reactions of butadiene with the C(100)-2x1 surface. One-dimer and three-dimer cluster models were used to represent the surface. Vibrational spectra of the product species were also calculated. Activation free energies suggest that the [4+2], or Diels-Alder mechanism, will be kinetically favored. The presence of adjacent unreacted surface dimers affects the orientation of the cycloaddition product. The adsorption of hydrogen on the surface has also been studied. Cluster size is seen to have a large effect on the vibrational spectrum of the adsorbed hydrogen. Theoretical results are compared to recent experiments.

Semiconductors
Room 306 - Session SC+EL+SS-WeM
Passivation and Etching of Semiconductors

Moderator: Y.J. Chabal, Bell Laboratories, Lucent Technologies

8:20am **SC+EL+SS-WeM1 Infrared Study of the Initial Stages of Etching of Si Electrode Surfaces in HF Solution***, Y. Kimura, Y. Kondo, J. Nemoto,* ***M. Niwano,*** Tohoku University, Japan

Porous Si has been a promising class of materials used for light-emitting devices and nano-scale electronic devices, and a number of theoretical and experimental investigations have been performed on the formation and optical properties of porous Si. A conventional method of synthesizing porous Si is to apply an anodic (positive) potential to a Si electrode in aqueous etching solutions such as dilute hydrofluoric acid (HF) solution. However, the mechanism of pore formation has not been fully understood. In order to control the structure of porous Si, we need an understanding of the microscopic etching process of Si electrode surfaces during immersion in etching solution. In this study, we have investigated in-situ and in real time the etching process on p-Si(100), (111), and (110) electrode surfaces in dilute HF solution, using infrared absorption spectroscopy (IRAS) in the multiple internal reflection (MIR) geometry, and analyzed infrared absorption spectra in the Si-H stretching vibration region of the electrode surface to examine how surface Si atoms are removed. At electrode potential below approximately 1 V, surface roughening occurs to produce hydride species in the vicinity of the electrode surface. At initial stages of etching of a Si(100) electrode, monohydride species is dominantly populated by the removal of dihydride species on the topmost layer of the electrode surface. We suggest that removal of monohydride species is favored over that of dihydride species, leading to the formation of pores on the etched surface. At electrode potential above 1 V, all the hydride species are etched away, leading to electropolishing of the surface. For electrochemical etching of Si(110), monohydride species are removed from the topmost layer to populate dihydride species on the second layer of the surface. For etching of the Si(111) surface, it appears that removal of surface Si atoms more favorably takes place at step sites than on terraces.

8:40am **SC+EL+SS-WeM2 Electrical Transport at Chemically Modified Silicon Surfaces***, O. Hul'ko, R. Boukherroub, C. Mark, S.N. Patitsas, H.Z. Yu,* ***G.P. Lopinski,*** National Research Council Canada

We are exploring methods for tailoring the electrical conductivity of silicon surfaces via the covalent attachment of atomic and molecular adsorbates. A method for studying the electrical transport properties of wet-chemically modified silicon surfaces has been developed and applied to study of chlorine terminated Si(111). Resistivity measurements (4-probe, van der Pauw geometry) were performed on low doped n-type Si (111) substrates patterned with titanium silicide contacts. These contacts were found to withstand the RCA clean and ammonium flouride etching procedures required to prepare the atomically flat, highly ordered hydrogen terminated Si(111) surfaces that are the starting point for fabricating chemically modified Si(111) surfaces. Chlorine-termination was achieved by UV irradiation of H/Si(111). The resulting surfaces were characterized by STM and Auger, indicating a monolayer of Cl in an ordered (1x1) structure. These Cl/Si(111) surfaces showed a significant (at least one order of magnitude) increase in conductivity with respect to H/Si(111). Under ambient conditions the conductivity decreased exponentially with a time constant of ~1hr., eventually returning to the value measured before chlorination. The enhanced conductivity of the Cl/Si(111) surface is attributed to increased carrier density in the near surface region due to upward band banding caused by the electron withdrawing nature of the adsorbed chlorine. In order to explain the increased conductivity this band bending must be sufficient to cause inversion (>0.6eV). Capacitance measurements indicate that the near surface carrier concentration is increased by at least a factor of 1000 upon chlorination, consistent with the observed conductivity change. Results on other chemically modified surfaces will also be presented.

9:00am **SC+EL+SS-WeM3 Using Micromachined Test Patterns to Study Surface Chemistry: An Investigation of Etchant Anisotrophy***,* ***M.A. Hines,*** *R.A. Wind,* Cornell University

We have developed a new technique for the rapid quantification of etchant anisotropy (i.e. orientation-dependent etch rates), which uses micromachined test patterns. Although macroscopic anisotropy cannot be inverted to provide detailed atomic mechanisms, macroscopic anisotropies do provide important clues to the underlying chemical reactions. For example, an etchant that produces atomically flat silicon surfaces -- a "perfect" etchant -- must selectively etch all defect sites, while leaving the flat surface virtually untouched. Macroscopically, this implies that a perfect etchant must attack vicinal surfaces much more rapidly than flat surfaces. Our standard test pattern consists of 180 1°-wide wedges arranged in an evenly spaced, circular array. Each wedge is bounded by a different set of vertical planes, so the sides of each wedge etch with a characteristic, face-dependent rate. Anisotropic etching leads to the development of a "flower pattern," which can be analyzed to yield absolute, face-spec ific etch rates of 180 surfaces simultaneously. Etch rates measured with this technique are in good agreement with those previously reported in the literature. This technique opens to door to a pseudo-combinatorial approach to etchant development. For qu a ntitative interpretation of these data, we constructed a simple model of orientation-dependent etching that is based on step-flow etching. We tested this model on a number of different anisotropic etchants, and the model performed surprisingly well. Interestingly, there was no evidence of direct step-step interactions or step coalescence on vicinal Si(111) surfaces during etching (within approx. 20° of the close-packed plane).

9:20am **SC+EL+SS-WeM4 Etching of BPSG Films Using Anhydrous HF***, A. Thorsness, G. Montano,* ***A. Muscat,*** University of Arizona

The absorption of water within BPSG films and its affect on the rate and the product distribution on the surface during etching with anhydrous HF (AHF) has been studied with transmission FTIR and ellipsometry. Gas phase HF chemistries are currently used to selectively etch doped oxide films relative to undoped films for both DRAM and MEMs applications, but often require a post-process water rinse. BPSG films containing 3.5%B/4.0%P were deposited to a nominal thickness of 5K Å on 8" Si wafers containing a 2K Å TEOS buffer layer. Sets of 25 wafers were annealed after deposition to four different temperatures: as deposited (400°C), 500°C, 750°C, and 900°C. The films were etched at atmospheric pressure and at temperatures from 25 to 75°C in a commercial gas phase oxide etching tool (FSI Excalibur ISR) using AHF in a nitrogen carrier. Water uptake by the films did not saturate but increased at a steady rate as a function of annealing temperature during storage in a cleanroom. Absorbed water reacted with P=O producing P-OH groups. The induction time to start etching decreased with water absorption and loss of P=O. Based on relative bond strengths AHF attacks the P-O bonds first opening up the silicon dioxide lattice and producing both a P-bearing acid and product water. The product water H-bonds to the P-bearing acid creating a thin liquid film on the wafer surface. The liquid film supports etching of the stronger Si-O-Si and B-O-Si bonds and solvates etching products. The water H-bonded to the P-bearing acid lowers the activation barrier to breaking Si-O bonds by forming a (SiO)HOH complex. The weakened Si-O bond is more amenable to attack by a polar HF molecule. Metaphosphoric acid, pyrophosphoric acid, boric acid, boron trifluoride, and water were present in the liquid films after etching. The relative amount of these products was a strong function of the annealing temperature.

9:40am **SC+EL+SS-WeM5 Etching of Polymer-like a-Si:H Films by Impact of H*, T. Zecho*,** *B. Brandner,* Universitaet Bayreuth, Germany*; J. Biener, J. Kueppers,* Max-Planck-Institut fuer Plasmaphysik (EURATOM Association), Germany

Etching of a-Si:H thin films with H atoms is a well known phenomenon from earlier studies. Nevertheless, the product distribution and the temperature dependence of the absolute etching rate could not be unambiguously determined. The present study was performed in order to quantify the etching rate by direct detection of the etching products during H admission and to determine to what extent higher silane species contribute to the etching process. A-Si:H films in a thickness range ca 1 to 100 nm were deposited at 300 K by ion-beam-deposition on a Pt(111) substrate and characterised by AES, TPD, HREELS and ELS. The films grow in a two-dimensional fashion and show a polymer like structure with a hydrogen content of about 40 %. The thermal stability of the films is limited by the formation of a Pt silicide commencing ab about 500 K which proceeds at the a-Si:H/Pt interface. In accordance with the exothermic formation of volatile silanes a constant etching rate of about 1 % between 100 K and 300 K was found with about equal contributions from the silane and higher silanes channels. In this temperature range even minor impurities lead to a decrease of the etching rate. From 300 K to 500 K the etching rate decreased roughly linear to 0.1 % due to the growing thermal instability of the higher silanes. Therefore at 500 K silane was the only detected etching product. The formation of both silane and higher silanes proceeds via a direct interaction of atomic hydrogen and the corresponding precursor species.

10:00am **SC+EL+SS-WeM6 Reaction Mechanism of Si(100) Etching by Mass- and Energy-Selected Cl+ Beams***, **S.M. Lee**, M. Lu, J.W. Rabalais,* University of Houston

Plasma etching of semiconductor materials is a standard manufacturing technique used in integrated semiconductor industries. Due to the high operational pressures used in this process, it is difficult to study the basic etching mechanism. While plasma etching is a dynamic process, many studies have been done on the more static systems using analysis techniques like temperature programmed desorption (TPD). In this work, the kinetic energy and temperature dependencies of Cl+ beam etching of Si (100) have been studied by Auger electron spectroscopy (AES), X-ray photoelectron spectroscopy (XPS), reflection high energy electron deflection (RHEED), and positive and negative energy-filtered secondary ion detection. Ion kinetic energies were varied over the hyperthermal range of 1 - 500 eV and sample temperatures were varied over the 25 - 700Â° C range. Chemical etching dominates in the low energy range, while both chemical and physical etching processes are prevalent at the higher energies. Both the AES and XPS results demonstrate that the amount of Cl deposited on the surface is a strong function of the ion energy. The RHEED study of the surface crystallinity clearly showed the existence of synergetic effects due to simultaneous ion bombardment and annealing. A nearly ideal (2x1) surface reconstruction was obtained under the conditions of 100 eV Cl+ etching at 600Â°C. AES analysis demonstrated that the main source of surface disordering at lower temperatures and lower kinetic energies is residual Cl in the surface region. The etching products, the kinetic energy distribution of each species, and the critical kinetic energy for the etching process have been measured for different temperatures by using the positive and negative ion detector. The overall reaction mechanism is discussed based on the results obtained.

10:20am **SC+EL+SS-WeM7 Deuterium Etching of the Si-rich SiC(0001)-(3x3) Surface Reconstruction***, **C.R. Stoldt**, C. Carraro, R. Maboudian,* University of California, Berkeley

The low-energy electron (LEED) pattern of the SiC(0001)-(3x3) surface reconstruction undergoes a conversion from (3x3) to (1x1) upon exposure to atomic hydrogen (and deuterium). Using high-resolution electron energy loss spectroscopy, Auger electron spectroscopy, LEED, and temperature programmed desorption, we have determined that this conversion is due to etching and disordering of the uppermost Si layers. With increasing deuterium exposure at 320 K, etching results in depletion of the Si adlayer and formation of SiD surface species. At high deuterium exposure, observation of the C-D stretch mode indicates the onset of bulk silicon carbide etching. SiD@sub 2@ and SiD@sub 3@ surface species, known intermediates in the Si etching process, are observed with deuterium exposure at 180 K.

10:40am **SC+EL+SS-WeM8 Variable Temperature Study of Hydrogen and Deuterium Passivation of the Si(100)-2x1 Surface using the Scanning Tunneling Microscope***, M.C. Hersam, **N.P. Guisinger**, K. Cheng, J. Lee, J.W. Lyding,* University of Illinois

Deuteration of dangling bonds at the Si/SiO@sub 2@ interface has led to a significant reduction of hot carrier degradation in complementary metal-oxide-semiconductor (CMOS) circuits. Although CMOS transistors are annealed in a D@sub 2@ environment, the presence of H in the oxide leads to the interface being unavoidably exposed to both H and D during the passivation process. Thus, an understanding of the parameters that affect the equilibrium quantities of H and D on Si surfaces is of notable interest. In this paper, the relative concentrations of H and D on the Si(100)-2x1 surface are studied following in situ passivation under conditions of equal H and D pressure. Electron stimulated desorption with a scanning tunneling microscope allows for atomically precise determination of the H and D levels. The ratio of D to H on the Si(100) surface is measured to be ~50 and ~5 following monolayer passivation at 350 K and 650 K respectively. This behavior can be qualitatively understood through a statistical thermodynamics model. Ultimately, the magnitude of the D:H ratio and its inverse relationship with passivation temperature result from the difference in the vibrational frequencies for Si-H and Si-D bonds. These results imply that the optimal deuteration of silicon dangling bonds in the presence of background H should occur at low sample temperatures. Since CMOS processes are continually reducing their thermal budgets to accommodate additional metal layers and novel materials (e.g., low k dielectrics), this paper fundamentally suggests that deuteration of the Si/SiO@sub 2@ interface could improve as processing temperatures are inevitably lowered in the future.

Semiconductors
Room Exhibit Hall C & D - Session SC+EL+SS-WeP
Poster Session

SC+EL+SS-WeP1 Selectivity in Attachment of a Model pi-conjugated Organic Molecule to a Group IV Semiconductor Surface: Styrene on Si(001)*, **M.P. Schwartz**,* University of Wisconsin, Madison*; M.D. Ellison,* Wittenberg University*; S.K. Coulter, R.J. Hamers,* University of Wisconsin, Madison

The bonding of styrene to the Si(001) surface has been investigated as a model system for understanding selectivity in the attachment of conjugated pi-electron systems to semiconductor surfaces. Scanning tunneling microscopy images show one primary bonding configuration, slightly off-center from the middle of a dimer row. Infrared spectra using isotopically-labeled styrene establish that attachment occurs in a highly selective way, bonding through the external vinyl group and leaving the aromatic ring almost completely unperturbed. The implications for the high degree of selectivity in understanding attachment of other conjugated pi-electron systems are discussed.

SC+EL+SS-WeP2 Ferrocene and Decamethylferrocene Adsorption and Decomposition on Ag(100) and Si(111)*, **C.M. Woodbridge**, D.L. Pugmire,* University of Nebraska, Lincoln*; N.M. Boag,* University of Salford*; M.A. Langell,* University of Nebraska, Lincoln

Although metallocenes show potential as Chemical Vapor Deposition (CVD) source molecules, there is comparatively little known about their interactions with oriented substrates. We have investigated the adsorption and decomposition of ferrocene (FeCp@sub 2@) and decamethylferrocene (FeCp@sub 2@*) on Ag(100) and Si(111) using High Resolution Electron Energy Loss Spectroscopy (HREELS), Temperature Programmed Desorption (TPD), and X-ray Photoelectron Spectroscopy (XPS). For weakly-interacting systems such as those which occur with Ag(100), both FeCp@sub 2@ and FeCp@sub 2@* are adsorbed molecularly at 130 K. Monolayers of both FeCp@sub 2@ and FeCp@sub 2@* are oriented such that their molecular axes are perpendicular to the plane of the Ag(100) substrate; monolayer desorption occurs at approximately 250 K for both metallocenes. While FeCp@sub 2@ desorption is clean, FeCp@sub 2@* shows significant amounts of metallocene dissociation competing with molecular desorption. The Si(111)/metallocene systems also show molecular adsorption at 130 K but are more reactive to thermal decomposition upon heating and decompose primarily through hydrogenation and ligand-metal dissociation mechanisms. Specific information about the orientation of the adsorbed species and decomposition intermediates will be discussed.

SC+EL+SS-WeP3 Lowering of Processing Temperature due to a High Pressure Deuterium Anneal for Improved CMOS Hot Carrier Reliability*, **J. Lee**, K. Cheng, K. Hess, J.W. Lyding,* University of Illinois, Urbana*; Y.K. Kim, Y.W. Kim, K.P. Suh,* Samsung Electronics Co., Ltd.

The deuterium (D) isotope effect has been found to be very effective in reducing hot carrier induced degradation in CMOS transistors of numerous technologies. The magnitude of lifetime improvement (10x to 100x) varies from one technology to the other, but it directly correlates with D incorporation at the gate SiO@sub 2@/Si interface. Secondary ion mass spectrometry (SIMS) depth profiling has been used to make this determination. We have recently implemented high pressure D annealing to enhance its incorporation at the interface. By increasing the D pressure, the concentration at the interface can be increased for a fixed annealing temperature. Consequently, lower temperatures and shorter anneal times can achieve equivalent transistor reliability. This promises to be a technologically significant result for future CMOS production which requires a much lower thermal budget process due to the introduction of advanced materials (e.g. low k dielectrics) and increased number of metal layers. This high pressure annealing technique has been applied to one of the most recent CMOS technologies from Samsung Electronics. For these short-channel (0.18 µm) and low operating voltage (1.5V) devices, the isotope effect is substantially enhanced (700x). Rather than being scaled away, deuterium reduction of hot electron damage appears more relevant in future generations of CMOS integrated circuits. In the current work, the annealing temperature has been lowered from 450@degree@C to 350@degree@C. Although the lifetime improvement is not as great, we do observe a significant lifetime improvement (300x) just from changes in pressure. More experiments are in progress to maximize the D incorporation at the low annealing temperature. In addition, SIMS depth profiles are being determined for devices that were sintered at different annealing conditions.

SC+EL+SS-WeP4 Investigation of the Penetration of Atomic Hydrogen from the Gas Phase into a SiO@sub 2@/GaAs System*, **V.A. Kagadei**,* Research Institute of Semiconductor Devices, Russia*; E.V. Nefedtsev,* Tomsk University of Control Systems and Radioelectronics, Russia*; D.I. Proskurovsky,* Institute of High Current Electronics, Russia

Introduction of hydrogen into near-surface layers of semiconductor materials (hydrogenation) substantially varies their properties. In some cases hydrogenation improves the electrophysical parameters of the material and allows one to create devices with improved characteristics, while in other cases the penetration of hydrogen into a solid accompanies a technological process and causes unwanted changes in the parameters of the material. Therefore, it appears urgent to investigate the penetration of hydrogen into a semiconductor material, and a better understanding of this process will make it possible to optimize the technology of hydrogenation. The hydrogenation of GaAs samples coated with thin (5 nm) SiO@sub 2@ film was investigated. Samples were treated in a flow consisting of a mixture of atomic and molecular hydrogen produced by a source whose operation is based on a reflected arc discharge with a hollow cathode and a self-heating element. The hydrogenation time was 5 - 30 min, the hydrogenation temperature was 150 - 300 C, and the hydrogen pressure was varied from 10@super -1@ - 10@super -3@ Pa. It has been established that an increase in discharge current results in an increase in the concentration of atomic hydrogen in the gas phase, N, and in a decrease in the number of atoms penetrating into samples, and this is in contradiction with the usual notions about the penetration of hydrogen atoms into a solid. The data obtained suggest that the amount of hydrogen penetrating into samples is more dependent on the probability of the penetration of hydrogen atoms into a solid body, F, rather than on N. It has been proposed that F decreases substantially with decreasing the energy of the hydrogen atoms arriving at the solid surface. The energy of the atoms emerging from the reflected-arc-discharge-based source is estimated to vary between 0.1 and 10 eV. It is determined by the operating voltage of the discharge and decreases with increasing discharge current. Another possible cause of the observed phenomena is the formation of a near-surface diffusion barrier constituted by immobile hydrogen molecules, which occupy interstitials and retard the diffusion of atoms. The contribution of each of the proposed mechanism is discussed.

SC+EL+SS-WeP5 a-SiC:H Thin Films Fabricated by the High Rate Deposition Method*, **B.G. Budaguan**, A.A. Sherchenkov,* Moscow Institute of Electronic Technology, Russia*; A.A. Berdnikov, V.D. Chernomordic,* Institute of Microelectronics of Russian Academy of Science*; A.A. Aivazov,* UniSil Corp.

The a-SiC:H alloys are considered to be a perspective wide band gap material for different optoelectronic utilization. For the commercial application it is necessary to increase the deposition rate. However the increase of the growth rate results in the increase of structural inhomogeneity and in the deterioration of electronic properties of amorphous layers. Recently we have shown that deposition rate of a-Si:H films with high electronic properties can be increased with using of low frequency (55 kHz) glow discharge. In this work we investigated the growth mechanism and microstructure of a-SiC:H thin films fabricated for the first time by this method. The a-SiC:H films were deposited at different methane content from 0 to 100%, substrate temperatures T@sub s@ from 160 to 320 °C, and different discharge regimes: continuous wave and square wave modulated (SQWM). It was shown that the increase of the deposition rate of a-SiC:H films (5.3-11.1 Å/s depending on the methane content in gas mixture) in comparison with the standard deposition technology (3 Å/s for 13.56 MHz PECVD) is caused by the close position of a-SiC:H precursors formation to the growth surface. The joint analysis with using of infrared/optical spectroscopy and atomic force microscopy measurements showed that a-SiC:H films has the island type microstructure where the clustering of C atoms occurs at the island surfaces in the form of C-H@sub n@ bonds. The increase of C-H@sub n@ configurations on islands surfaces at high C content facilitate the relaxation of rigid a-SiC:H network through formation of flexible sp@super 2@-sites. The incorporation of Si-C bonds in the interior of islands determines the optical bandgap while the clustering of CH@sub n@ and SiH at the islands surface leads to the formation of graphite-like microstructure. It was shown that the suppression of formation of graphite-like microstructure at low T@sub s@ and in SQWM plasma allows to fabricate device quality alloys.

SC+EL+SS-WeP6 Mechanism for and Site of the Dissociative Chemisorption of XeF@sub 2@ on Si(100)2x1 Below 1 ML of Fluorine Coverage*, J.R. Holt,* *R.C. Hefty, M.R. Tate, S.T. Ceyer,* Massachusetts Institute of Technology

Upon exposure of a clean Si(100)2x1 reconstructed surface to a beam of xenon difluoride incident with an average kinetic energy of 0.9 kcal/mol, the XeF@sub 2@ dissociatively chemisorbs by atom abstraction solely on the Si dangling bonds up to a fluorine coverage of one monolayer (ML) before it begins to react with the Si-Si lattice bonds. This conclusion is based on the observations of scattered XeF and the preservation of the 2x1 dimer row reconstruction at 1 ML fluorine coverage. The scattered XeF is detected by a line-of-sight and differentially pumped mass spectrometer while the order of the surface is monitored by He diffraction. A clean Si(100)2x1 surface is characterized by three primary features in a He diffraction spectrum: a specular feature due to the smoothness and general order of the surface, a half-order feature due to diffraction perpendicular to the dimer rows, and a first order feature due to diffraction parallel to the dimer rows. The presence of the half-order feature at a fluorine coverage of 1 ML provides evidence that even the Si-Si sigma dimer bonds are undisturbed, preserving the original dimer rows. The reaction exothermicity of approximately 230 kcal/mol does not destroy the surface order. Molecular fluorine has previously been observed to react with a clean Si(100)2x1 surface in a similar manner by atom abstraction, saturating the Si dangling bonds at a coverage of 1 ML. The 2x1 periodicity is maintained. However, after saturation of the dangling bonds, F@sub 2@ ceases reacting with the surface while XeF@sub 2@ continues to deposit fluorine on the surface by its reaction with the Si-Si sigma dimer bonds and the Si-Si lattice bonds. The surface order is destroyed as a result of the continued fluorine deposition and ultimately etching occurs by the formation of volatile SiF@sub 4@.

SC+EL+SS-WeP7 STM Investigations of the Initial Ad- and Desorption Sites of Molecular Hydrogen on Si(001)*, M. Dürr,* Philipps University Marburg, Germany*; A. Biedermann, Z. Hu,* Columbia University*; U. Höfer,* Philipps University Marburg, Germany*; T.F. Heinz,* Columbia University

Whereas the extremely small sticking coefficients for dissociative adsorption of H@sub 2@ on Si surfaces indicate a high, the almost thermal energy distribution of the desorbing H@sub 2@ molecules points to a low barrier in the reaction channel. Recent molecular beam experiments have shown that this apparent contradiction is in full accordance with the principle of detailed balance and can be understood in terms of phonon-assisted sticking.@footnote 1@ To shed light on the underlying microscopic mechanisms, we have adsorbed H@sub 2@ on Si(001) at temperatures below the onset of H diffusion and investigated the site distributions with scanning tunnelling micrcoscopy (STM). The STM images show configurations of 4 adsorbed H atoms indicating a two-step process with an inter-dimer rather than the commonly assumed intra-dimer adsorption path as the relevant initial step. In the inter-dimer path, H@sub 2@ interacts with two dangling-bonds on adjacent Si dimers and forms a transition state with relatively large lattice distortion. Single-shot laser-induced thermal desorption experiments from nearly perfect hydrogen monolayers reveal distributions of unsaturated dangling bonds which indicate that the reverse path is also active in desorption. The influence of coverage, minority reaction channels as well as the consequences of the results on the reaction kinetics will be discussed. @FootnoteText@ @footnote 1@ M. Dürr, M. B. Raschke, and U. Höfer, J. Chem. Phys. 111, 10411 (1999).

SC+EL+SS-WeP8 Photoemission Study on Initial Oxidation of Si(001) Surfaces with Supersonic O@sub 2@ Molecular Beams*, Y. Teraoka,* Japan Atomic Energy Research Institute, Japan*; A. Yoshigoe,* Japan Atomic Energy Research Institute

We made a new surface reaction analysis apparatus at a soft x-ray beamline (BL23SU) in the SPring-8 (Super Photon ring-8GeV) to study incident energy effects for reactant chemisorption on semiconductor surfaces. As the first step, initial oxidation of Si(001) with O@sub 2@ has been investigated because that is not only interesting for surface reaction analysis but also important as electronic device development. The maximum incident energy was 3 eV in calculation. The clean Si(001) surfaces were irradiated by the supersonic O@sub 2@ molecular beams with various incident energy to achieve saturated adsorption. The oxygen amount on the surface was evaluated by measuring O-1s photoemission intensity. The intensity depended on the incident energy and two thresholds of 1.0 eV and 2.6 eV were found. These values are very resemble to the predicted values of 0.8 eV and 2.4 eV from the first-principles calculation, showing potential energy barriers for dimer backbond oxidation and oxygen insertion between the second and the third layer. Si-2p photoemission spectra were obtained at room temperature and 873 K by using high resolution soft x-rays from the beamline. In the case of room temperature, the maximum silicon oxidation number increased with increasing the incident energy from Si@super 2+@ to Si@super 4+@. Whereas a peak corresponding to SiO@sub 2@ was minor even in the case of 2.9 eV at room temperature, the peak was apparent in 873 K cases. Thermal energy may drive oxygen migration to form the SiO@sub 2@ structure. Even at such high temperature, incident energy affected in sub-oxide peak composition. The sub-oxide peak for Si@super 3+@ was increased with increasing the incident energy and was dominant in the case of 2.9 eV whereas the peak for Si@super 2+@ was primary in the case of 0.6 eV. The variation may be resultant from the Si@super 3+@ increase due to oxidation of dimer and sub-surface silicon atoms depending on the incident energy.

SC+EL+SS-WeP9 The Effect of Time and Moisture on the Adhesion Bond between Silica Particle and Silicon Oxide Substrate*, J.W. Feng*, *A.A. Busnaina,* Clarkson University

Adhesion of silica particles to silicon wafers is a problem that affects semiconductor manufacturing processes. The particle adhesion forces are greatly affected by the environment such as humidity, temperature and adhesion induced stress between the particle and the wafer following the particle deposition. The adhesion forces considered in the process include van der Waals, capillary force, double layer force and hydrogen bonding. In this study, silica particles are deposited onto wet and dry thermal oxide silicon wafers, then the samples are aged in different relative humidity environments. Results show that the largest increase in contact area between silica particles and thermal oxide wafers occur when the particle is first deposited on wet surface then aged in relative humidity above 55%. Higher humidity, results in higher adhesion force and lower removal efficiency. Results also indicate that adhesion force increases by more than two order of magnitude after the aging process. This suggests that hydrogen and covalent bonds are responsible for the increase in the adhesion force especially in humid environments.

SC+EL+SS-WeP10 Influence of Growth Direction on Order-Disorder Transition in (GaAs)@sub (1-x)@(Ge)@sub 2x@ Semiconductors*, A.G. Rodriguez,* ***H. Navarro-Contreras****, M.A. Vidal,* University, Mexico

We provide direct evidence of the dependence on the growth direction of the critical concentration of IV atoms at the order-disorder transition in ternary metastable (III-V)-IV, zincblende-diamond semiconductor alloys. The excellent agreement between the experimental and model predicted critical concentrations is evidence that the atomic ordering in these alloys is ruled almost entirely by substrate geometry. We report the observation of the critical concentration dependence on substrate orientation in (GaAs)@sub (1-x)@(Ge@sub 2@)@sub x@ metastable alloys, epitaxially grown on (001), (111), (112) and (113) GaAs. A different long-range order parameter behavior with Ge concentration is obtained for each growth direction, 0.36, 0.96, 0.59, and 0.50 ± 0.03, respectively, numbers that compare well with results of a Montecarlo simulation of the growth, 0.33, 1.0, 0.64 and 0.54, respectively.

SC+EL+SS-WeP11 Surface Electronic Structure of p-type GaN(000-1)*, P. Ryan*, *Y.C. Chao, K.E. Smith,* Boston University

Our investigation sought to describe the surface electronic characteristics of MBE grown (Mg-doped) wurtzite p-GaN (0001'). Four surface bands were mapped within the surface Brillouin zone. The peaks have been removed by atomic hydrogen exposure and three of the peaks show pz orbital configuration, the fourth an s orbital. The most interesting peak is a highly dispersing surface state which sweeps from the bulk valence band into the forbidden bulk band gap, approaches the Fermi level then returns to the bulk valence band. We compare this state to previously predicted mid-gap surface states.

SC+EL+SS-WeP12 Ultrafast Dephasing of Coherent Phonons by Lattice Defects in n-GaAs*, M. Kitajima,* *M. Hase, K. Ishioka,* National Research Institute for Metals, Japan*; K. Ushida,* RIKEN, Japan

GaAs is a key material for ultrafast switching and THz radiation because the carrier lifetime of low-temperature grown (defective) GaAs is ultrafast (sub-picosecond). In doped GaAs, the plasmon and the LO phonon form coupled modes through Coulomb interactions, and the frequencies of the LO phonon-plasmon coupled (LOPC) modes depend on the carrier density. We report the effect of active lattice defects on dephasing of coherent LOPC modes in He-ion irradiated n-GaAs by using a femtosecond pump-probe technique. The time-domain oscillations of the coherent LOPC modes in He@super +@ irradiated n-GaAs have been precisely measured for the different ion doses. The samples used were n-type GaAs with carrier density of ndop= 1.4x10@super 18@cm@super -3@. In order to examine the effect of point defects, 5 keV He@super +@ were irradiated to n-GaAs samples at doses of 9.4x10@super 12@ and 3.0x10@super 14@ He@super +@/cm@super 2@ in a UHV chamber with base pressure of 3x10@super -9@ Torr. The light source was a mode-locked Ti:sapphire laser with a pulse width of 25 fs. The anisotropic reflectivity change revealed coherent oscillations which shows beating pattern for the as-grown n-GaAs. This beating pattern in the time-domain data is due to an existence of the strong LO mode and the L@sub -@ mode. The mode beating changed clearly as increasing the ion dose, and the pattern of the Lmode disappeared at doses higher than 3.0x10@super 13@ He@super +@/cm@super 2@. The results suggest that defect-induced carrier trapping dominate annihilation of the coherent coupled modes. In addition we will also discuss on an anormalous behavior of dephasing of the coherent LO-phonon.

SC+EL+SS-WeP13 High Density Plasma Via Hole Etching In SiC*, H. Cho,* Miryang National University, South Korea*; K.P. Lee, P. Leerungnawarat,* University of Florida*; S.N.G. Chu,* Lucent Technologies, Bell Laboratories*; F. Ren,* University of Florida*; C.-M. Zetterling,* Royal Institute of Technology (KTH), Sweden*; S.J. Pearton,* University of Florida

Through-wafer vias ~100µm deep were formed in 6H-SiC substrates by Inductively Coupled Plasma etching with SF@sub 6@/O@sub 2@ at rates up to 0.8 µm·min@super -1@ and employing Al masks. Selectivies of @>@40 in SiC over Al were achieved. Electrical (C-V, I-V) and chemical (AES) analysis techniques showed that the etching produced only minor changes in reverse breakdown voltage, Schottky barrier height and near-surface stoichiometry of the SiC and had high selectivity over common front side metallization. The SiC etch rate and etch yield were measured as a function of plasma composition along with the selectivity over Al. This process is attractive for power SiC transistors intended for high current, high temperature applications.

SC+EL+SS-WeP14 RHEED Study of Ion-beam Induced Carbonization for 3C-SiC Heteroepitaxial Growth on Si(100)*, N. Tsubouchi*, *A. Chayahara, A. Kinomura, Y. Horino,* Osaka National Research Institute, Japan

3C-SiC heteroepitaxial film formation on a Si substrate is a very important when we consider compatibility with the silicon fabrication technology. So far, it has been reported that a carbonization process as buffer layer formation using various film-growth methods is effective for the heteroepitaxial film growth of 3C-SiC on Si while the lattice mismatch between 3C-SiC and Si is as large as 20 %. These methods reported for this reaction process, however, require high-temperatures ranging 700--1000°C, causing serious problems of redistribution of dopants and crystal defects such as dislocations and stacking faults especially at the heterointerface. In addition, carbonization reaction between provided gases including carbon atoms and Si substrates also results in promotion of defect formation in the Si-SiC interface. For solving these problems, a newly process, that is, ion-beam induced carbonization process of Si(100) with mass-separated energetic carbon ion species (e.g., @super 12@C@super -@, @super 12@C@sub 2@@super -@, @super 12@C@super +@ ions) was tried and investigated by RHEED measurements. The kinetic energies of ions and substrate temperatures were in the range 20-1200 eV and 400-700 °C, respectively. Such energetic species have possibility to lower a growth temperature inducing a decrease in defects and dislocations at the SiC/Si interface, in comparison with conventional methods. We report on the SiC growth condition during the carbonization process, i.e., ion-beam energy and substrate temperature dependence together with structural information.

SC+EL+SS-WeP15 Auger Depth Profile Analysis: Process Window Definition of 0.2 micron Aluminum RIE Interconnections*, C. Dziobkowski,* *L. Clevenger,* IBM Corporation*; M. Honda,* Toshiba, Japan*; R. Ramachandran,* Infineon Technologies

For fabrication of devices with dimensions of less than 0.2 microns, processing requirements become more demanding. New design requirements for the 256 Mbit DRAM also have higher aspect ratios. Process temperature control becomes very important because of the effects of temperature on the RIE etch, theta-Al2Cu precipitate distribution and texture. Eventually, even the electrical properties are affected resulting in device shorts and open circuits. This paper gives a description of the methodology developed to provide Auger depth profile analysis to characterize the copper distribution in the AlCu metallurgy. Copper segregation at the Al/Ti interface also affects the RIE process etching window. The information obtained from the Auger depth profiles can be used to define a window for VLSI devices with these small dimensions.

SC+EL+SS-WeP16 Epitaxial Growth of Cubic SiC Thin Films on Silicon Using New Single Molecular Precursors by MOCVD*, J.-H. Boo,* *S.-B. Lee,* Sungkyunkwan University, Korea*; K.-W. Lee, Yunsoo Kim, K.-S. Yu, S.H. Yeon, I.N. Jung,* Korea Research Institute of Chemical Technology, Korea

Heteroepitaxial cubic SiC thin films have been deposited on silicon substrates at temperatures in the range of 750 - 1000 ° C using newly developed single molecular precursors by MOCVD method. Single-crystalline, crack-free stoichiometric cubic SiC films were successfully grown on both Si(001) and Si(111) substrates without surface carbonization at as low as temperature of 920 ° C with 1,3-disilabutane (DSB), H@sub 3@Si-CH@sub 2@-SiH@sub 2@-CH@sub 3@, as a liquid single source precursor which contains silicon and carbon in 1:1 ratio. Cubic SiC thin films highly oriented in the [001] direction were also obtained on Si(001) using either a liquid mixture of 1,3,5-trisilapentane (TSP), H@sub 3@Si-CH@sub 2@-SiH@sub 2@-CH@sub 2@-SiH@sub 3@, and 2,4,6-trisilaheptane (TSH) at 980 ° C or 2,6-dimethyl-2,4,6-trisilaheptane (DMTSH), H@sub 3@C-SiH(CH@sub 3@)-CH@sub 2@-SiH@sub 2@-CH@sub 2@-SiH(CH@sub 3@)-CH@sub 3@ at 950 ° C without carrier gas. These growth temperatures were much lower than conventional CVD growth temperatures, and this is the first report of cubic SiC film growth using the single molecular precursors of trisilaalkanes.

SC+EL+SS-WeP17 Optical and Contact Properties of Indium Tin Oxide on p-GaN*, D.W. Kim,* *Y.J. Sung, J.W. Bae, G.Y. Yeom,* Sungkyunkwan University, Korea*; H.S. Kim,* University of Strathclyde, Scotland

Because Gallium nitride(GaN) is an attractive material which has an wide direct band gap, GaN-based optoeletronic devices such as light emitting diodes(LEDs) and laser diodes(LDs) in blue and ultraviolet wavelength regions have been studied intensively and fabricated successfully. However, the contacts to GaN-based LEDs are currently made by depositing metal layers on the top of GaN-based LEDs, therefore, significant optical loss is inevitable. In this study, we applied multilayers containing transparent conducting oxide such as indium tin oxide(ITO) to p-GaN and the effect of the optically more transparent contacts to p-GaN on the electrical and optical properties were investigated. As substrates, Mg-doped p-GaN layers were used. ITO thin films were deposited on p-GaN at room temperature using an oxygen radical assisted electron beam evaporator system. To improve the contact properties to p-GaN, various ITO/very thin metal multi-layer contact systems were also attempted and their electrical, structural, and optical properties were investigated. A semiconductor parameter analyzer and a four point probe were used to measure contact and electrical properties of ITO and mutilayer films on p-GaN. X-ray diffractometry(XRD) and Auger electron spectroscopy(AES) were used to investigate the structural properties of the contact during the annealing process, and an optical spectrophotometer was used to investigate the optical properties. The deposited ITO thin films showed the optical transmittance above 80 % at 420 nm(blue) with the sheet resistance of 40 ohm/sq. With ITO contact to p-GaN alone, Schottky contacts were generally obtained. However, depending on the applied very thin metal inter-layer and followed annealing conditions, different electrical and contact properties, which could be applicable to GaN devices, were obtained.

SC+EL+SS-WeP18 Visible Emission from Electroluminescent Devices using an Amorphous AlN:Cu, Mn, and Cr Thin Film Phosphor*, M.L. Caldwell,* *V.I. Dimitrova, M.E. Kordesch, H.H. Richardson, P.G. Van Patten,* Ohio University

Electroluminescence (EL) studies of AlN:Cu, Mn, and Cr alternating-current thin-film electroluminescent (ACTFEL) devices were performed at 300 K. Thin films of Cu, Mn, and Cr doped AlN, ~ 200 nm thick, were grown on p-doped silicon (111) substrates using RF magnetron sputtering in a nitrogen atmosphere. A transparent layer utilizing indium tin oxide was employed as the top layer contact. A strong bluish-green emission from the AlN:Cu films was observed under reverse bias due to electron impact excitation of the Cu atoms. The emission spectrum consisted of one broad peak in the visible region of 475 nm. a strong red emission from the AlN:Mn films was observed also under reverse bias due to electron impact excitation of the Mn atoms. There were two sharp emission peaks in the visible region at 680 nm and 700 nm. Studies of incorporationg the Cr@super +3@ ion will be performed to try to overcome the charge compensation problem. Temperature-dependent cathodoluminscence (CL) and photoluminscence (PL) studies will be performed between 30 - 450 K to determine the relationship of them to the EL results and show the optimum conditions for device performance.

SC+EL+SS-WeP19 Organic Contamination Removal on Silicon Substrate by Low Temperature Remote Plasma, ***H. Kang,*** *H. Soh, H. Seo, Y.C. Kim,* Hanyang University, Korea*; H. Jeon,* Hanyang University, Korea, South Korea

Organic contamination on silicon substrate deteriorates the film adhesion and forms deleterious decomposition during heating process. Organic impurities absorbed on the Si substrate surface generally desorbes in the form of volatile compounds by radio frequency (RF) remote oxygen and hydrogen plasma at relatively low temperatures. In this study, organic contamination removal and Si substrate surface microroughness by RF remote oxygen and hydrogen plasma will be described. The remote plasma system and analysis systems were connected by ultrahigh vacuum transfer system to avoid recontamination such as carbon absorption in the air. Organic impurity were intentionally contaminated and removed by hydrogen and oxygen remote plasma system. Surface contamination concentration and bonding state changes were analyzed by Auger electron spectroscopy (AES) and x-ray photoelectron spectroscopy (XPS). Surface morphology and microroughness were observed by scanning tunneling microscope (STM) and atomic force microscope (AFM). After remote hydrogen and oxygen plasma cleaning, carbon impurity was significantly reduced below detection limit of AES and the Si-C peaks of XPS were not observed. The surface microroughness generally degraded with increasing plasma power and exposure time.

SC+EL+SS-WeP20 Studies of the Surface Morphology, Chemical and Structural Changes of Ion Bombarded Silicon Carbide, ***P. McCarty,*** University of Alabama, Huntsville*; C.I. Muntele, I. Muntele,* Alabama A&M University*; M.A. George,* University of Alabama, Huntsville*; D. Ila,* Alabama A&M University*; D.B. Poker, D.K. Hensley,* Oak Ridge National Laboratory

Silicon carbide is gaining increasing interest for high temperature/harsh environment applications including miniature integrated sensors. In the past few years, efforts have been made toward controlling the defects and impurification that occur during various growth and fabrication processes. This work is intended to analyze the surface damage that occurs during ion implantation of silicon carbide, and the evolution of these defects. In order to correlate the effects that surface damage has on the sensing properties of ion implantation based silicon carbide gas sensors we have characterized these sensors under various conditions. We present the results of our investigation of the morphological, electrical and spectroscopic characteristics of ion implanted silicon-face 6H-SiC. In this work we have used He, O, Pd, and Au at energies between 100 keV to 8 MeV at fluences between 1 x 1015/Cm2 to 3 x 1017/Cm2. The ion bombardments were performed at both room temperature (300oK) and at elevated temperature (773oK). Atomic force microscopy, surface potential measurements and electric field microscopy was performed before and after ion implantation, as well as after the post-implantation high temperature annealing. This study is correlated with results obtained using micro-Raman, FTIR and Rutherford Backscattering Spectrometry. @FootnoteText@ We would like to thank Dr. David Larkin, NASA Glenn Research Center. Research sponsored by the NASA Grant No. NG3-2302, and partially by the Center for Irradiation of Materials, Alabama A&M University and the Division of Materials Sciences, U.S. Dept. of Energy, at the Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U. S. Department of Energy under contract DE-AC05-00OR22725

SC+EL+SS-WeP21 Gallium Oxide Deposition and Radical Oxidation on GaAs(001)-(2x4) Investigated with STM, ***S.I. Yi,*** *P. Kruse, M. Hale, A.C. Kummel,* University of California, San Diego

Growth of metal oxide on GaAs with a low interface defect density is necessary for development of GaAs based metal oxide semiconductor field effect transistor (MOSFET). Vapor deposition of gallium oxide on GaAs(001) is emerging as a viable method for this objective. Using STM, we have investigated deposition of gallium oxide on GaAs(001)-(2x4) during the initial period and oxidation of the surface by atomic oxygen. Deposition of gallium oxide results in an atomically abrupt interface with the GaAs(001)-(2x4) surface, without disrupting the (2x4) surface order. In contrast, oxidation of GaAs(001)-(2x4) by atomic oxygen results in disordering of the surface characterized by formation of undimerized As surface atoms with half filled dangling bonds and As@subGa@ antisites. The stark difference in these two methods of oxide preparation has a profound implication for development of GaAs based MOSFET devices.

SC+EL+SS-WeP22 Density Functional Theory Studies of Semiconductor Surfaces, *G.S. Hwang,* California Institute of Technology*;* ***C.B. Shin,*** Ajou University, South Korea

Density functional theory (DFT) simulations have been proven to be a reliable and tractable tool in condensed matter physics. Indeed, these simulations are now successfully used to treat not only simple ordered solids but also complex systems such as surfaces and point-like/extended defects. We present the results of our recent pseudopotential based DFT studies which included: (i) the dynamics and configurations of Si(100) and (ii) the adsorption of hydrogen molecules on the surface. It is now rather well known that dimers on Si(100) are alternatively buckled at the ground state. However, the details of their geometry and dynamics at room temperature are still an issue of controversy. Our studies illustrate a tied flipping behavior of two consecutive dimers: the buckling of adjacent outer dimers becomes stronger while two inner dimers switch their orientations. Contrary to popular speculation, in most cases, the dimers undergo thermal fluctuations between two unequal energy minima, thereby preserving the 2x anticorrelation of dimer buckling along a row even at room temperature. Based upon such understanding of the dynamical behaviors of Si(100) at finite temperature, we have looked into dissociative adsorption of H@sub 2@ on Si(100), which is still ambiguous. This study reveals that intradimer @pi@-bonding disruption caused by thermal induced dimer stretching is mainly responsible for the anomalously strong surface temperature dependence of H@sub 2@ adsorption on the clean Si(100) surface.

SC+EL+SS-WeP23 Investigation of Polycrystalline Silicon Grain Structure by Single Wafer Rapid Thermal Chemical Vapor Deposition (RTCVD), ***H. Bu,*** *C. Hu, M. Bevan, L. Tsung,* Texas Instruments*; L. Luo,* Applied Materials

It is known that the grain structure in poly-Si gate electrode can directly affect dopant activation and gate electrode depletion (GED). It is highly desirable to control the grain size and orientation during processing for improved IC device yield and reliability. This paper demonstrates the capability of tuning and generating a specific poly-Si grain structure with a lamp based and a heater based single wafer rapid thermal chemical vapor deposition (RTCVD) reactor at reduced pressure regime. Nitrogen gas is used as the carrier gas. The deposition temperature is varied from 650°C to 700°C. The effect of the concentration of intentionally added hydrogen during deposition is examined. Films deposited at various process conditions are characterized by TEM and XRD analysis. The results show that poly-Si grain size and orientation are sensitive to the hydrogen concentration. With a carefully selected process temperature and hydrogen concentration combination, the RTCVD technique is able to engineer the poly-Si grain size and orientation. The effect on poly-Si grain structure on electrical parameters such as electrical oxide thickness (EOT) and gate electrode depletion (GED) will be discussed.

SC+EL+SS-WeP24 Buried Low-Temperature (T@sub s@ <500 °C) Lateral Epitaxial Overgrowth of Si on SiO@sub 2@ Using Solid-Metal-Mediated Epitaxy, ***T. LaFave Jr.,*** *N. Lakshminarayana, A. Faik, M.-A. Hasan,* University of North Carolina

Buried lateral epitaxial overgrowth of Si on thin SiO@sub 2@ layers (<100 nm) using a thick solid Al layer as growth mediator was demonstrated using a newly developed solid-metal-mediated molecular beam epitaxy (SMM-MBE) method. The experiments were carried out at growth temperatures T@sub s@ < 500 °C using electron beam evaporation for Si and thermal evaporation of Al from an effusion cell. Si(100) wafers were thermally oxidized and patterned to provide seed/oxide strips ranging from 2/2 to 50/500 microns. Each seed/oxide strip was repeated within an area of ~ 1.25x2.00 cm@super 2@ and all patterns were placed on the same wafer. The wafers were then thermally etched at T@sub s@ = 900 °C under UHV conditions to desorb the remnant native oxide from the seed areas followed by deposition of Al at room temperature. Si deposited on the resulting structure at T@sub s@ < 500 °C re-grew epitaxially at the buried Al/Si interface and growth was extended laterally over the oxide layer. Initial TEM results demonstrated lateral growth of single crystalline Si over the oxide layer. This SOI method described above is based on SMM-MBE. In SMM-MBE, silicon grows epitaxially at a buried Al/Si interface during thermal evaporation of Si. Si atoms diffuse through the Al overlayer to the interface where low-energy atomic Si sites act as sinks for the diffusing Si atoms. This process is fundamentally different from surfactant assisted growth in which a small concentration of a metal (typically a fraction of a monolayer) is used to enhance epitaxial growth. In SMM-MBE, the Al layer can be thousands of monolayers thick (solid). The new findings may lead to new silicon-on-oxide fabrication method. Also, it provides a procedure for combined metallization and heavy p-type doping, e.g. in MOS device structure. Applications of this method in device fabrication will be discussed.

SC+EL+SS-WeP25 Field-Assisted Metal-Induced Crystallization of Amorphous Silicon Films*, **A. Khakifirooz**, S.S. Mohajerzadeh, S. Haji,* University of Tehran, Iran

Recently, metal-induced crystallization has gained special attention for low-temperature fabrication of polysilicon thin-film transistors. Metal-induced lateral crystallization, has been successfully utilized for obtaining high-performance TFTs. Very large silicon grains, free of metal contamination, are formed as a result of this lateral growth, providing a high carrier mobility. However, the lateral growth rate is still low and very long time annealing is required for practical applications. It has been reported that applying an electric field may enhance the growth rate. We have also observed this effect and the obtained results will be reported. Amorphous silicon films with a thickness of 1000Å are deposited on 50µm thick glass substrates via e-beam deposition. A 1000Å thick passivation oxide layer is subsequently deposited with e-beam and windows are opened for metal pads. A 1000Å thick nickel film is then deposited and patterned using photolithography. Samples are annealed on a hot plate while a DC voltage up to 100 V is applied between the pads. Growth rate is monitored using optical microscopy. SEM, TEM, and XRD are also used to investigate the crystalline structure of the films. A 300 µm crystallization was observed in samples annealed at 400°C for 30 min. when a 100 V/cm field applied. This is much higher than the previously reported growth rates. This may be explained by the fact that we have applied the field directly to metal pads, allowing a considerable current to pass through the a-Si film. Three regions with different crystalline structure are clearly observed in the laterally crystallized area when a high voltage is applied. The mechanism behind these phenomena will be discussed. In addition to filed-enhanced diffusion of Ni atoms, which has been supposed to be responsible for enhanced growth rate, we study the role of energetic electrons. Effect of impurities on the growth kinetics will be also reported.

SC+EL+SS-WeP26 Medium Range Order in Amorphous Silicon Films as a Function of Low-Energy Particle Bombardment During Growth*, **J.E. Gerbi**, J.R. Abelson,* University of Illinois at Urbana-Champaign*; P.M. Voyles,* University of Illinois and NEC Research Institute*; M.M.J. Treacy,* NEC Research Institute*; J.M. Gibson,* Argonne National Laboratory

Medium range order (MRO) refers to atomic correlations on a length scale of 1-2 nm. The recently developed TEM fluctuation microscopy technique@footnote 1@ is directly sensitive to MRO, as opposed to diffraction-based methods which are notably insensitive. In this work, we quantitatively compare the MRO in nominally amorphous hydrogenated Si thin films grown by significantly different vapor phase methods: plasma enhanced CVD, hot-wire (HW) CVD, and reactive magnetron sputtering (RMS). All films show significant MRO in the as-deposited state; the MRO decreases upon light soaking or thermal annealing, indicating the existence of a metastable state in the starting material. We investigate the roles of various particle bombardments in producing MRO with the RMS and HW-CVD growth processes. In previous work, we showed that bombardment by ions or neutrals promotes the formation of nanocrystalline or polycrystalline Si, depending on hydrogen addition and substrate temperature. We compare the MRO of a-Si:H, a-Si:D, and a-Si grown by RMS under high argon ion flux with that of a-Si:H grown by HW-CVD, which involves essentially no particle bombardment. We discuss how these bombardments affect the "structure" of a-Si in terms of MRO, and explain how this structure evolves during growth using the model of a frustrated polycrystalline growth surface which yields a highly strained, fine-grained "paracrystalline" structure. Such a structure looks amorphous in conventional diffraction methods, but is topologically crystalline. By contrast, the model of a continuous random network structure, as usually assumed for amorphous films, does not fit the data for as-deposited material. @FootnoteText@ @footnote 1@ J.M. Gibson, et al. Appl. Phys. Letts. 73 3093 (1998).

SC+EL+SS-WeP27 Cluster Deposition Study by Molecular Dynamics Simulation: Al Cluster and Cu Cluster*, **J.-W. Kang**, K.-S. Choi, E.-S. Kang, K.-R. Byun, H.-J. Hwang,* Chung-Ang University, Korea

Ionized cluster beam deposition for semiconductor interconnection technology has attracted much attention as a promising method for growing high-quality films at low substrate temperature. Therefore, it is important to understand the interaction between energetic cluster and substrate. In this work, we investigated energetic copper and aluminum clusters deposition and cluster-surface interactions. In the work, we used copper and aluminum clusters with the face centered cubic structure, a classical molecular dynamics simulation, and the second-moment approximation of tight-binding scheme. We simulated cluster deposition and investigated the variations of substrate temperature and the number of disordered atom as a functions of time, energy, and cluster size. The maximum substrate temperatures after energetic cluster impact on surface had linear relationship with total cluster energy and energy per atom, but we could not find any specific relationship with time taken for substrate temperature to reach its maximum. In this work, the correlated collisions between atoms in the cluster played a very important role in the impact on substrate surface and the correlated collision effect was proportional to the cluster size and kinetic energy per atom. For each impact angle and energy, we calculated the average properties such as sputter yield, sticking probability, average reflection angle of the impact cluster, and average emission angle of the sputter products. The calculated properties were compared with that of single atom deposition.

Semiconductors
Room 306 - Session SC+EL+SS-WeA
Semiconductor Alloys

Moderator: P. Desjardins, Ecole Polytechnique de Montreal

2:00pm **SC+EL+SS-WeA1 Si-Ge Heterostructures***, **K.L. Wang**,* University of California, Los Angeles **INVITED**

PLEASE SEND US AN ABSTRACT. Thank you.

2:40pm **SC+EL+SS-WeA3 Critical Behavior of Epitaxial Si@sub 1-x@Ge@sub x@/Si(001) Islands***, **R.A. Budiman**, H.E. Ruda, D.D. Perovic, B. Bahierathan,* University of Toronto, Canada

We study the island size distributions of three-dimensional Si@sub 1-x@Ge@sub x@/Si(001) islands of varying Ge fractions (x = 0.4-0.7) and thicknesses grown by ultrahigh vacuum chemical vapor deposition. The size distributions of the percolating islands obey the dynamic scaling hypothesis due to random percolation process, only in the small island limit. Morphologies of the islands strongly suggest a presence of Smoluchowski ripening mechanism, in which islands collide and ripen. We therefore combine random percolation and Smoluchowski ripening to analyze the size distributions. To understand the critical behavior of the islands as exhibited by their size distributions, we formulate a mean-field theory of coherently strained island formation by incorporating surface energy and strain relaxation. The resulting phase diagram shows that the island formation in Si@sub 1-x@Ge@sub x@/Si(001) is located near the critical region. Order parameter fluctuations can be estimated by calculating the curvature energy for such a system and we find that the strain fluctuation is indeed relevant to properly describe the island formation in the Si@sub 1-x@Ge@sub x@/Si(001) system.

3:00pm **SC+EL+SS-WeA4 Growth of Coherent Three-dimensional Si Islands on Ge(111)***, **A. Raviswaran**, C.P. Liu,* University of Illinois, Urbana-Champaign*; J.M. Gibson,* Argonne National Laboratory*; D.G. Cahill,* University of Illinois, Urbana-Champaign

We study the evolution of three-dimensional islands during Si/Ge(111) epitaxy. The strain due to lattice mismatch (4.2% tensile) and the difference in the surface energies (@gamma@@sub Si@>@gamma@@sub Ge@) contribute to the formation of the three-dimensional Si islands. We grow Si islands on pseudomorphic Si@sub 0.15@Ge@sub 0.85@ buffer layers (deposited on Ge(111) substrates) in the temperature range 500°C - 650°C using MBE; the (111) orientation is used because the critical thickness of Si layers on Ge(111) is larger than that on Ge(001). We characterize the morphology and relaxation of the Si islands using ex situ AFM, TEM and SEM. Islanding occurs at 1 BL Si coverage, i.e., without the formation of a wetting layer. We observe high densities (~ 10@super 12@ cm@super -2@) of coherent, circular base islands for growth temperatures 500°C - 600°C and low Si coverage (< 2 BL Si). The density and shape of the islands is insensitive to the growth temperature. Beyond a critical width the islands relax plastically, by the nucleation and glide of misfit dislocations; this critical width is ~ 16 nm at 550°C and ~ 25 nm at 600°C. We observe large, incoherent, irregularly shaped islands at higher temperatures (> 600°C) and coverages (> 4 BL Si). As the islands transform from coherent to incoherent, coarsening occurs which results in an increase in the island width and a reduction in the island density. The high temperature (> 600°C) growths show a secondary maximum in the island density near 4 BL Si coverage.

3:20pm **SC+EL+SS-WeA5 Adatom Assisted Stabilization of Ad-dimers on Ge(001)***, **E. Zoethout**, H.J.W. Zandvliet, B. Poelsema,* University of Twente, The Netherlands

Studies of the early stage of near room temperature growth of silicon on Ge(001) have revealed an inconsistency between experimental@footnote 1@ and theoretical@footnote 2@ work. Experimentally a stable cluster has been labeled to be a trough dimer oriented perpendicular to the substrate dimer bonds (D-dimer). The same type of cluster is found in the early stage of near room temperature homoepitaxial growth on Ge(001). Theoretically such a D-dimer is predicted to be energetically unfavorable. It turns out that the apparent D-dimer is actually comprised of three rather than two atoms. The three-atom cluster of Ge or Si on Ge(001) is shown to differ from a trough dimer orientated along the substrate dimer bonds, from a small epitaxial island and also from a three-atom Si cluster on Si(001). The three-atom cluster of Ge or Si on Ge(001) is composed of an ad-dimer in the D-configuration and an adatom on the neighboring substrate dimer row. @FootnoteText@ @Footnote 1@W. Wulfhekel, B.J. Hattink, H.J.W. Zandvliet, G. Rosenfeld, and B. Poelsema, Phys. Rev. Lett. 79, 2494 (1997). @Footnote 2@S.V. Khare, R.V. Kulkarni, D. Stroud and J.W. Wilkins, Phys. Rev. Lett. 60, 4458 (1999).

3:40pm **SC+EL+SS-WeA6 C Incorporation during the Growth Of Ge@sub 1-y@C@sub y@/Ge(001) from Hyperthermal Beams***, **J. D'Arcy-Gall**, D. Gall, P. Desjardins, I. Petrov, J.E. Greene,* University of Illinois, Urbana

C-containing group-IV semiconductor alloys are of interest due to the potential they offer for both band gap and strain engineering in microelectronics. This investigation focuses on the effects of incident particle energy and film growth temperature T@sub s@ on the distribution of C lattice configurations in Ge@sub 1-y@C@sub y@ epitaxial layers grown on Ge(001) from hyperthermal beams obtained by ultra-high vacuum ion-beam sputtering using Kr@super +@. All Ge@sub 1-y@C@sub y@ (y @<=@ 0.03) layers, grown at T@sub s@ = 245-415 °C, are fully-coherent and free of extended defects as judged by high-resolution x-ray diffraction, reciprocal lattice mapping, and transmission electron microscopy. The strain-state of epitaxial Ge@sub 0.99@C@sub 0.01@ alloys grown at T@sub s@ = 300 °C changes from in-plane tension to compression as the Kr@super +@ energy E@sub Kr@ is increased from 300 to 900 eV. This results from an increasing fraction of C incorporated in Ge-C split interstitial sites as a result of the trapping, by substitutional C, of Ge self-interstitials formed due to irradiation by the increasing fraction of sputtered Ge atoms in the high energy tail of the energy distribution. These results are supported by TRIM simulations which show that the number of displaced lattice atoms per incident hyperthermal Ge increases from 0.10 with E@sub Kr@ = 300 eV to 0.24 at 900 eV, and ab initio calculations of layer strain for different C lattice configurations. All Ge@sub 1-y@C@sub y@ alloys grown at E@sub Kr@ = 900 eV are in a state of in-plane compression, which decreases with increasing T@sub s@. Raman scattering results show that the substitutional C concentration in these layers is negligible. Comparison of experimental results with ab initio calculations reveals that an increasing fraction of C incorporates as C pairs as T@sub s@ is increased due to the higher C-C encounter probability on the growth surface.

4:00pm **SC+EL+SS-WeA7 Growth and Characterization of Metastable Ge@sub1-x@C@subx@ Thin Films on Si(100) Substrate.***, **W. Li**, D. Guerin, S.I. Shah,* University of Delaware

The Ge-C system is of interest due to the possibility of band gap engineering on Si. For strain free deposition of Ge@sub1-x@C@subx@, a carbon concentration in excess of 10% is required, assuming that the system obeys Vegard's law. The maximum equilibrium solubility of C in Ge, however, is only 10@super8@/cm@super3@. Molecular beam epitaxy and chemical vapor deposition have been used to grow metastable Ge@sub1-x@C@subx@ thin films with x up to 2.5%. We have used a bias assisted sputter deposition using Ge and C magnetrons to obtain the epitaxial Ge@sub1-x@C@subx@ films with extended carbon solubility. Without any applied substrate bias and C flux, a Ge epitaxial layer on Si(100) substrate was obtained at 750°C with proper substrate preparation. Based on the results of pure Ge epitaxy, C was systematically added. Without the substrate bias, x-ray diffraction analyses show that the films were polycrystalline. With the application of a substrate bias, we were able to obtain epitaxial Ge@sub1-x@C@subx@ films. The Ge (400) XRD peak shifts to higher 2@theta@ were observed indicating C incorporation in the Ge lattice. Extended x-ray absorption fine structure (EXAFS) analyses confirmed that the C was indeed incorporated on the substitutional sites in the Ge lattice. C concentration was determined from XRD, X-ray photoelectron spectroscopy (XPS) and Rutherford backscattering spectroscopy (RBS). A C concentration of up to 5 at.% was obtained. Depth profiles of samples by XPS show that carbon is uniformly distributed in the film. Experiments are underway to study the effects of bias and thickness on the epitaxial deposition of Ge@sub1-x@C@subx@ with even further extension of the concentration of substitutionally situated C in germanium lattice.

4:20pm **SC+EL+SS-WeA8 Electrical and Optical Properties of Silicon : Germanium Alloys prepared by DC Magnetron Sputtering***, **A. Subrahmanyam**, S. Karthikeyan, J. Asbalter,* Indian Institute of Technology, Madras, India*; P. Amirtharaj,* National Institute of Standards and Technology

The Silicon: Germanium (Si:Ge) alloys are being used in various semiconductor devices. As is well known, these alloys offer advantages in band gap engineering, and can integrate well with the existing silicon technology. Several studies have been made on these alloys. In the present paper, we report the electrical and optical properties of Si:Ge alloys prepared by DC Magnetron sputtering technique. A 7.5 cm diameter circular magnetron cathode has been designed and fabricated. The balanced magnetron cathode is operated at low pressures (4.0 x 10@super -3@ mbar). Argon is the sputter gas. The target is prepared by bonding commercially available Silicon wafer to the water cooled copper backing plate. A small portion of the erosion area on the magnetron cathode is covered with pure germanium wafer. The alloys of Si:Ge (undoped) are prepared (at room temperature 25°C) on glass and Si substrates. The growth parameters in the present study are : flow rate of argon (180 - 250 sccm), Magnetron power (80 - 225 watts) and germanium content in the alloy. The thickness and refractive index of the films is measured by ellipsometer in the wavelength range 300 - 700 nm. The thickness of these alloy films is about 150 nm. The alloy films have been found to be amorphous. The germanium content in the alloy films is varied between 15 - 30 atomic % and is estimated by EDAX and RBS analysis. The optical absorption and photo conductivity measurements have been made on these alloys. The optical band gap of these alloys is in the range 1.45 - 1.6 eV. The dark conductivity is in the order 10@super-@ mho cm@super-1@. The deposition rate is observed to be linear with the magnetron power till 120 watts.

4:40pm **SC+EL+SS-WeA9 Preparation and Characterization of Highly Li-doped a-Se Alloy Films for Thermal Neutron Detectors***, **K.C. Mandal**, B. Dille, R.D. Rauh,* EIC Laboratories, Inc.*; A. Burger,* Fisk University*; R.N. Bhattacharyya,* National Renewable Energy Laboratory

This paper describes our recent research in developing highly Li-doped a-Se alloys and thin films for thermal neutron detector applications. The grown Li-doped (35 a/o) a-Se alloy thin films have shown high promise for this application due to the presence of Li in high concentrations, high dark resistivity (2x10@super 14@@ohm@. cm), good charge transport properties (mu-tau@sub e@ = 3.2x10@super -6@ cm@super 2@/V), low cost and relatively easy scale up. Highly Li-doped a-Se alloy has been synthesized in controlled ambient and used for making large area films up to 4x4 sq. inch. The vacuum evaporated a-Se alloy films have been characterized by X-ray diffraction (XRD), atomic absorption (AA), differential thermal analysis (DTA), Raman spectroscopy and X-ray photoelectron spectroscopy (XPS). The detectors fabricated from these films have demonstrated potential for thermal neutron detection for the first time. Details of various steps involved in detector fabrication and testing of these devices will also be presented.

5:00pm **SC+EL+SS-WeA10 Instability in Atomic Step Morphology during the Sublimation of Si(111)***, **Y. Homma**, P. Finnie,* NTT Basic Research Laboratories, Japan

A morphological instability has been predicted to occur during step-flow crystal growth.@footnote 1@ Recently we experimentally demonstrated transitions between stability and instability@footnote 2@ during epitaxial growth on an ultra-flat Si(111) terrace - a terrace which is atomically flat on a 100 µm scale. In this paper, we show that such instability can also occur during step-flow sublimation at high temperatures. Step motion due to sublimation was tracked with in situ scanning electron microscopy. When the size of a terrace becomes comparable to the adatom diffusion length, a new step is nucleated, forming the edge of a new, monolayer-deep crater at the center of an ultra-flat terrace. As a result of successive expansion and nucleation, steps become distributed in a concentric circular pattern. The spacing between steps can be controlled by varying the annealing temperature. When the spacing is less than about 20 µm, the innermost step is typically smooth and nearly circular. For larger spacings, the innermost crater is irregularly shaped while it is still relatively small. The crater becomes smoother as it expands. The instability is manifest when the width of the lower terrace is much smaller than that of the upper terrace. Since the adatom flux from a step to a neighboring terrace depends on the terrace width, by reducing the size of the stabilizing terrace the instability can be initiated. The behavior of a subliming surface is thus similar to that of the growing surface. @FootnoteText@ @footnote 1@ G. S. Bales and A. Zangwill, Phys. Rev. B 41 (1990) 5500 @footnote 2@ P. Finnie and Y. Homma, Phys. Rev. Lett. to be published.

Semiconductors
Room 306 - Session SC+EL+SS-ThM
Hydrogen On and In Semiconductors

Moderator: J.T. Yates, Jr., University of Pittsburgh

8:20am **SC+EL+SS-ThM1 Step Structures and Energies on Vicinal Si(001) Monohydride Surfaces: Dependence on H Chemical Potential***, **A. Laracuente**, L.J. Whitman,* Naval Research Laboratory

It is well known that foreign adsorbates can alter the equilibrium step structure on surfaces and often have a dramatic effect on film growth. Given that most semiconductor devices are fabricated in hydrogen-rich environments on silicon substrates, a comprehensive understanding of how hydrogen affects Si step energies is essential to the development of accurate models of semiconductor growth and processing. We have determined the equilibrium step structures and step formation energies for the whole range of monohydride-terminated (001)-terrace-plus-step surfaces. Compared with the clean surfaces, hydrogen termination alters the atomic-scale step edge structure and, in many cases, causes large-scale changes in the surface morphology. The structural modifications result directly from a change in the relative energies of the possible single- and double-layer step configurations. On nominal Si(001), the S@sub B@ steps are mostly non-rebonded and rougher after H passivation. A kink distribution analysis reveals that H reduces the nearest neighbor interaction across the S@sub B@ steps by an order of magnitude. Whereas the nearest neighbor interaction strongly depends on H@sub 2@ pressure, i.e. the H chemical potential, the step formation energies do not. On D@sub B@-stepped surfaces, such as Si(1 1 11), a statistical analysis of the steps shows that H lowers the formation energy of non-rebonded D@sub B@ and S@sub B@ steps, making them close in energy to the rebonded D@sub B@ steps. Post annealing a monohydride Si(1 1 11) surface without H significantly changes the n-D@sub B@/r-D@sub B@ ratio, indicating that the D@sub B@ step formation energies strongly depend on H chemical potential.

8:40am **SC+EL+SS-ThM2 Si(100) Surface Roughening and H Atom Absorption: Surface and Bulk Characterizations.***, **S.K. Jo**, J.H. Kang,* Kyung Won University, S. Korea*; X. Yan, J.M. White, J.G. Ekerdt,* University of Texas at Austin*; J. Lee,* Seoul National University, S. Korea*; J.Y. Maeng, S.H. Kim,* Korea Advanced Institute of Science and Technology

Absorption of thermal-energy gaseous hydrogen atoms by Si(100), exceeding by far the dopant and other impurity concentrations, occurs within a narrow substrate temperature (T@sub s@) window centered at ~ 460 K. The absorbed hydrogen persists in the crystalline bulk as highly mobile species before migrating out and desorbing as molecular hydrogen at T@sub s@ as high as 900 K, well above the recombinative desorption temperatures of surface-adsorbed H. Developing and sustaining atomic-scale surface roughness, by H-induced silicon etching, is a prerequisite for H absorption and determines the T@sub s@ window. In support of these conclusions are our TPD, Raman, SIMS, TEM, and STM data for this fundamental and interesting phenomenon of thermal H atom absorption by Si(100).

9:00am **SC+EL+SS-ThM3 Dissociation Pathways of Molecular Hydrogen on Silicon Surfaces@footnote 1@***, **U. Höfer**,* Philipps Universität Marburg, Germany **INVITED**

The dissociative adsorption of H@sub 2@ on Si(001) has emerged as a prototype for activated chemical reactions on semiconductor surfaces. One of the most distinctive features of this basic reaction is the low sticking probability for dissociative adsorption (< 10@super -11@) and the fact that thermally induced distortions of the Si lattice enhance the reactivity by many orders of magnitude. In order to reveal the atomic-scale motion responsible for "phonon assisted sticking" we have performed a series of experiments employing optical second-harmonic generation (SHG), supersonic molecular beam dosing, and scanning tunnelling microscopy (STM). It will be demonstrated that, similar to thermally activated dynamical distortions, the reactivity can be enhanced by static distortions of the surface by precoverage with atomic hydrogen or by steps. The barriers to adsorption at these well-defined sites were determined. They revealed systematic trends that could be reproduced by density functional calculations and traced back to the interplay between electronic structure and local distortions of the Si surface. We find that hydrogen adsorption proceeds via inter-dimer reaction pathways in all cases. Whenever the energy splitting between the reactive dangling-bond states of adjacent dimers may be reduced by low-energy displacements of Si atoms, the adsorption barrier is found to be low. @FootnoteText@ @footnote 1@ Work performed in collaboration with W. Brenig, A. Biedermann, M. Dürr, T. F. Heinz, M. Hilf, Z. Hu, P. Kratzer, E. Pehlke, M. B. Raschke and M. Scheffler.

9:40am **SC+EL+SS-ThM5 Hydrogen Bonding on Compound Semiconductor Surfaces***, **R.F. Hicks**, Q. Fu,* University of California, Los Angeles*; L. Li,* University of Wisconsin, Milwaukee*; C.H. Li,* University of California, Los Angeles

Hydrogen adsorption on gallium arsenide and indium phosphide (001) surfaces has been studied by scanning-tunneling microscopy and internal-reflection infrared spectroscopy combined with ab initio molecular cluster calculations. The calculations are based on a series of clusters that accurately simulate the group III and V dimer termination of the surface. Good agreement has been achieved between the vibrational frequencies predicted by the theory and those observed in the experiments. On the anion-rich surfaces, hydrogen adsorbs on arsenic (or phosphorous) dimers to form isolated and coupled monohydrogen bonds and dihydrogen bonds. Conversely, on the cation-rich surface, hydrogen adsorbs on gallium (or indium) dimers to form terminal and bridged metal hydrides. The latter species occur in isolated or coupled structures involving two or three metal atoms. The implications of these results for the surface science of compound semiconductors will be discussed at the meeting.

10:00am **SC+EL+SS-ThM6 Scanning Tunneling Microscopy of Low Temperature Adsorption H2 on GaAs(001)***, **H. Xu**,* National University of Singapore, Singapore*; Y. Lee, J. Lee, A. Lee,* National University of Singapore

The variable temperature scanning tunneling microscope (VT-STM) has been used to study in-situ the transition of 2x6 reconstruction of GaAs (001) at low temperature. High resolution STM images show that the metastable As dimers rows of 2x6 reconstruction in GaAs (001) becomes unstable under the attack of the dissociated adsorption H@sub2@. As dimers were broken firstly due to the formation of double atom lines structure by the attacking of hydrogen on As dimers atoms. Furthermore, the opened As atoms rows on the top of this surface were twisted gradually up to coalesce together with a width of 3 As dimers. Unexpectedly, these compressed As atoms suddenly extend along the original As dimers rows direction(-110) gives rise to form a metastable trimer As rows.

10:20am **SC+EL+SS-ThM7 Theoretical Approaches for Predicting SiGe Heteroepitaxy***, **C. Mui**, S.F. Bent, C.B. Musgrave,* Stanford University

The demand for silicon-germanium devices has been growing in recent years due to potential applications in areas such as infrared photodetection, wireless communications and quantum nanostructures. The need for improved SiGe processing has motivated efforts to better understand the detailed reaction mechanisms of SiGe heteroepitaxy, including the adsorption of gas phase precursors and the removal of hydrogen from SiGe surfaces. We have used Becke3LYP density functional theory to study the effect of Ge alloying on the energetics and kinetics of H2 desorption from SiGe surfaces. We have investigated H2 desorption from the Si-Si homodimer, the Si-Ge heterodimer and the Ge-Ge homodimer sites. We found that in the transition state the two desorbing hydrogen atoms are localized above one surface atom, such that the structure resembles a dihydride species. The transition states on all three types of dimers have similar geometries, independent of the identity of the surface dimer atoms. Furthermore, the activation barriers depend only on the identity of the dimer atom not bonded to the desorbing hydrogens. For example, the activation barrier for H2 desorption from the Si site of a Si-Ge heterodimer is lower than that from a Si-Si homodimer by 10.6 kcal/mol. However, the barrier for desorption from the Ge-Ge homodimer is the same as that from the Si site of a Si-Ge heterodimer. We also found that the activation barrier for H2 desorption is only affected by surface Ge, and not Ge in the bulk. Calculations on a three dimer cluster showed that the activation barriers are dependent on cluster size, indicating that charge transfer and surface strain play a role in the desorption process. Finally, we will present results concerning additional surface reactions including the adsorption of germane on SiGe surface dimers.

10:40am **SC+EL+SS-ThM8 Real-time Monitoring of H@sub 2@ Adsorption on C(001) at High Temperature by Ultraviolet Photoelectron Spectroscopy***, **Y. Takakuwa**, M. Asano,* Tohoku University, Japan

The hydrogen-terminated diamond surface has attracted much attention not only as a high efficiency electron emitter because of its electron affinity being negative (NEA) but also as a p-type conductive surface for field-effect-transistor devices. On the other hand, H@sub 2@ desorption on the hydrogen-terminated diamond surface occurs appreciably at higher temperature than 900@super o@C. This suggests that during the synthesis of diamond thin films by chemical vapor deposition using hydrocarbon gases such as methane the diamond-growing surface could be terminated by hydrogen and therefore NEA, even though the growth temperature is as high as 800-1000@super o@C. In this study, the electron affinity, secondary electron emission and pinning position of the Fermi level during exposing a diamond C(001) surface to H@sub 2@ at 700@super o@C and 1x10@super -5@ Torr were investigated by a real-time monitoring method of ultraviolet photoelectron spectroscopy. It was observed that (1) molecular hydrogen not activated by a hot tungsten filament absorbs dissociatively on the C(001) surface, wile it takes about 120 min to cover wholly the surface with hydrogen; (2) the electron affinity decreases from +0.4 eV for the clean surface to a negative value when the hydrogen coverage is about 90%; (3) the Fermi level is positioned at 0.61 eV above the valence band maximum just when the diamond surface changes to NEA; (4) the secondary electron yield increase with the hydrogen exposure time even after the complete termination of the surface with hydrogen. On the basis of the observed results, the time evolution of the surface electronic state during the hydrogen adsorption on the C(001) surface is discussed.

11:00am **SC+EL+SS-ThM9 Infrared Studies of Hydrogen on Diamond (100)***,* ***J.N. Russell, Jr.,*** Naval Research Laboratory*; J. Hovis, R.J. Hamers,* University of Wisconsin*; G.T. Wang, S.F. Bent,* Stanford University*; M.P. D'Evelyn,* General Electric CRD*; J.E. Butler,* Naval Research Laboratory

Hydrogen atoms play a critical role in the chemical vapor deposition of diamond thin films. Currently, hydrogen plasmas are used to produce reproducible, clean, smooth, diamond (100) single-crystal surfaces. The use of diamond films for microelectronic or surface acoustic wave devices requires a fundamental understanding of the diamond surface termination and its interaction with adsorbed species. The hydrogen terminated diamond (100) surface is comprised of two 2x1 domains of monohydride surface dimers. Using s- and p-polarized multiple internal reflection infrared spectroscopy, the symmetric and asymmetric stretches of the HCCH surface dimer are easily resolved and are compared to ab initio calculations of the frequencies. The thermal dependence of the CH stretches is monitored as a function of the anneal temperature. When the hydrogen terminated surface is covered with a condensed layer of physisorbed molecules, the surface CH vibrational frequency is significantly influenced. We discuss the implications of these observations.

11:20am **SC+EL+SS-ThM10 Fundamental Connection Between the ESD of H/D at Silicon Surfaces and at Oxide/Silicon Interfaces***,* ***K. Cheng****, J. Lee, Z. Chen, J.-P. Leburton, E. Rosenbaum, K. Hess, J.W. Lyding,* University of Illinois, Urbana-Champaign

Parallels can be drawn between electron stimulated desorption (ESD) of hydrogen at silicon surfaces in UHV and the ESD of hydrogen at the oxide/silicon interface in CMOS transistors. In particular, the multiple carrier vibrational heating mechanism for ESD, and the giant hydrogen/deuterium isotope effect play important roles in interface degradation. In this paper we will present results demonstrating the primary role of channel hot carriers in the degradation of the oxide/silicon interface of transistors. Experiments performed on p-channel MOSFET's show essentially no isotope effect for the creation of interface traps when carriers are injected into the oxide. However, a large isotope effect, consistent with vibrational heating, is observed when carriers flow along the oxide/silicon interface. One key difference between a H-passivated silicon surface and a H-passivated oxide/silicon interface is that there is a distribution of Si-H bond strengths at the interface due to variations in the amorphous oxide matrix. Experimental results will be presented which directly measure this distribution as well as show its ramifications in terms of rapid interface trap creation. The significance of this study comes from the fact that it is still a widely held view that the dominant transistor degradation mechanisms arise from carrier injection into the oxide, and therefore will be scaled away as industry trends progress. However, by performing new experiments and using basic surface science as a setting for their interpretation, we are able to show that there are fundamental problems with this view. Our results are supported by the fact that even state-of-the-art 0.18mm, 1.5 V CMOS chips show hundreds times lifetime improvement when hydrogen is substituted by deuterium.

11:40am **SC+EL+SS-ThM11 Depth-Resolved Determination of the Hydrogen Concentration at Buried SiO@sub 2@/Si(100) Interfaces by Resonant Nuclear Reaction Analysis***,* ***M. Wilde****, M. Matsumoto, K. Fukutani,* University of Tokyo, Japan*; Z. Liu, Y. Kawashima,* NEC Corp., Japan

Hydrogen at the SiO@sub 2@/Si interface has been discussed to affect the electronic performance of MOS diodes by influencing the density of states at the interface. Drastic improvements of the reverse current resistance were reported after H@sub 2@-annealing of such devices.@footnote 1@ In this study the hydrogen concentration at the SiO@sub 2@/Si interface is measured directly by a Nuclear Reaction Analysis (NRA, based on the @sup 1@H(@sup 15@N, @alpha@@gamma@)@sup 12@C reaction), and the influence of H@sub 2@-annealing is investigated. Oxidized Si(100) samples with SiO@sub 2@ films of (19.0 - 41.5 nm) thickness were studied. In the as-oxidized condition, H near the SiO@sub 2@/Si interface is identified at a concentration lower than 4x10@sup 19@ cm@sup -3@. In the NRA depth profiles of all samples the center of the near-interface H-distribution appears at a depth (5±1) nm shallower than the interface location determined by ellipsometry. While no H is found in the silicon substrate, hydrogen is accumulated in a several nm wide layer within the oxide film adjacent to the interface. This result supports the idea of a transition region between the mere interface and the SiO@sub 2@ material, where stoichiometry and strain-induced defects may act as local bonding sites for hydrogen. In-situ annealing of the oxidized wafers in ambient H@sub 2@ gas causes a substantial increase of the H-concentration near the SiO@sub 2@/Si(100) interface, whereas the width of the H-distribution and its position within the oxide film remain unchanged. The H-distribution is thermally stable below the annealing temperature of 400@deg@C. On heating to higher temperatures in vacuum depletion of H from the interface layer occurs to a concentration level below the as-oxidized condition. Hydrogen can be replenished at the interface by repeating the H@sub 2@-annealing procedure. @FootnoteText@ @footnote 1@ S. Fujieda, H. Nobusawa, M. Hamada, T. Tanigawa, J. Appl. Phys. 84 (1998) 2732.

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.

Friday Morning, October 6, 2000

Semiconductors
Room 306 - Session SC+EL-FrM
III-Nitride Processing and Devices

Moderator: D.D. Koleske, Naval Research Laboratory

8:20am **SC+EL-FrM1 Process Development For Small-Area GaN/AlGaN HBTs***, **K.P. Lee**, G. Dang, A.P. Zhang, F. Ren,* University of Florida*; J. Han,* Sandia National Laboratories*; W.S. Hobson,* Lucent Technologies, Bell Laboratories*; C.R. Abernathy, S.J. Pearton,* University of Florida*; J.W. Lee,* Plasma Therm

A self-aligned fabrication process for small emitter contact area (2x4 µm@super 2@) GaN/AlGaN heterojunction bipolar transistor is descried. The process features dielectric-spacer sidewalls, low damage dry etching and selected-area regrowth of GaAs(C) on the base contact. The junction I-V characteristics were evaluated at various stages of the process sequence and provided an excellent diagnostic for monitoring the effect of plasma processes such as CVD or etching. A comparison will be given with large emitter-area (2.5x10@super 4@ µm@super 2@) devices fabricated on the same material. The small-area devices are alternative for microwave power switching applications.

8:40am **SC+EL-FrM2 Morphology on HDP-Etched III-Nitride Materials***, T.-N. Kuo, J.-H. Yeh, H.-J. Lee, C.-A. Chen, **D.G.-K. Jeng**,* Nano-Architect Research Corporation, Taiwan

Needle-shaped morphology or highly textured surface was often observed after GaN/GaInN multiple layered structures have been etched in high-density plasma; this phenomenon was not so often observed in structures containing GaN alone. It is attributed to layers containing indium under certain chemical environments. An experimental procedure was carried out for the characterization of materials etching. It turned out that the needle-shaped morphology or textured surface was possibly the consequence of a micro-masking effect due to low-vapor pressure compound formed on the etched surface, which prohibits underneath layers from being etched. The experiments were conducted in a high-density plasma equipment with a novel plasma source designed exclusively by the authoring group. This equipment has the capability for a typical etch-rate of 7000-8000 Å/min for all types of III-nitride compound materials and structures with good surface morphology.

9:00am **SC+EL-FrM3 Effects of Etch Processing on Contacts to n-GaN***, **R. Singh**, C.R. Eddy, Jr.,* Boston University*; H.M. Ng,* Lucent Technologies*; T.D. Moustakas,* Boston University

We report studies on the effects of high density plasma etching on the properties of ohmic contacts to n-GaN. Samples deposited by plasma-assisted MBE on a-plane sapphire and doped with Si are used in this study. Inductively coupled high density chlorine plasmas are applied to etch the surfaces of GaN and subsequent contacts (Ti/Al) to these etched surfaces are evaluated. We identify degradation of contact ohmicity even for very low rf bias powers (ion energies) as a function of the doping level in the GaN film. For films of high doping levels (3x10@super 18@ cm@super -3@), as might be encountered in a laser or LED structure, the degree of contact degradation, compared to the control sample, is a modest factor of 2 (4x10@super -4@ @ohm@cm@super -2@ to 1x10@super -3@ @ohm@cm@super -2@). However, for lower doping level films (10@super 17@ cm@super -3@), as might be encountered in electronic devices, the specific contact resistance is higher by almost two orders of magnitude for the same treatment (5x10@super -3@ @ohm@cm@super -2@ to 2x10@super -1@ @ohm@cm@super -2@). These as-deposited contacts are then rapid thermal annealed (700°C) in a nitrogen atmosphere, where specific contact resistance is monitored as a function of annealing time. Although there is improvement in contact resistivity, the effect of plasma exposure is still evident even at a cumulative rapid thermal annealing time of 280 seconds. We show that even modest ion energies in highly reactive chemistries can lead to contact degradation and that care must be taken in applying such processes if highly efficient power devices are to be routinely realized. In an effort to identify the cause of the degradation, we will also report SEM, AFM and surface sensitive photoluminescence measurements of the as etched surfaces. We will also discuss in-situ and ex-situ efforts to eliminate such degradation.

9:20am **SC+EL-FrM4 Growth of Ga(In)NAs/GaAs Alloys by Plasma-Assisted Molecular Beam Epitaxy***, **A.L. Holmes, Jr.**,* University of Texas at Austin **INVITED**

In recent years, the addition of nitrogen into GaInAs, created via energetic nitrogen species from a RF-plasma or decomposition of hydrazine-based precursors,has attracted a great deal of interest due to the large negative bowing parameter of the resultant semiconductor alloy. As a result, GaNAs/GaAs and GaInNAs/GaAs heterostructures can be grown which emit light at wavelengths applicable for lasers and detectors for fiber-optic communications or absorb wavelengths which make solar cells more efficient. While nitrogen leads to a significant reduction in the band gap of the resultant material, the addition of nitrogen (on the order of a few atomic percent) also leads to a significant reduction in luminescence intensity which has significant consequences for optoelectronic devices. In this talk, growth of the GaInNAs/GaAs alloy system will be discussed. The effects of important growth-related parameters such as growth temperature, RF plasma conditions, indium composition, and arsenic over-pressure will be described. The resultant materials are characterized by x-ray diffraction, photoluminescence, and SIMS to create a picture of how nitrogen is incorporated and how this incorporation affects the resultant material properties. These properties are then compared to GaNAs-based photodetectors which show outstanding device performance with nitrogen concentrations as high as 2.5%.

10:00am **SC+EL-FrM6 Field Electron Emission and Surface Properties of as-grown and Modified AlGaN Films***, A. Bensaoula, I. Berishev, E. Kim,* University of Houston*; M. Ugarov, V. Ageev, E. Loubnin, A. Karabutov,* General Physics Institute, Russia*; **A. Tempez**,* University of Houston

The correlation between surface morphology and composition, Si substrate orientation and field emission properties of Al@sub x@Ga@sub1-x@N and GaN/AlN films was investigated. It was demonstrated that a high Ga surface density provides thin films with better field electron emission characteristics such as a higher emission current and lower voltage threshold. It was found that a proper choice of the substrate orientation is crucial to obtaining the desired electronic properties since it plays a major role in the resulting thin film surface microstructure. A post-growth modification by X-ray irradiation was also performed on these films. Our results show a significant improvement in the field emission characteristics of the Al@sub x@Ga@sub1-x@N surfaces. The threshold field was reduced by up to three times and current density increased up to 10 A/cm@super2@. These results are consistent with data previously obtained for field emission and laser photoconductivity enhancement by X-ray irradiation of BN thin films. The effect of the X-ray induced generation of additional density of states in the nitride material band gap, on the changes in film conductivity and surface potential barrier height will be discussed. The project was funded in part by a CRDF Grant assistance program (Project # RP0-698), a Russian Federation for Basic Research grant (# 99-02-16653) and a NASA Cooperative agreement #NCC8-127 to the Space Vacuum Epitaxy Center.

10:20am **SC+EL-FrM7 Effect of Annealing and Carbon Concentration on the PL Intensity from GaN:Er and GaN:Eu***, **M.E. Overberg**, C.R. Abernathy, S.J. Pearton,* University of Florida*; J.M. Zavada,* U.S. Army European Research Office, UK

An attractive alternative for emission in the visible and near-IR are rare earth doped III-Nitrides, whose emission wavelength is host-material insensitive and less susceptible to thermal quenching than conventional narrow gap semiconductors. GaN doped with Er and Eu during growth by molecular beam epitaxy (MBE) has been found to produce strong room temperature emission at 1540 nm and 621 nm, respectively. In addition to the electronic characteristics of the host material, impurities such as C and H are expected to play an important role in the emission process. In this study, the effects of carbon doping and annealing in either nitrogen or forming gas on the luminescence intensity from Er-doped and Eu-doped GaN has been investigated. In samples with no added carbon, annealing was found to decrease the room temperature emission. The addition of carbon to the GaN during growth however, not only improved emission relative to non-carbon doped material but also produced material which improved with annealing. For carbon co-doped material the presence of hydrogen in the annealing ambient produced the greatest improvement in emission intensity, suggesting that both C and H are beneficial to the emission process. The effect of annealing on surface morphology and structural quality will also be presented as will a model for the observed PL behavior.

10:40am **SC+EL-FrM8 Probing Nanoscale Electronic Properties in Nitride Semiconductor Heterostructures***, **E.T. Yu**, K.V. Smith, X.Z. Dang,* University of California, San Diego **INVITED**

III-V nitride heterostructures are of outstanding current interest for both optoelectronic and electronic device applications. However, the high concentrations of point and extended defects typically present even in device-quality nitride semiconductor material necessitates detailed characterization and understanding of local structure and electronic properties at atomic to micron length scales for optimization of device performance. In particular, the presence of a variety of defect structures in combination with strong piezoelectric and spontaneous polarization effects in nitride semiconductors leads to pronounced variations in local electronic properties. Experimental characterization, theoretical analysis, and numerical simulation of these effects, especially in the context of nitride heterostructure field-effect transistor (HFET) structures, will be described. Scanning capacitance microscopy has been used extensively to characterize local electronic structure in AlGaN/GaN HFET structures. Measurement and analysis of capacitance contrast as a function of bias voltage allows submicron-scale lateral variations in transistor threshold voltage, nanoscale depleted regions within the channel of the transistor in the vicinity of negatively charged threading dislocations, and evidence of piezoelectric fields arising from local strain in the vicinity of dislocation lines to be observed. Application of large bias voltages during the imaging process is found to give rise to localized trapping of charge in deep levels. Measurement and analysis of the resulting contrast allows the distribution of trapped charge both laterally and as a function of depth to be probed.

11:20am **SC+EL-FrM10 GaN and AlGaN Power Rectifiers***, **A.P. Zhang**, G. Dang, F. Ren, X.A. Cao, K.P. Lee, S.J. Pearton,* University of Florida*; J. Han,* Sandia National Laboratories*; J.I. Chyi,* National Central University,Taiwan*; C.M. Lee, C.C. Chuo,* National Central University, Taiwan

We fabricated the GaN & AlGaN rectifiers and p-i-n rectifiers on a range of different MOCVD-grown materials. The reverse breakdown voltages of lateral GaN&AlGaN rectifiers on 3µm thick resistive GaN&AlGaN were in a range of 2.3~4.3kV with a 30µm Schottky metal and Ohmic metal spacing. The p-i-n diodes on 4µm thick GaN epitaxial layer showed a reverse breakdown voltage of 500V with turn-on voltage of ~5V (100A/cm@super 2@). Different edge termination methods were used to improve the performance of GaN rectifiers, including Schottky metal overlap, guard rings, and float rings and junction barrier control (JBS). The edge termination has a strong effect to prevent catastrophic breakdown at the contact periphery. The lowest R@sub ON@ was 0.14 @ohm@.cm@super 2@ for GaN rectifiers and 2.6 @ohm@.cm@super 2@ for AlGaN rectifiers. Figure-of-merit (V@sub RB@)@super 2@/R@sub ON@ are in the 6 -55 MW.cm@super -2@ range, emphasizing the potential of these devices for power switching applications. For the devices we fabricated, we invariantly observed the negative temperature coefficient for V@sub RB@ most likely due to the influence of defects in the heteroepitaxial GaN. For the similar reverse breakdown voltage, current densities are higher in the p-i-n structures, at the expense of higher turn-on voltage, but the on-voltages still need improvement in the Schottky rectifiers. A comparison will be given with state-of-the-art Si and SiC power rectifiers.

11:40am **SC+EL-FrM11 Growth and Characterization of Gadolinium Oxide Gate Dielectric on Gallium Nitride***, **B.P. Gila**, K.N. Lee, K.K. Harris, W. Johnson, V. Krishnamoorthy, C.R. Abernathy, F. Ren, S.J. Pearton,* University of Florida

Fabrication of high performance metal oxide semiconductor field effect transistors (MOSFETs) on gallium nitride will require both good interfacial electrical characteristics and good thermal stability. While dielectrics such as SiO@sub 2@ and GaGdO have demonstrated low to moderate interface state densities, questions remain about their thermal stability and reliability, particularly for use in high power or high temperature widebandgap devices. In this talk we will discuss the utility of gadolinium oxide, Gd@sub 2@O@sub 3@, as a gate dielectric material on GaN. Gadolinium oxide deposited by gas source molecular beam epitaxy from elemental Gd and an electron cyclotron resonance (ECR) oxygen plasma has been found to produce layers with excellent surface morphologies as evidenced by SEM and AFM, with a surface roughness of less than 1 nm. Surface preparation techniques, both in-situ and ex-situ, have been explored to produce films of different crystal morphologies as evidenced by RHEED and TEM. Stoichiometric films can be easily obtained over a range of growth temperatures, growth rates and oxygen flows. This talk will describe the relationship between deposition conditions and film characteristics for Gd@sub 2@O@sub 3@, and will present electrical characterization and thermal stability of capacitors fabricated from Gd@sub 2@O@sub 3@ on GaN.

Author Index

Bold page numbers indicate presenter

Author Index

Author Index