## Semiconductors
## Room 122 - Session SC+SS-MoM
## Oxidation of Semiconductors

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

10:00am **SC+SS-MoM2 Coexistence of Active and Passive Oxidation Areas on the Si(100) Surface under Oxygen Cluster Beam Impact***, **D.V. Daineka**,* A.F. Ioffe Physicotechnical Institute, Russia, France*; F. Pradère, M. Chatelet,* CNRS, Ecole Polytechnique, France*; E. Fort,* Universités Paris VI et Paris VII, France

The Si(100) oxidation by cluster beam impact has been studied in ultrahigh vacuum for surface temperatures from 850 to 1100°C. Neutral oxygen clusters with an average size of 2000 molecules and a translational energy of 0.26 eV/molecule were delivered by a supersonic beam with the maximal flux density of 10@super 15@ cluster/cm@super 2@s. The analysis of surface profiles after the beam exposure at T 2SiO(g), is characterized with a steep inner wall and a gradual decrease of its depth towards the outer edge. In the central part of the impact spot, surrounded by the groove, no surface etching occurs due to the formation of a protective oxide layer. The revealed effect is attributed to the gaussian flux density distribution in the cluster beam cross section. The abrupt drop of the etching rate at the inner wall of the groove corresponds to the transition from active to passive oxidation. Only active oxidation with formation of a single etch pit was observed at T>1000°C. The reaction is steady-state and close to first-order. It has been found that there is no pronounced temperature dependence of the etching rate, which is in contrast with the previous results obtained with molecular oxygen.@footnote 1,2@ Etching rates as high as 6 µm/min were measured for T>1000°C. This enhanced reaction efficiency is attributed to the role of the oxygen clusters. The obtained results show that the knowledge of the flux density distribution in the beam is extremely important when supersonic sources are used to study surface reactions. @FootnoteText@ @footnote 1@ Y. Ono, M. Tabe, H. Kageshima, Phys. Rev. B48(1993) 14291 @footnote 2@ S. Hildebrandt, A. Kraus, R. Kulla, H. Neddermeyer, Appl. Surf. Sci. 141(1999) 294 .

10:20am **SC+SS-MoM3 An Ab Initio Study of the Initial Oxidation of the Si(100)-(2x1)***, Y. Widjaja, **C.B. Musgrave**,* Stanford University

As the dimensions of metal-oxide-semiconductor (MOS) devices keep shrinking, O@sub 2@ molecule is increasingly used as the oxidizing species over H@sub 2@O as it oxidizes silicon more slowly and hence results in better control of film thickness. Here, we use density functional theory to investigate the detailed chemical mechanism of O@sub 2@ reaction with the Si(100)-(2x1) surface using cluster approximations, in which larger clusters are used to examine reactions across dimers as well as to investigate nonlocal effects. Our proposed mechanism confirms the trapping-mediated mechanism previously observed by molecular beam experiments. We find that O@sub 2@(g) initially adsorbs on the "up" silicon atom of the surface dimer with an adsorption energy of 31 kcal/mol. The adsorption is site specific and reaction on the "down" silicon atom is unstable. The adsorbed O@sub 2@(a) then reacts and forms a peroxide bridge structure, which subsequently dissociates and inserts into the dimer bond and the backbond. Reactions involving neighboring dimers also exhibit an adsorbed state in which the O@sub 2@(a) molecule is adsorbed in between the two silicon dimers. In addition to investigating the initial adsorption of oxygen molecules, we also study the atomistic mechanisms leading to the SiO(g) desorption observed at high temperature. The desorption barrier calculated is 65 kcal/mol, which explains the high thermal energy required before SiO(g) desorption occurs.

11:00am **SC+SS-MoM5 Oxidation of Si(100): Mechanisms of Oxygen Insertion, Migration and Agglomeration***, **K. Raghavachari**,* Agere Systems

Understanding the formation of thin oxides on silicon surfaces is of prime importance as developments in microelectronics demand oxide thicknesses of the order of a few atomic layers. We have carried out first-principles quantum chemical calculations with cluster models to investigate the structural and mechanistic aspects of the initial oxidation of a Si(100) surface. The microscopic steps related to the initial oxygen incorporation as well as oxygen migration and agglomeration on annealing are considered in detail. The calculated activation energy barriers suggest an interesting competition between the steps involved in oxygen insertion and oxygen migration and agglomeration. The presence of surface hydrogen causes significant perturbations on the calculated energy barriers and has important implications to the reaction mechanisms. Our results are used to provide novel interpretations of experimental infrared spectroscopic data.

11:20am **SC+SS-MoM6 Fundamental Aspects of Silicon Oxidation: O@sub 2@ and H@sub 2@O Reaction with Si(100) and H-passivated Si Surfaces***, **Y.J. Chabal**,* Agere Systems*; A. Esteve,* LAAS, France*; X. Zhang, E. Garfunkel,* Rutgers University*; K. Raghavachari,* Agere Systems

Examining the initial oxidation steps of both clean and H-passivated silicon surfaces is important to unravel the mechanism for oxygen insertion and oxide formation in realistic environments. We have combined high resolution infrared absorption spectroscopy (IRAS) with quantum chemical (QC) cluster calculations and kinetic Monte Carlo (KMC) simulations to determine the energetics and kinetics of O@sub 2@ and H@sub 2@O thermal oxidation of Si(100) and H-passivated Si(100) and Si(111) surfaces. Specific local structures are determined by comparing experimental IRAS data of both Si-O and Si-H vibrational modes with vibrational frequencies determined from first principles QC calculations of energetically stable model structures. KMC simulations are then used to analyze the cumulative effect of a series of elementary reaction steps on extended growth of an oxide layer. For the clean Si(100)-(2x1) surface, oxygen is readily incorporated into the surface from either O@sub 2@ or H@sub 2@O with a thermodynamic propensity to agglomerate but with different kinetics. KMC simulations show that oxide growth is governed by two fundamental phenomena: (i) charge transfer arising from oxygen insertion into the Si-Si bonds and (ii) hydrogen passivation and/or dangling bond formation at the surface. The charge transfer strongly affects the energetics (thermodynamics) of further oxygen agglomeration (the ability for an oxygen atom to leave an oxygenated dimer unit); the presence/absence of dangling bonds then compounds this effect by further modifying the oxygen migration kinetics. For H-passivated surfaces, both O@sub 2@ and H@sub 2@O are found to incorporate into the Si-SiH backbonds without loss of surface hydrogen. We find an oxygen insertion energy of 1.6 - 1.7 eV, while the oxidation kinetics of different surface structures appear to be dominated by O2 access to Si-Si bonds (locally blocked by unreactive Si-H species).

11:40am **SC+SS-MoM7 Displacement of Surface As Atoms by Insertion of Oxygen Atoms into As-Ga Backbonds***, **M.J. Hale**, S.I. Yi, J.Z. Sexton, A.C. Kummel,* University of California, San Diego

Stable and metastable oxide structures resulting from the reaction of GaAs(001)-(2x4) with O and O@sub 2@ are investigated using scanning tunneling microscopy (STM). The relative stability of these oxide structures is examined using density functional calculations. STM images show that when GaAs(001)-(2x4) is exposed to O atoms, the O atom will either remove an As atom from its original dimer position and take its place or insert into an As-Ga backbond and create a metastable state. As the O atom coverage increases, O atoms increasingly occupy the position of two As atoms across two neighboring dimers, while the number of metastable states remain constant. These experiments show that As is preferentially removed as a pair (As@sub 2@) with one removed As atom originating from each of two neighboring As-As dimers instead of two As atoms from the same As-As dimer. This displacement of As@sub 2@ is consistent with the propensity of the unit cell to relax into a charge-balanced morphology. Furthermore, the charge-imbalance from oxygen chemisorption is the driving force for As@sub 2@ displacement. DFT calculations demonstrate both the charge imbalances in the metastable states and the relative stability of the final chemisorption state. The displaced arsenic atoms form As@sub Ga@ antisites which pin the Fermi level and prevent thermal oxidation from forming an electrically passive interface on GaAs in contrast to vapor deposited oxides.

## Semiconductors
## Room 124 - Session SC-MoM
## Band-Engineered Electronic Materials

**Moderator:** R.S. Goldman, University of Michigan

9:40am **SC-MoM1 III-N-V: A Novel Class of Compound Semiconductors for Electronic and Photonic Applications***, **C.W. Tu**,* University of California, San Diego **INVITED**

Recently there is much interest in III-N-V compound semiconductors, because only a small amount of nitrogen incorporation (less than 5%) in conventional GaAs- and InP-based III-V compounds results in very large bandgap bowing, which is mainly from the downward movement of the conduction band edge. We demonstrated that InNAsP/GaInAsP single-quantum-well microdisk lasers exhibit a large characteristic temperature, as a result of a large conduction band discontinuity and electron confinement in the quantum well. An application of more interest is using GaInNAs/GaAs heterostructures on GaAs substrates for 1.3 micron edge-emitting and vertical-cavity surface-emitting lasers (VCSELs), utilizing the well developed GaAs/AlAs distributed Bragg reflectors (DBRs). We demonstrated even longer wavelength (1.5 micron) room-temperature photoluminescence (PL) from self-assembled GaInNAs QDs. We have also utilized the low-bandgap GaInNAs as the base of a heterojunction bipolar transistor (HBT), which exhibits a 0.4 V reduction in the turn-on voltage for low-power applications. Besides bandgap bowing, incorporating nitrogen in GaP also results in a change in the band structure. We have demonstrated that with only 0.5% nitrogen, the Ga(N)P bandgap changes from being indirect to direct, with strong PL emission in the red (650 nm). We have fabricated light-emitting diodes (LEDs) from GaNP/GaP heterostructures grown with one-step epitaxy, which is simpler than the commercial process of GaAs substrate removal and wafer bonding to a transparent GaP substrate for high-brightness AlInGaP LEDs. We are also exploring GaInNP on GaAs for HBT applications because of near-zero conduction band offset.

10:20am **SC-MoM3 Microstructure and Optical Properties of (InGa)(AsN) Alloys and Nanostructures***, **X. Weng**, S. Clarke, A. Daniel, J. Holt, S. Krishna, S. Kumar,* University of Michigan, Ann Arbor*; J. Sipowska,* University of Michigan, Flint*; V. Rotberg, R. Clarke, A. Francis, P.K. Bhattacharya, R.S. Goldman,* University of Michigan, Ann Arbor

Mixed anion nitride-arsenide compound semiconductor heterostructures are promising for devices with emission or detection wavelengths throughout the near infrared range. However, a limited miscibility of InGaAsN on the anion sublattice leads to the formation of phase separation-induced alloy nanostructures.@footnote 1,2@. We have synthesized InGaAsN alloys and nanostructures by N ion implantation into GaAs and InAs, with a variety of implantation and rapid thermal annealing conditions. We have analyzed the composition, structure, and properties of the resulting alloys and nanostructures, using nuclear reaction analysis, transmission electron microscopy (TEM), x-ray energy dispersive spectrometry, x-ray diffraction, photoluminescence, and cathodoluminescence spectroscopy. For 50 keV N ion implanted GaAs and InAs substrates, high resolution cross-sectional TEM reveals ~5nm diameter amorphous nanostructures surrounded by crystalline matrices. For 100 keV N ion implanted GaAs epilayers, crystalline nanostructures surrounded by disordered matrices are apparent. Electron and x-ray diffraction indicate that these nanostructures are cubic phases with lattice parameters similar to that of pure GaN. The crystalline nanostructures exhibit significant photoluminescence in the near infrared range. The apparent lowering of the fundamental band gap of the GaN nanostructures is consistent with strain-induced band gap narrowing of a GaN-rich cluster.@footnote 1@. We will discuss the mechanisms of formation and coarsening of these nanos truc tures, correlations between their optical and structural properties, and comparisons with similar alloys and nanostructures synthesized by molecular beam epitaxy. @FootnoteText@@footnote 1@R. S. Goldman et al., Appl. Phys. Lett. 69, 3698 (1996), J. Electr. Mater. 26, 1342 (1997). @footnote 2@H. P. Xin et al., Appl. Phys. Lett. 74, 2337 (1999).

10:40am **SC-MoM4 Measurement of Charge Separation Potentials In GaAs(1-x)N(x)***, **S.W. Johnston**, R.K. Ahrenkiel,* National Renewable Energy Laboratory*; C.W. Tu, Y.G. Hong,* University of California, San Diego

The ternary alloy GaAs(1-x)N(x) is interesting as a semiconductor that can be grown epitaxially on GaAs. As is well known, the bandgap can be reduced by as much as 0.4 eV by changing the nitrogen concentration from 0% to 3%. We measured the spectral response and photoconductive lifetime of the alloys, as a function of temperature. In this work, the films were grown by gas-source molecular beam epitaxy on semi-insulating GaAs substrates. All measurements were made using the contactless, resonant-coupled photoconductive decay (RCPCD) method. Our data shows that the spectral or excitation spectra of GaAs1-xNx alloys consists of photoconductive band tails that extend well into the infrared (beyond the nominal bandgap). For example, the photoconductive bandtails extend to about 1.8 mm for GaAs(0.97)N(0.03). The primary photoconductive decay times are in the range of 200 to 300 ns. At temperatures below about 200 K, the decay rate begins to decrease with lowered temperature. By plotting the inverse lifetime versus 1/T, one generates the standard Arrhenius plot of a thermally activated process. These data fits produce activation energies that increase with the N-content. The activation energies, DE, for compositions x = 0.011, 0.023, and 0.033 are 67, 72, and 83 meV, respectively. These energies represent the potential barriers which inhibit recombination. The increase of DE with x is indicative of charge separation being related to N-atom clustering. Our model suggests that these barriers originate from the inhomogenous band structure produced by the random distribution of the nitrogen impurity.

11:00am **SC-MoM5 Characterization of GaPN Layers Grown by Molecular Beam Epitaxy on Si Substrates***, **M.A. Santana-Aranda**, M. Melendez-Lira, M. Lopez-Lopez,* Centro de Investigacion y de Estudios Avanzados del IPN, Mexico*; K. Momose, H. Yonezu,* Toyohashi University of Technology, Japan*; S. Jiménez-Sandoval,* Cinvestav-IPN, Unidad Querétaro, Mexico

The heteroepitaxial growth of III-V-N alloys with high crystal quality on Si substrates could make possible the monolithic integration of III-V-N based light-emitting devices with the Si based microelectronics. However the III-V-N/Si heteroepitaxy present serious problems like the lattice mismatch and the difference in thermal expansion coefficients. In order to solve these problems, we have been studying the growth of GaPN with a N concentration of 2% that is lattice-matched to the Si substrate. The epilayers were grown by molecular beam epitaxy employing an RF plasma source to produce active nitrogen species. First, a 3.2µm Si homoepitaxial layer was grown on the substrate, followed by a thin (20nm) GaP layer to avoid the strong interaction of nitrogen with Si. Then, the GaP@sub 0.98@N@sub 0.02@layer was grown with a thickness of 400nm. In order to avoid the generation of crystal defects induced by the different thermal expansion coefficients the epilayer was capped first with a 16nm thick GaP layer and finally with a 300nm thick Si layer. The structural and optical properties of this sample were compared with those of a GaPN layer on GaP/Si but without the capping layers, and with those of a GaPN layer on a GaP substrate. Transmission electron microscopy showed that the capped heterostructure was free of crystal defects. While the other samples presented dislocations and cracks. The photoluminescence at 10K associated to GaP was blue shifted in the capped structure confirming that the GaP layers were coherently strained to the Si lattice. Raman spectroscopy showed narrow peaks in the capped structure reflecting the high structural quality of this sample, for the other samples the Raman peaks were wide suggesting the presence of disorder.

11:20am **SC-MoM6 Nanoscale Phase Formation at Cu(In,Ga)Se@sub 2@ Surfaces***, **Y.M. Strzhemechny**, G.H. Jessen, J.I. Choi, L.J. Brillson,* The Ohio State University*; D.-X. Liao, A. Rockett,* University of Illinois at Urbana-Champaign

Copper indium gallium diselenide (CIGS) exhibits unique optical properties that make it well suited for thin film devices as a polycrystalline material. The engineered electronic properties of CIGS heterojunctions depend sensitively on the CIGS near-surface region. The nanoscale electronic structure and chemistry of this layer and, specifically, point defect segregation and surface phases are thought to be critical to such device structures, yet they are relatively unexplored. We employed low-energy depth-resolved cathodoluminescence (CL) and Auger Electron Spectroscopy (AES) to measure the local band and defect properties as well as composition variations of CIGS films grown epitaxially with (001), (110), and (112) orientations on GaAs wafer substrates. CL spectra reveal near band edge (NBE) emissions of 1.10 to 1.15 eV, depending on growth and orientation as well as the presence of a deep-level transition with energy 0.89-0.93 eV confined to within a few hundred nm of the free CIGS surface. The NBE energies vs. AES compositions agree with the reported variation in band gap vs. Cu/(In+Ga) ratio. The deep defect-associated feature relative to the higher lying peak has maximum intensity at the surface and decreases exponentially into the bulk with a decay length of ca. 50 nm. Auger depth profiles for (110) and (001) orientations show 16% and 20%, respectively, depletion in Cu content within tens of nanometers of the surface. Deep level and NBE energies exhibit a strong dependence on surface Cu and Ga content. Both increase by tens of meV away from the free surface, in line with the increased band gap and changes in composition. The Cu-deficient surface layers are consistent with an ordered vacancy compound proposed for the CIGS surface. The observed gap and composition changes confirm the existence of a nanoscale surface phase whose properties can impact charge generation and recombination for solar energy-generating structures.

11:40am **SC-MoM7 Metal-organic Vapor Phase Epitaxial Growth and Photoluminescent Properties of ZnMgO and ZnCdO Thin Films***, **W.I. Park**, G.-C. Yi,* Pohang Univ. of Science and Technology, Korea (ROK)

ZnO, a wide-gap semiconductor oxide, has attracted considerable attention due to its large exciton binding energy (~60 meV) and bond strength, which might make reliable high efficiency photonic devices based on ZnO. Recently it has also been reported that ZnMgO was grown with maximum

Mg incorporation up to 36 at.% without phase separation and that the room temperature luminescence energy in this film blue-shifted from 3.3 to 4.0 eV. Since a ZnMgO containing MgO over 4 at.% is in a thermodynamically metastable state, this result indicates that the solubility limit of Mg in ZnO depends on growth mechanisms as well as growth conditions. Meanwhile, current research on the growth of ZnO-related alloys is restricted to pulsed laser deposition and molecular beam epitaxy. Despite the epitaxial growth of high quality ZnO and related alloys using the methods, they might have disadvantages in mass production, due to high cost and low throughput. In this talk, we demonstrate that metal-organic vapor phase epitaxy (MOVPE), which has great advantages in terms of large area deposition and atomic composition control feasibility, is an excellent technique for the epitaxial growth of high quality ZnO and related alloy films. In addition, the structural and optical characterizations of ZnMgO and ZnCdO thin films will be reported. By increasing Mg content up to 47 at.%, the c-axis constant of ZnMgO films decreased from 0.521 nm to 0.515 nm and no significant phase separation in the ZnMgO films was observed as determined by x-ray diffraction measurements. Furthermore, the near-band-edge (NBE) emission peak position showed blue shifts of 100, 430, and 570 meV at Mg content levels of 9, 21, and 47 at.%, respectively. Photoluminescent properties of the ZnMgO and ZnCdO alloy films will also be discussed.

## Semiconductors
## Room 122 - Session SC+SS-MoA

### Semiconductor Surfaces

**Moderator:** D.Y. Petrovykh, Naval Research Laboratory

2:20pm **SC+SS-MoA2 Indium-Induced Charge Redistribution and Surface Electronic Structure of the Si(111)-(7x7) Surface***, **M. Yoon**, R.F. Willis,* The Pennsylvania State University

The adsorption mechanism and the origin of the In-induced surface electronic states of the Si(111)-(7x7) surface have been studied using bias-dependent scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS). At very low In coverages, bias-dependent STM images show that some of adatoms have either slightly higher or lower apparent height in the filled-state image, while the empty-state images are completely identical to those of the clean Si(111)-(7x7). These peculiar features are interpreted as being caused by two adsorption mechanisms: charge redistribution due to the adsorption of In atoms on Si dangling bond and the substitution of In for Si atoms in the 7x7 adatom positions, opening the bandgap by removing intrinsic metallic surface states caused by Si adatom dangling bond. As the coverage increases, a self-assembly of a superlattice of two-dimensional non-metallic In nanodots on the Si(111)-(7x7) surface begin to develop on both halves of the 7x7 unit cell which indicates a metal-insulator transition occurring on the surface. This confirms that the origin of the metallicity of the Si(111)-(7x7) surface is the delicate charge transfer between adatom and restatom Si dangling bonds in the center of the 7x7 unit cell.

2:40pm **SC+SS-MoA3 Study of GaAs(100) Surface Cleaning Using Synchrotron Radiation Photoemission Spectroscopy***, **Z. Liu**, Y Sun, F. Machuca,* Stanford University*; W.E. Spicer, P. Pianetta,* Stanford Synchrotron Radiation Lab*; R.F.W. Pease,* Stanford University

Atomic surface cleanliness is required for novel NEA electron emission devices fabricated from GaAs and is also very important for GaAs MBE growth. Chemical cleaning of the GaAs (100) surface has been studied with high-resolution photoemission spectroscopy using synchrotron radiation (in the range of 55 eV to 750 eV) at the Stanford Synchrotron Radiation Laboratory. The high surface sensitivity of the technique has allowed us to identify the chemical state of the surface species after both the chemical cleaning and final vacuum processing steps. In order to eliminate contamination from the surroundings, all chemical cleaning steps were performed in an Ar or N@sub 2@ purged glove box attached to the load-lock allowing samples to be transferred into the system without being exposed to air. Samples were etched in H@sub 2@SO@sub 4@:H@sub 2@O@sub 2@:H@sub 2@O solution and then heat cleaned at 500°C (both diluted and concentrated solutions were studied). After chemical etching in the dilute (4:1:100) solution, elemental As (>1ML), As sub oxide (~0.1ML), Ga sub oxide and C (0.5~1ML) are found on the surface. Subsequent annealing at 500°C in UHV produces a stoichiometric, oxide free surface as determined by valence band and core level photoemission. In addition, C has been reduced to less than 10% of its initial level. We believe that the C can be removed by heating because the elemental As from the earlier cleaning step tends to protect the GaAs surface.

3:00pm **SC+SS-MoA4 Steady-State Fluctuations of High-T Vicinal Si(111): Investigation of Step-Step Correlation Function of REM Data@footnote 1@***, **T.L. Einstein**,* University of Maryland, College Park*; S.D. Cohen,* UM,CP*; J.J. Métois,* University of Aix-Marseilles III, France*; H.G. Bantu,* UM,CP*; H.L. Richards,* Texas A&M University*; E.D. Williams,* UM,CP

To estimate from experimental data the strength of step interactions on vicinal surfaces, one typically studies the terrace-width distribution (TWD), i.e. the separation distance between adjacent steps. From a theoretical perspective, it is simpler to study instead the step-step correlation function h(L), i.e. the probability of finding two steps separated by some distance L, regardless of how many steps lie between them.@footnote 2@ In fact, to the extent that traditional 1+1 D fermion models are applicable, exact results are available for h(L).@footnote 3@ We apply this new approach to extensive REM (reflection electron microscopy) data for the intriguing case of vicinal Si(111) at high temperatures T: 1100, 1200, and 1250°C. To compensate for the sublimation in this regime (e.g. 0.015 ML/s at 1100°C), Si is evaporated onto the sample to maintain steady state.@footnote 4@ Digitizing the data posed several unusual challenges, some of which made this system particularly appropriate for analysis via h(L) rather than TWD. The key question is whether the step stiffness and step-step repulsion of these steady-state systems are consistent with (higher-T extrapolation) of equilibrium results obtained at lower T. @footnote 5,6@ @FootnoteText@ @footnote 1@ Work at UM supported by NSF-MRSEC. @footnote 2@ T.L. Einstein et al., Surface Sci., in press [cond-mat/0012274] & refs. therein. @footnote 3@ P.J. Forrester, J. Stat. Phys.72 (1993) 39. @footnote 4@ S. Stoyanov, J.J. Métois, & V. Tonchev, Surface Sci. 465 (2000) 227. @footnote 5@ H.-C. Jeong & E.D. Williams, Surface Sci. Reports 34 (1999) 171 & refs. therein. @footnote 6@ C. Alfonso, J.M. Bermond, J.C. Heyraud, & J.J. Métois, Surface Sci. 262 (1992) 371.

3:20pm **SC+SS-MoA5 Simplified Bond-Charge Model for the Analysis of Second-Harmonic-Generation Data: Application to Si/Dielectric Interfaces***, **J.F.T. Wang**, G.D. Powell, R.S. Johnson, G. Lucovsky, D.E. Aspnes,* North Carolina State University

We develop a simplified bond-charge model for the analysis of second-harmonic-generateion (SHG) data, and apply it to study interfaces between singular and vicinal (001) and (111) Si substrates and various oxides, nitrides and oxynitrides. We model SHG microscopically as the 2@omega@t component of dipole radiation generated by the nonsinusoidal motion of electrons in bonds with anharmonic restoring forces, where the bonding electrons are driven by the @omega@t incident field. The simplfying assumption, which makes the treatment of SHG simpler than that of linear optics, is that only the anharmoic polarizability along the bond axis need be considered owing to the expected symmetry of the bond. Using this approach we analyze the azimuthal intensity dependence of SHG in the 800 to 900 nm spectral range of Si interfaces of various orientations and surface terminations. We find for example that a knowledge of the azimuthal dependence of the p-p signal for vicinal (111)Si allows us to predict the p-s, s-p, and s-s signals, and to determine the real and imaginary parts of the nonlinear polarizability associated with the different bonds. For interfaces between vicinal (001) Si samples and thin (less than 10 nm) thermally grown oxides, the essential absence of a 4-fold contribution to the azimuthal intensity dependence shows that these interfaces are double-domain. This result allows us to assign both SHG and RD signals of these interfaces to steps. Differences among oxidized samples and samples nitrided in various ways are relatively small, but systematic.

3:40pm **SC+SS-MoA6 STM Studies of the Ca/Si(111) System***, **J.W. Dickinson**,* Virginia Commonwealth University*; S.C. Erwin,* Naval Research Laboratory*; J.A. Carlisle,* Argonne National Laboratory*; A.A. Baski,* Virginia Commonwealth University

The Ca/Si(111) system forms a series of odd-order nx1 (n = 3,5,7,etc.) reconstructions that culminate with a 2x1 phase at 0.5 ML.@footnote 1@ Similar to group I metals, group II Ca forms a 3x1 phase at low coverage, where a previous model based upon Si honeycomb-chain-channel (HCC) chains accounts well for the observed STM data. In contrast to the group I metals that form the 3x1 phase at 1/3 ML, however, Ca forms this phase at 1/6 ML,@footnote 2@ presumably due to the fact that Ca has twice the number of available electrons. Another interesting behavior unique to Ca is the presence of a 2x1 phase that reaches completion at 1/2 ML. We have proposed a model for the 2x1 phase based upon pi-bonded Seiwatz Si chains, where Ca rows form between the Si chains. The variety of odd-order nx1 phases (5x1, 7x1, etc.) that occur between these end-point 3x1 and 2x1 phases are then appropriate combinations of the 3x1 HCC chains and 2x1 Seiwatz chains. For example, a 5x1 unit cell is composed of one HCC chain and one Seiwatz chain, where two Ca rows are found per unit cell. Calculated surface energies based on the HCC and Seiwatz models correctly predict that for increasing Ca coverage, the 3x1, 5x1, and 2x1 phases each appear as stable phases. @FootnoteText@ @footnote 1@ A.A. Baski, S.C. Erwin, M.S. Turner, K.M. Jones, J.W. Dickinson, J.A. Carlisle, Surf. Sci. 476, 22 (2001). @footnote 2@ G. Lee, D. Shin, J. Koo, H. Kim, S. Hong, Abstract #S25-8, APS 2001 March meeting.

4:00pm **SC+SS-MoA7 Growth of Semiconductor (Si, Ge)/Insulator (CaF@sub 2@) Heterostructures on Si(111)***, **A. Klust**, M. Bierkandt, C. Deiter,* Universität Hannover, Germany*; J. Falta,* Universität Bremen, Germany*; M. Grimsehl,* Universität Hannover, Germany*; R. Feidenhansl, C. Kumpf,* Riso National Laboratory*; T. Schmidt,* Universität Bremen, Germany*; Y. Su,* Universität Hamburg, Germany*; J. Wollschläger,* Universität Hannover, Germany

Silicon-fluorite superlattices exhibit strong photoluminescence at room temperature@footnote 1@. The origin of this novel behavior, not found in bulk silicon, may be electron confinement and/or interface effects. An important contribution to understanding these effects is detailed knowledge of the epitaxial semiconductor/insulator interface structure, which we find to be different for the Si-on-CaF@sub 2@ and CaF@sub 2@-

on-Si interfaces. The CaF@sub 2@/Si(111) interface was investigated using x-ray standing wave (XSW) excited photoelectron spectroscopy (XPS). This combination exploits the large binding energy difference between interface and bulk emission to separately locate these sites relative to the Si substrate. The XSW results show that interface Ca atoms are well ordered even at growth temperatures as low as 370°C. Furthermore, we used surface x-ray diffraction (SXRD) to study growth of Si and Ge on thin CaF@sub 2@ films. In contrast to surfactant mediated growth of Si on CaF@sub 2@,@footnote 2@ Si films grown on pristine CaF@sub 2@ films exhibit the same crystallographic orientation as the CaF@sub 2@ film. For the CaF@sub 2@-on-Si interface, the orientation of the substrate and overlayer are rotated by 180° at growth temperatures used here. These differences in interface structure are attributed due to different interface reaction chemistry.@FootnoteText@ @footnote 1@F. Bassani et al., J. Appl. Phys. 79 (1996) 4066. @footnote 2@B. R. Schroeder et al.. Appl. Phys. Lett. 77 (2000) 1289.

4:20pm **SC+SS-MoA8 Structural Relaxation at SiO@sub 2@/Si(100) Interfaces Studied by Coaxial Impact Collision Ion Scattering Spectroscopy*, H. Ikeda,* *S. Goto, K. Honda, M. Sakashita, A. Sakai, S. Zaima, Y. Yasuda,* Nagoya University, Japan

With downsizing the ULSI devices, atomic bonding structures at the SiO@sub 2@/Si interface have become a serious factor to determine the device performance. Nevertheless, there are few studies about the interfacial structure. By using coaxial impact collision ion scattering spectroscopy (CAICISS), we have studied the structural changes extending over the first several layers from oxidized Si(100)-2x1 surfaces and claimed that the inward oxidation occurs before the lateral oxidation finishes.@footnote 1@ In the present study, we clarify Si atomic structures at the SiO@sub 2@/Si interface, which depend on the thickness of the oxide films and the oxidation temperature. An ion scattering simulation which is based on the consecutive calculation of the He@super +@ ion trajectories was used for the analysis of CAICISS spectra. Below an oxide thickness of 2.3 ML, the structural relaxation of a Si lattice at the SiO@sub 2@/Si interface occurs similarly in the range of room temperature to 700°C. The CAICISS spectra show only horizontal displacement of the second-layer Si atoms in these samples. In the following oxidation stage, the oxidation process depends on the temperature. At room temperature, the oxide thickness saturates at 2.3 ML, which is probably due to the restriction of oxygen adsorption on the distorted Si-Si bond sites. The CAICISS spectra of oxidation at above 300°C indicate interface structures that consist of Si atoms existing at normal lattice sites. Furthermore, vertical displacement of the second-layer Si atoms can be detected as well as horizontal one. From these results, it can be concluded that the vertical displacement of the second-layer Si atoms is a trigger of the formation of an amorphous structure and, moreover, a very abrupt SiO@sub 2@/Si interface is realized. @FootnoteText@ @footnote 1@ M. Wasekura, M. Higashi, H. Ikeda, A. Sakai, S. Zaima, Y. Yasuda, Appl. Surf. Sci., 159-160 (2000) 35.

4:40pm **SC+SS-MoA9 Two Dimensional Scattering-images of Lateral Structured GaAs/AlAs Systems as an Example for Diffuse X-ray Scattering at Interfaces*, J. Stuempel,* *I. Busch,* Physikalisch-Technische Bundesanstalt, Germany

Two-dimensional X-ray scattering pattern in reciprocal space (space map) is measured by the reflection of X-rays at grazing incidence. These images are composed of specular and diffuse scattered components. The essential information about the statistical parameters of the interfaces (roughness, correlation length, lateral symmetries, etc.) is contained in the diffuse part of the scattered radiation. As an example of highly structured interfaces we use an GaAs/AlAs multilayer system. The interfaces of a multilayer grown on a substrate with a small miscut (angle about 2 °) between the surface and the (100)-plane reconstructs to a lateral correlated system with step hights of some nanometers. The measured space maps of these systems will be presented in detail. Due to a quantitative data interpretation the results will be compared with numerical simulated data. The simulation is based on a modified scattering theory. The underlaying theory will be presented within the talk.

## Semiconductors
## Room 124 - Session SC-MoA

### GaN Surfaces, Interfaces, and Devices

**Moderator:** A. Rockett, University of Illinois

2:00pm **SC-MoA1 The Influence of Active Nitrogen Species and Substrate Polarity on the Growth and Doping of GaN Grown by RF Plasma-assisted Molecular Beam Epitaxy*, T.H. Myers,* *A.J. Ptak,* West Virginia University*;* *L.T. Romano,* Xerox Palo Alto Research Center **INVITED**

Growth of GaN by molecular beam epitaxy (MBE) is typically limited by increased desorption of Ga from the growing surface. We will report on the relative reactivity of the various active nitrogen species produced by rf plasma sources: low and high energy ions, atoms and metastables. Studies of growth rate as a function of temperature suggest the GaN surface is prone to "attack" by neutral and ionic atomic nitrogen above 700oC, promoting decomposition. This leads directly to the observed lower than expected temperature for a significant decrease in growth rate, while this decrease is not observed when the active nitrogen flux consists primarily of nitrogen metastables. Dramatically improved electrical properties are observed in epilayers grown using nitrogen metastables. Similar to most compound semiconductors, GaN lacks inversion symmetry that leads to different chemical terminations on different crystal planes. The two most common surfaces, the (0001) (or Ga-polar) and the (000-1) (or N-polar) surfaces exhibit quite different properties. Results illustrating the differences in basic growth kinetics related to surface polarity will be presented. Surface polarity also has a pronounced influence on doping. A pronounced dependence of Mg incorporation on surface polarity was observed in a series of Mg step-doped epitaxial GaN layers. Measurements indicate surface accumulation of Mg occurs during growth, with stable accumulations of close to a monolayer of Mg on the Ga-polarity surface. This surface layer can cause surface inversion to occur. Beryllium incorporation was also studied for both Ga-polarity and N-polarity GaN. Unlike magnesium, surface polarity-related incorporation differences were less pronounced for Be. Preliminary results, however, indicate a strong dependence of compensation, e.g. point defect formation, on surface polarity. Polarity related issues for O-incorporation will also be discussed.

2:40pm **SC-MoA3 "Functionalizing" the GaN(0001) Surface: The Chemisorption of Organic Amines*, V.M. Bermudez,*** Naval Research Laboratory

The emergence of "molecular electronics" has led to interest in the synthesis of hybrid organic/semiconductor structures. Surfaces "functionalized" by attachment of unsaturated hydrocarbons provide the possibility of subsequently building complex electro- or photoactive molecular films using, e.g., photochemical or cycloaddition reactions. Previous work@footnote 1@ with NH@sub 3@ shows that amines are highly reactive with the Ga-polar GaN(0001) surface. Here we use mainly XPS, UPS and ELS to study chemisorption of amines involving @pi@-bonded hydrocarbons, focusing on a primary amine (aniline, C@sub 6@H@sub 5@-NH@sub 2@) and a secondary amine (3-pyrroline, C@sub 4@H@sub 6@NH) having N in a 5-member ring with one C=C bond. Dosing near 300 K with either amine causes rapid elimination of the GaN 3.4 eV surface-state loss in ELS and growth of a C=C @pi@-@pi@@super *@ loss at 6.5 eV (aniline) or 7.2 eV (3-pyrroline). The background-corrected xray-excited C KLL and N KLL band areas indicate a saturation coverage of about 0.40 molecules per surface Ga site for either species. In contrast, benzene (C@sub 6@H@sub 6@) does not adsorb under these conditions. HeII UPS shows rich orbital structure, differing from that of either free molecule, which has been analyzed with the aid of ab-initio DFT calculations. The results suggest adsorption via the amine N-atom with the hydrocarbon ring remaining intact. UPS has also been used to measure changes in band bending and in electron affinity (@delta@@chi@) with adsorption. This permits construction of energy-level diagrams showing the alignment of the molecular HOMO and LUMO with the GaN band edges. For aniline (3-pyrroline), the surface dipole layer leads to @delta@@chi@ of about -0.55 (-0.92) eV, vs. the clean-surface @chi@ of 3.3 eV. This large reduction in @chi@ may be useful in electron emission devices. @FootnoteText@ @footnote 1@ V.M. Bermudez, Chem. Phys. Lett. 317 (2000) 290.

3:20pm **SC-MoA5 STM Study of Dislocation-Mediated Surface Morphology of GaN Grown by ECR-Plasma Assisted MBE*, Y. Cui,*** *L. Li,* University of Wisconsin

The surface morphology of GaN films grown on the 6H-SiC substrates by ECR-plasma assisted molecular beam epitaxy was studied by reflection high-energy electron diffraction (RHEED) and in situ scanning tunneling microscopy (STM). Clean SiC substrates were prepared by a two-step method of etching in hydrogen atmosphere at 1600 °C and annealing under Si beam in ultrahigh vacuum at 950 °C. These processes remove the polishing damages of the SiC substrates. The resulting surfaces are composed of atomically flat terraces that are separated by triple-layer steps. At temperature between 550 and 600 °C and plasma power of 30 W, two-dimensional growth was observed. The surface morphology of the films can be characterized by two dislocation-mediated structures: pinned steps and spiral hillocks. Straight-pinned steps along the {1120} directions were found for film thickness of 500 Å, created due to the emergence of screw and mixed dislocations at the crystal surface from the bulk of the film. By counting the number of the steps, the dislocation density is estimated to be in the order of 10@super10@ cm@super-2@. At film thickness greater than 1000 Å, these pinned steps grow outward and around the dislocation, forming spiral hillocks with a density in the order of 10@super8@ cm@super-2@. The reduction of the density is explained by annihilation of the dislocations during the formation of the spirals. These results and their implications for GaN epitaxy will be presented at the meeting. This research is supported by NSF DMR-0094105.

4:00pm **SC-MoA7 Search for the Missing Group-III Flux during AlGaN OMVPE***, **J.R. Creighton**, M.E. Coltrin, R.P. Pawlowski,* Sandia National Laboratories

At normal operating conditions, most AlGaN OMVPE reactors exhibit non-ideal behavior with respect to the group-III precursor concentration. The deposition rate can be considerably less than the predicted transport-limited rate, and the solid AlGaN alloy composition is typically a nonlinear function of the gas-phase composition. It is generally thought that gas-phase "parasitic" reactions between trimethylgallium (TMGa), trimethylaluminum (TMAl), and ammonia are responsible for removing group-III material from the deposition process. We have explored many possible mechanisms for the parasitic pathways using both experimental techniques and complex reactive flow simulations. As expected, TMGa and TMAl react with ammonia to form adducts, which we have unambiguously identified with mass spectroscopy and FTIR. We have measured the vapor pressure of the adducts and their mixtures near room temperature and found that physical condensation can be an important process, especially at higher reactor pressures and higher TMAl concentrations. However, over the 0-100°C range we have found no evidence of significant irreversible decomposition reactions, such as methane elimination, which have often been postulated to be the source of the decrease in group-III flux. As the temperature is raised in this range, the adducts simply dissociate back into the original reactants at rates consistent with equilibrium calculations. The lack of evidence for a low temperature parasitic reaction pathway is consistent with our reactive flow simulations, which indicate that the parasitic reaction pathway occurs at high temperatures near the growing surface. The simulations utilized deposition rate measurements from a rotating disk reactor over a wide range of operating conditions chosen to accentuate the differences between possible high-temperature and low-temperature pathways. Recent results examining possible high-temperature pathways will be presented.

4:20pm **SC-MoA8 Models, Concepts and Realizations of Pyroelectronic Heterostructure Devices***, **P. Vogl**, G. Zandler, S. Hackenbuchner, J.A. Majewski, O. Ambacher,* Technische Universitaet Muenchen, Germany*; K. Chu, V. Tilak, R. Dimitrov, L.F. Eastman,* Cornell University **INVITED**

High field transport in semiconductors that possess high internal spontaneous electric fields opens up a new field of "pyroelectronics". The pyroelectric character of group-III-nitrides with wurtzite crystal structure yields a novel degree of freedom in designing and tayloring devices for modern microelectronic applications. We present both theoretical and experimental studies of III-nitride based high electron mobility field effects transistors (HEMT´s) that demonstrate these devices to be optimally suited for high power and high frequency transistors as well as microwave amplifiers. On the theory side, we have employed first principles calculations to determine spontaneous and piezoelectric polarization charges at interfaces and surfaces of GaN based heterostructures and superlattices. Based on this calculated set of electronic structure data, we have performed extensive high field transport simulations for submicron HEMT devices. In addition, we show how the built-in electric fields can be utilized to produce high hole densities as a function of gate voltage in these devices. Experimentally, undoped and pyroelectric AlGaN/GaN HEMT´s have been processed on c-Al@sub 2@O@sub 3@, Si(111) and 6H-SiC substrates that show excellent device characteristics. With gate length down to 150 nm, we have reached an electron transit velocity and intrinsic transit time frequency of 1.3x10@super 7@ cm/s and 106 GHz, respectively, at room temperature. Experimental results for the first microwave amplifier build by a combination of 4x4 AlGaN/GaN HEMTs will be presented.

5:00pm **SC-MoA10 Ni/Au Ohmic Contacts to p-GaN Epilayers***, B. Liu, E. Lambers, **P.H. Holloway**,* University of Florida*; T. Johnson, D. Guiterrez, K. Kidney, W.B. Alexander,* Uniroyal Optoelectronics

The deposition and properties of evaporated thin Ni (5 nm)/Au (5 nm) contacts on MOCVD p-GaN has been studied. After annealing the bi-layer structure in an oxidizing environment, the contact is transformed from a Schottky to an ohmic behavior. The Ni underlying the Au top layer was found to have largely diffused to the surface and formed NiO during the anneal. The Au formed a porous film between the NiO and p-GaN which allowed between 50 and 85% transmission of 450 nm light, depending upon the deposition and annealing conditions. The porous Au network also allowed good sheet resistance with typical values of 300 @ohm@. X-ray photoelectron spectroscopy indicated that the NiO reached to the GaN interface, however a Ni-Ga-Au ternary metallic phase also formed at the interface. This phase modified the capillary forces and resulted in formation of the porous Au network. In the absence of this metallic phase, the Au film broke into islands with a very high sheet resistance. Formation of the porous network will be discussed in terms of a total energy model of thin film morphology. The consequences of forming NiO and forming the ternary metallic layer upon achieving an ohmic contact will also be discussed.

## Semiconductors
## Room 124 - Session SC-TuM
## Semiconductor Interfaces and Thin Films

**Moderator:** L.J. Brillson, The Ohio State University

8:20am **SC-TuM1 Nanometer-scale Studies of Possible Dislocation Charging at GaN Interfaces***, **J.P. Pelz**, H.-J. Im, Y. Ding, E.R. Heller,* The Ohio State University*; B. Heying, J.S. Speck,* University of California, Santa Barbara*; W.J. Choyke,* University of Pittsburgh **INVITED**

Threading dislocations (TDs) in III-Nitride films are thought to be electrically active and of major concern for device applications. Several recent studies of GaN and AlGaN/GaN films suggested that TDs might develop significant fixed negative charge (up to 1 e- every c-axis lattice spacing) at or near the TD core. We have quantified possible dislocation charging near metal/GaN interfaces using ultra high vacuum Ballistic Electron Emission Microscopy (BEEM) measurements of identifiable TDs, which were compared with electrostatic modeling of conduction band (CB) bending due to fixed local negative charge. Surprisingly, measurements of TDs in GaN films (grown by molecular beam epitaxy (MBE) under Ga droplet conditions) do not indicate any negative charge at TDs close to the metal-GaN interface, with an estimated upper limit of ~0.25 (e-)/c along the TDs. In contrast, we generally observe a mild decrease in the local CB at TDs as well as at step edges, which may be due to piezoelectric surface charge induced by local stress variations. We will discuss on-going measurements of near-interface dislocation charging of III-Nitride films grown under different conditions (MBE Ga-poor, MOCVD, etc.) to investigate how growth conditions affect local dislocation charging and local transport behavior. Time permitting, we will also discuss on-going measurements of how the Schottky Barrier height on metal/SiC contacts depends on SiC polytype, interface orientation, and deposited metal. This work was supported by the Office of Naval Research.

9:00am **SC-TuM3 Nanometer-scale Studies of Phase Separation in Compound Semiconductor Alloys***, **B. Shin**, A. Lin, K. Lappo, R.S. Goldman,* University of Michigan*; M.C. Hanna, S. Francoeur, A.G. Norman, A. Mascarenhas,* National Renewable Energy Laboratory

Thin films of compound semiconductor alloys can be grown with a wide range of band gap energies and lattice constants, useful for the development of novel electronic and optoelectronic devices. In most of these systems, growth conditions have been reported for which phase separation occurs. Yet, the thermodynamic versus kinetic origin of phase separation, as well as the experimental conditions for determining the presence of phase separation has been the subject of debate for nearly 20 years.@footnote 1,2@ In thin films of compound semiconductor alloys, both the difference in binary bond lengths and the film/substrate misfit are expected to play a significant role in the initiation of alloy phase separation. In this work, we have examined phase separation in the misfit-free InAlAs/InP system using ultra-high vacuum cross-sectional scanning tunneling microscopy (XSTM) and x-ray reciprocal space mapping. For p-doped thin InAlAs layers, XSTM reveals the presence of isotropic non-uniformities which consist of nanometer-sized clusters. For thicker, undoped InAlAs layers, longer wavelength quasi-periodic modulations perpendicular to the growth direction are apparent. These lateral modulations are observed in both topographic and conductance XSTM images, suggesting that they are due to a combination of compositional and strain variations. A signature of these modulations is also apparent in x-ray reciprocal space maps. Interestingly, the modulation wavelengths increase with film thickness and are notably lower than those reported for similar films grown at higher temperatures.@footnote 3@ Together, these results suggest that phase separation is a thermally activated kinetic process which may be significantly affected by the presence of impurities such as dopants. @FootnoteText@@footnote 1@G. B. Stringfellow, J. Cryst. Growth 65, 454 (1983). @footnote 2@A. Zunger and S. Mahajan, in Handbook on Semiconductors (North-Holland, Amsterdam, 1994), Vol. 3, p. 1399. @footnote 3@H. K. Cho et al, Mat. Sci. Eng. B 64, 174 (1999).

9:20am **SC-TuM4 Scanning Tunneling Spectroscopy on Adsorbate Induced Two Dimensional Electron Systems on InAs(110)***, **J. Klijn**, M. Morgenstern, Chr. Meyer, D. Haude, R. Wiesendanger,* Hamburg University, Germany

Two dimensional electron systems (2DES) are usually prepared in heterostructures and thus buried below the surface. Scanning probe methods are consequently restricted to resolutions above 100 nm.@footnote 1@ To increase the spatial resolution, we have prepared an adsorbate induced 2DES close to the surface on n-type InAs(110).@footnote 2@ We measured the local density of states of this 2DES in zero and in finite magnetic field (T=6K, B<=6T). The data at zero field reflect the scattered wave functions at the residual dopants. The corresponding Fourier transformation identifies the k-vector of the undisturbed 2DES as the strongest contribution. However, mixing with other k-vectors due to the potential scattering leads to broadening of the k-space features. The magnetic field data show Landau quantization of the 2DES and exhibit distinct changes in the local density of states. @FootnoteText@ @footnote 1@ S.H. Tessmer et al., Nature 392(1998)51; N.B. Zhitenev et al., Nature 404(2000)473; P. Weitz et al., appl.Surf.Sci. 157(2000)349 @footnote 2@ M. Morgenstern et al., Phys. Rev.B 61(2000)13805.

9:40am **SC-TuM5 InAs Surface Passivation for Electronics and Biosensors***, **D.Y. Petrovykh**,* University of Maryland, College Park*; M.J. Yang, L.J. Whitman,* Naval Research Laboratory

Many semiconductor-based chemical and biological sensors operate by detecting changes in the device conductivity caused by adsorption of organic or inorganic molecules on the sensor surface. The conductivity is affected by the surface charge induced by adsorbates, so sensors based on very thin films or nanostructures should be inherently more sensitive. InAs is a natural material for these applications, because the charge accumulation layer, naturally formed on its surface, provides intrinsic conductivity down to nm-scales. To be used in chemical/biological sensors, InAs films and nanostructures must be properly passivated and functionalized. Ammonium sulfide treatment, commonly used in GaAs processing, is known to effectively remove the oxide and other surface contaminants. We show that it also offers sub-5 nm etching, and the resulting S-passivated surface resists oxidation during short-term exposure to ambient air, or immersion in water (with a range of pH) or organic solvents. We will discuss the possibility of using alkanethiol films for longer-term stability and surface functionalization, including the use of selective deposition by dip-pen nanolithography. For sensor applications, it is also important to control the surface Fermi level pinning. We use conductivity measurements and electron spectroscopy to examine band bending in InAs films and the effects on the conductivity of different capping layers, passivation treatments and other common device processing steps. @FootnoteText@ This work was carried out at the Naval Research Laboratory and supported by the Office of Naval Research, National Nanotechnology Initiative Program on the Nanoscience Basis for Miniaturized, Intelligent Sensors.

10:00am **SC-TuM6 Formation of Co Silicides on Si@sub 0.7@Ge@sub 0.3@ Layer in the Presence of Thin Interposing Au Layer and Capping Ti Layer***, **W.W. Wu**, T.F. Chiang, S.L. Cheng, H.H. Lin, L.J. Chen,* National Tsing Hua University, Taiwan, R.O.C.*; H.H. Cheng, Y.H. Peng,* National Taiwan University, Taiwan, R.O.C.

Strained SiGe alloys offer the possibility of bandgap engineering for silicon-base devices. Due to their high mobility, SiGe/Si heterostructures have been investigated for use as SiGe channels in MOSFET@super '@s as well as high speed and high transconductance MODFET@super '@s, elevated source-drain contacts and gate material in CMOS technologies. Silicide/Si@sub 1-x@Ge@sub x@/Si(001) heterostructures are promising structures for use in devices such as the heterojunction bipolar transistor and infrared detectors with high cutoff wavelength. Due to its low resistivity, low Schottky barrier, good thermal stability, and possibility of self-aligned formation at relatively low temperatures, CoSi@sub 2@ is an attractive contact material for submicron Si devices. However, in the Co/Si@sub 0.7@Ge@sub 0.3@ system, the CoSi@sub 2@ tended to agglomerate at relatively low temperatures. The formation of Co silicides on Si@sub 0.7@Ge@sub 0.3@ alloys with a thin interposing Au layer and capping Ti layer has been investigated. CoSi@sub 2@ was observed to be the only silicide phase in Si@sub 0.7@Ge@sub 0.3@ samples annealed at 650-950 °C with a thin interposing Au layer and capping Ti layer. The sequence of phase formation is the same as the reaction of Co with single-crystal Si. The presence of Au was found to decrease the formation temperature of CoSi@sub 2@ by about 300 °C compared to that of Co(30nm)/Si@sub 0.7@Ge@sub 0.3@ samples. In addition, a thin capping Ti layer improves the uniformity and thermal stability of CoSi@sub 2@ layer. For Ti(5nm)/Co(30nm)/Au(1nm)/Si@sub 0.7@Ge@sub 0.3@ system, the process window of CoSi@sub 2@ was extended to 650-950 °C. SIMS analysis indicated that a large amount of Au diffused from the Co/Si@sub 0.7@Ge@sub 0.3@ interface to disperse in CoSi@sub 2@ layer during annealing.

10:20am **SC-TuM7 Intrinsic Defects of Cl-doped ZnSe Epitaxial Layers Examined by Photothermal Spectroscopy**, ***K. Yoshino,*** Miyazaki University, Japan; *M. Yoneta, K. Ohimori, H. Saito, M. Ohishi,* Okayama University of Science, Japan

Photothermal (PT) measurements have recently been carried out as one of the new methods to study the physical properties of semiconductors. One of the great advantages of the PT measurements is that the nonradiative carrier recombination processes are measured directly. Therefore, the PT may complement a photoluminescence (PL) and PL excitation (PLE). Furthermore, the PT also is much easier than deep-level transient-capacitance spectroscopy (DLTS) since no electrodes are needed in the PT system. In our previous paper,@footnote 1@ the PT measurements were carried out for nondoped and N-doped ZnSe epitaxial layers grown by molecular beam epitaxy (MBE), and we obtained the nonradiative carrier recombination centers in those samples. In this paper, we carried out the PT and PL measurements on Cl-doped ZnSe epitaxial layers from 80 to 300 K. The net carrier concentration is from 5.8 ´ 10 @super 17@ to 2 ´ 10@super 18 cm@super 3@. Three distinct peaks correspond to bandgap energy of ZnSe and two kinds of Cl related centers are observed. The activation energies of the Cl defects are estimated to be about 25 and 250 meV. The energy of 25 meV is known to be an activation energy of Cl atom in the Se site and the energy of 250 meV is not unknown. The emission due to the deep defect is not observed in the PL spectrum. Therefore, it indicates the defect with an activation energy of 250 meV acts the nonradiative carrier recombination center. @FootnoteText@ @footnote 1@ K. Yoshino et al., J. Crystal Growth 214&215 (2000) 572.

10:40am **SC-TuM8 Metal-Induced States and Polytype Transformations at SiC Interfaces**, ***S.P. Tumakha,*** *L.J. Brillson, G.H. Jessen,* Ohio State University; *R.S. Okojie, D. Lukco,* NASA-Glenn Research Center

We have used low energy electron-excited nanoluminescence (LEEN) spectroscopy to probe electronic structure at chemically-treated and metallized 4H and 6H-SiC interfaces. SiC high temperature electronics requires metal contacts with controllable barriers and minimal deep level electronic states. LEEN spectra over incident electron beam energies E from 0.5 to 5 keV identify the presence of localized states and their spatial distribution on a nanometer scale. With increasing E, the electron cascade and resultant generation of free electron-hole pairs peak at increasing depth ranging from 10 nm at 0.5 keV to 200 nm at 5 keV. The resultant band-to-band and band-to-defect luminescence is detected selectively at the intimate metal-SiC interface, the near-interface region extending tens of nanometers into the SiC, or the bulk SiC up to 0.2 microns into the solid. Pt/Ti/SiC junctions were prepared by standard cleaning, oxidation, and etching methods. 6H-SiC exhibits optical emission that varies with depth from the intimate interface and with surface chemical preparation. The depth-dependent spectra exhibit 2.9 eV near band edge (NBE) features of 6H-SiC for bulk excitation vs. a disordered and/or defected region within a few nm of the metal contact. Spectra from the near interface region indicate the existence of a SiC polytype with a higher band gap of ca 3.4 eV - resembling 4H-SiC as well as a discrete deep level, i.e., emission energy = 1.9 eV, for a specific surface treatment. Metal-induced features on 4H-SiC are similar. In addition, oxidation before or after metallization produces 2.5 eV emission extending hundreds of nm into the 4H bulk, characteristic of polytype conversion to 3C-SiC and confirmed by TEM. A strong impurity doping dependence suggests that oxidation or metallization-induced strain drives this transformation. The structural as well as electronic changes at SiC interfaces have significant device and processing implications.

11:00am **SC-TuM9 Growth and Electrical Characterization of Ultra-Dense Phosphorous Delta-Doping Layers in Silicon**, ***T.-C. Shen,*** *J.-Y. Ji,* Utah State University; *M. Zudov, R.-R. Du,* University of Utah; *J.S. Kline, J.R. Tucker,* University of Illinois

If dopant atoms substitute a substantial fraction of a monolayer of the Si atoms within a crystal, the resulting 2D dopant sheet may provide unique electrical properties for novel nano-scale devices. We have demonstrated that depositing phosphine molecules onto Si(100) surfaces in ultrahigh vacuum, followed by 35-50ML of Si epitaxy at T<500K, can yield a conducting layer that does not freeze out even at 0.3K. At 1/4ML saturation coverage at room temperature, the positive phosphorous ions create very large electric fields in the growth direction, producing a tightly confined 2D electron system. Within the plane, however, wavefunctions for these bound electrons are expected to couple across relatively large distances of a few Bohr radii (~2.5nm for P-atom donors), opening up new possibilities for lateral tunnel junctions. Initial magnetotransport measurements reveal an electron density of ~ 2.6x10@super 14@cm@super -2@ (~1/4ML) at 0.3K indicating complete electrical activation of the donor layer. From 60 to 0.3K the sheet resistance grows logarithmically with decreasing T, yielding a resistance of 1.16 k@ohm@/sq and a mobility of 21cm@super 2@/Vs at 0.3K. Studies of the correlation between electrical characteristics and phosphine deposition parameters will be presented. In addition, a new paradigm for devices based on selectively patterned 2D electron/hole systems will be discussed.

## Semiconductors
## Room 122 - Session SC+SS-TuA
### Semiconductor Nanostructures and Processing

**Moderator:** D.G. Cahill, University of Illinois, Urbana

2:00pm **SC+SS-TuA1 Nanoparticles for Fabrication of Zero- and One-dimensional Quantum Objects**, ***L. Samuelson***, *M. Bjork, K. Deppert, J. Ohlsson, M.H. Magnusson, A. Persson, C. Thelander, R. Wallenberg,* Lund University, Sweden

Quantum dots and quantum wires are of great interest for their possible use in quantum devices, such as single-electron transistors. In many cases these quantum objects are fabricated using different forms of self-organized epitaxial growth. We will report the use of aerosol techniques for fabrication of nanoparticles which are used as building blocks for quantum devices and which also allow us to controllably grow semiconducting, III-V, nanowhiskers. We will first describe our method for controlled fabrication of crystalline nanoparticles of metallic and semiconducting nanoparticles. Then we will turn to description of the way we grow nanowhiskers or nanoneedles using size-controlled nanoparticles as catalytic seeds which control the dimension and the location of the nanowhiskers. Transmission electron microscope characterization of chemical and structural properties of nanoparticles and nanowhiskers will be presented. Finally we will discuss electrical data from quantum devices obtained via nanomanipulation of nanoparticles and nanowhiskers, a technique that has allowed ohmic electrical contacts as well as tunnel-injecting contacts to be formed to these quantum objects.

2:20pm **SC+SS-TuA2 Growth of Ag Nanowires on Atomically Flat Ag films Formed on GaAs(110) Surfaces**, ***H.B. Yu***, *C.-S. Jiang, C.-K. Shih,* University of Texas at Austin

By using the scanning tunneling microscopy, we study the growth and evolution of Ag nanowires on atomically flat Ag films deposited onto GaAs(110) substrates. We show the ability to grow Ag nanowires with a well-defined width and very large aspect ratio (>150:1). For atomically flat Ag-film on GaAs(110), it has been shown that the surface has a quasi-periodic superstructure with long (L) and short (S) wavelength modulations arranged according to the Fibonacci sequence.@footnote 1,2@ We find that for the Ag nanowires grown on such a surface, the width of the nanowires is quantized in units of L (1.7 nm) or S (1.3 nm) segments. Very long (> 1 micron) nanowires of such a well-defined width can be formed on the surface with its ends terminated at the edge of the voids on the Ag film. The formation mechanism and the electronic properties of such nanowires will be discussed. @FootnoteText@@footnote 1@A.R. Smith, K.-J. Chao, Q. Niu, and C.K. Shih, Science 273, 226 (1996). @footnote 2@Ph. Ebert, K.-J. Chao, Q. Niu, and C.K. Shih, Phys. Rev. Lett. 83, 3222 (1999).

2:40pm **SC+SS-TuA3 Ge Nanoclusters Prepared from Solution with Chemically Tailored Surfaces**, ***B.R. Taylor***, Lawrence Livermore National Laboratory; *S.M. Kauzlarich,* University of California, Davis; *L.J. Terminello, A.W. van Buuren, C.F.O. Bostedt, T.M. Willey,* Lawrence Livermore National Laboratory

Ge nanoclusters have been prepared by a solution reaction between the Zintl salt Mg@sub 2@Ge and GeCl@sub 4@ in refluxing diglyme@footnote 1@ and triglyme.@footnote 2@ The nanoclusters are produced in a range of sizes from 2 to 10 nm in diameter, and are quantum confined. The particles were characterized by high-resolution transmission electron microscopy and Fourier transform infrared spectroscopy. The shift in band gap of the nano clusters was measured by optical spectroscopy and X-ray photoelectron spectroscopy . @FootnoteText@ @footnote 1@ Taylor, B. R.; Kauzlarich, S. M.; Lee, H. W. H.; Delgado, G. R. Chem. Mater., 1998, v. 10, 22-24. @footnote 2@ Taylor, B. R.; Kauzlarich, S. M.; Lee, H. W. H.; Delgado, G. R. Chem. Mater., 1999, v. 11, 2493-2500.

3:00pm **SC+SS-TuA4 X-Ray Absorption and Emission Studies of Diamond Nanoclusters**, ***T. van Buuren***, *J. Plitzko, C.F.O. Bostedt, N. Franco, L.J. Terminello,* Lawrence Livermore National Laboratory

The conduction and valence band structure of bulk diamond and diamond nanoclusters have been measured using x-ray absorption and x-ray emission spectroscopies. The diamond nanoclusters are commercially available products from the Straus chemical corporation and are synthesized in a detonation wave from high explosives. X-ray diffraction and TEM show that the nanodiamond powder is crystalline and approximately 3.5 +/- 1.0 nm in diameter. The nanodiamond K-edge absorption and emission show the same spectral features as bulk diamond with low impurity levels. The C1s core exciton feature clearly observed in the K-edge absorption edge of bulk diamond is not observed in the nanodiamond spectra. A possible explanation for this is a broadening due to a distribution of particle size. The depth of the second gap in the nanodiamond spectra is shallower than that of bulk diamond. This effect has been observed previously and attributed to quantum confinement. We note that no blue shift measured in the position of nanodiamond conduction edge when compared to the bulk diamond contrary to a recent publication that has reported large conduction band shifts in CVD grown diamond nanoclusters.@footnote 1@ Experiments are in progress to measure the nanodiamond conduction band edge from the EELS spectra acquired with a field emission TEM. We compare our conduction band data to the published measurements and comment on the differences. Soft x-ray emission measurements of the valence band structure of the diamond nanocluster will also be presented. The electronic structure of the nanodiamond will be compared to recent results on Si and Ge nanoclusters and the effects of reduced sizes on the electronic structure of group IV semiconductors will be discussed.@footnote 2@ The work is supported by the US-DOE, BES Ma-terial Sciences under contract W-7405-ENG-48, LLNL. @FootnoteText@ @footnote 1@ Y.K. Chang et.al. PRL 82, 5377 (1999). @footnote 2@ van Buuren et.al. PRL 80, 3803 (1998).

3:20pm **SC+SS-TuA5 AFM Tip-mediated Nucleation and Growth of Passivated Au Nanocrystal Islands**, *M.D.R. Taylor,* ***P. Moriarty***, University of Nottingham, UK; *M. Brust,* University of Liverpool, UK

Recent molecular dynamics simulations by Luedtke and Landmann@footnote 1@ have highlighted the rich dynamics associated with diffusion of Au clusters on surfaces. However, although there is a significant amount of work related to the diffusion of clusters formed in gas-aggregation (and related) sources, to date there have been no experimental studies of the dynamic properties of passivated Au nanoparticles@footnote 2@ deposited onto a surface from a colloidal suspension. We report non-contact mode and tapping mode (including phase imaging) atomic force microscopy (AFM) observations of the evolution of close-packed layers of 1.5 nm diameter thiol-passivated Au clusters on SiO2. The morphology of 1.5 nm cluster overlayers differs dramatically to that observed for dodecanethiol passivated clusters of 6 nm diameter.@footnote 3@ Furthermore, during each NC-AFM scan dramatic morphological changes occur - faceted holes develop, islands appear and grow, steps change appearance - which we attribute to strong tip-cluster interactions. Dynamic force-distance spectroscopy curves indicate that instabilities in the feedback loop are responsible for significant mass transport during (nominally) non-contact mode AFM scanning. @FootnoteText@ @footnote 1@ Luedtke WD and Landmann U 1999 Phys. Rev. Lett. 82 3835 @footnote 2@ Brust M, Walker M, Bethell D, Schiffrin DJ and Whyman R 1994 J. Chem. Soc., Chem. Comm. 801 @footnote 3@ Fractal Aggregation of Polydisperse Au Nanoclusters on Silicon, M. D. R. Taylor, P. Moriarty and M. Brust, submitted.

4:00pm **SC+SS-TuA7 Chemically Enhanced Electron Beam Induced Micromachining of SiO@sub 2@**, *J.H. Wang, A.R. Guichard, D.P. Griffis,* ***P.E. Russell***, North Carolina State University

While material removal using chemically enhanced focused ion beam micromachining is well known, utilization of electron beam induced chemistry for material removal is relatively unexploited. If practical techniques can be developed utilizing electron beam induced chemistry for material removal, issues involving the implantation or "staining" by the Ga ion beam generally used for micromachining can be avoided. In this study, the utilization of XeF@sub2@ for electron beam induced selective etching of SiO@sub 2@ is investigated. The influence of electron dose, electron beam energy and XeF@sub2@ pressure is presented. An etch rate of 10nm/sec over a square micron has been achieved at a chamber pressure of 8x10@super -6@ Torr. At low electron beam doses, material is deposited (rather that etched). This deposited material and micromachined features have been characterized by AFM, SEM and EDS. These results clearly demonstrate the ability to micromachine SiO@sub 2@ using XeF@sub2@ enhanced electron beam induced etching.

4:20pm **SC+SS-TuA8 Surface Passivation Effects of Deposited Ge-Nanocrystal Films Probed with Synchrotron Radiation*, C.F.O. Bostedt*[1]**, *T. van Buuren,* Lawrence Livermore National Laboratory*; T. Moller,* Hasylab at Desy, Germany*; L.J. Terminello,* Lawrence Livermore National Laboratory

Clusters and nanocrystals represent a new class of materials that exhibit promising novel properties. The production of these nanostructures in the gas phase gives control over not only the size of the nanoparticles, but also over surface passivation â€“ often not possible in other growth modes. The clusters are condensed out of supersaturated Germanium-vapor that is cooled down in a He-atmosphere and are subsequently deposited on a variety of substrates. Their surface is then subsequently passivated with different materials evaporated into the vacuum chamber. This approach allows us to probe in a controlled and dynamic fashion the effect of surface passivation on nanocluster properties. The clusters are spherical in shape and their sizes are determined by atomic force microscopy (AFM) and confirmed by transmission electron microscopy (TEM). X-ray absorption spectroscopy (XAS) was performed on thin films of Germanium (Ge) clusters. We find that the passivating agent strongly alters the electronic structure of the clusters. In general the absorption edge shifts to significantly higher energies compared to cluster films without surface passivation. This can be explained with a stronger confinement effect in the passivated films compared to unpassivated ones due to a reduction of the cluster-cluster interactions. @FootnoteText@ C. Bostedt acknowledges a fellowship from the German Academic Exchange Service DAAD in the HSP-III program, N. Franco from the Spanish Education and Culture Office. The work is supported by the US-DOE, BES Material Sciences under contract W-7405-ENG-48, LLNL.

4:40pm **SC+SS-TuA9 Surface Nanostructuring by Ion Sputtering: The Early Stages*, F. Buatier de Mongeot*,** *D. De Sanctis, C. Boragno, U. Valbusa,* Universita' di Genova, Italy

Ion sputtering is commonly used in surface science as a standard sample cleaning procedure. Recently, we have demonstrated that prolonged exposure to an ion beam can lead to the formation of regular patterns on surfaces, which have a spatial periodicity in the nanometer range.@footnote 1@ However, it is not trivial to understand how a random process, like the impingement of ions on the surface, can lead to a regular spatial organization.@footnote 2@ In order to investigate this aspect, we studied the early stages of the process by a Variable Temperature Scanning Tunneling Microscope VT-STM. The ion flux was reduced in order to follow the time evolution of the surface self-organization, starting from the single-impact events and until the formation of ripples on an Ag(110) surface occurred. We fixed the ion impact angle to 70 deg from the normal and low substrate temperatures, in order to enhance the erosive contribution.@footnote 1@ Under these experimental conditions, prolonged exposure to the ion beam leads to the formation of a regular ripple pattern parallel to the ion beam direction with a wavelength in the nm range. Surprisingly, in the early stages, after exposing the surface to an ion dose as low as 0.03 ML the surface morphology shows a well defined correlation along the crystallographic directions and only at higher fluences the correlation figure alignes with the ion beam. In this contribution we discuss the relevant parameters of this phenomenon. @FootnoteText@ @footnote 1@ S.Rusponi, G.Costantini, F.Buatier de Mongeot, C.Boragno and U.Valbusa, Appl.Phys.Lett. , 75 (1999) 3318 @footnote 2@ G. Costantini, F. Buatier de Mongeot, C. Boragno and U. Valbusa, Phys. Rev. Lett. 86 (2001) 838.

## Semiconductors
## Room 124 - Session SC-TuA
## Semiconductor Heterojunctions

**Moderator:** G. McGuire, MCNC

2:00pm **SC-TuA1 Characterization of SiGe/Si Heterostructures with Abrupt Interfaces*, Y. Shiraki,*** The University of Tokyo, Japan **INVITED**

2:40pm **SC-TuA3 Indium Segregation and its Effect on Interfacial Bonding at the GaSb-on-InAs Heterojunction: A Cross-Sectional Scanning Tunneling Microscopy Study@footnote 1@*, J. Steinshnider*,** *M. Weimer,* Texas A&M University*; E.M. Shaw, Z. Mi, T.C. Hasenberg,* University of Iowa*; R. Kaspi,* Air Force Research Laboratory

We describe how scanning tunneling microscopy (STM) may be used to determine the chemical composition across the nearly-lattice-matched, non-common-atom GaSb-on-InAs heterojunction with atomic-scale precision. An ideal, compositionally-abrupt GaSb-on-InAs interface is composed of either InSb-like or GaAs-like bonds whose character is easily distinguished with STM.@footnote 2@ Indium segregation, on the other hand, leads to compositional grading within the subsequent GaSb layers that compromises interfacial abruptness. We have quantified the indium fraction in successive gallium planes and find this compositional grading is described by the same microscopic model previously applied to antimony segregation at the InAs-on-GaSb interface.@footnote 3@ We discuss how indium segregation at the GaSb-on-InAs heterojunction is linked with the surface reconstruction of the underlying InAs template and consider the effect of this segregation on the interfacial bonding. @FootnoteText@ @footnote 1@Work supported by the National Science Foundation (Division of Materials Research) and Air Force Research Laboratory @footnote 2@J. Steinshnider, M. Weimer, R. Kaspi, and G.W. Turner, Phys. Rev. Lett., 85, 2953 (2000). @footnote 3@J. Steinshnider, J. Harper, M. Weimer, C.-H. Lin, S.S. Pei, and D.H. Chow, Phys. Rev. Lett., 85, 4562 (2000).

3:00pm **SC-TuA4 Dislocations and Microstructure Evolution in Semiconductor Thin Films*, A. Sakai,*** Nagoya University, Japan **INVITED**

The utilization of high-quality heteroepitaxial films is the key to realizing high performance optoelectronic and electronic semiconductor devices. In general, a lattice mismatch between a heteroepitaxial film and a substrate induces strain into the film and the strain relaxation is achieved by the introduction of misfit dislocations. This, in most cases, results in threading dislocations in the film, which severely degrade the properties required for the device operation. In order to reduce the threading dislocation density, we have performed novel heteroepitaxy which is based on the idea that misfit dislocations are confined at the hetero interface regions without leaving their threading arms in the film. Two successful demonstrations for GaN and SiGe thin films are presented. 1) Facet-initiated epitaxial lateral overgrowth (FIELO) allows us to obtain GaN films on sapphire substrates with threading dislocation densities on the order of 10@super 7@ cm@super -2@ which is two orders of magnitude smaller than that of the conventional epitaxy. Transmission electron microscopy analyses revealed that the reduction of the threading dislocation density was mainly due to dislocation bending in the FIELO GaN layer. Mechanisms of dislocation propagation which is closely related to the appearance of the facets early in ELO are discussed. 2) Strain-relaxed SiGe buffer layers on Si(001) substrates with low threading dislocation densities have been grown. The process consists of annealing of the first low-temperature-grown SiGe layer and growth of the second SiGe layer on the first layer. A thin capping Si layer formed before the annealing effectively suppressed surface roughening during the annealing. Periodic undulation was formed on the second layer surface, conformably to the alignment of interface misfit dislocations. This undulation plays an important role in introducing the dislocations uniformly and in suppressing the entanglement of threading arms of the dislocations.

3:40pm **SC-TuA6 The Strain Relaxation Mechanism of SiGe Growth with a Low Temperature Si Buffer Layer by Molecular-beam Epitaxy*, S.W. Lee*,** National Tsing Hua University, Taiwan, R.O.C.*; Y.H. Peng,* National Taiwan University, Taiwan, R.O.C.*; H.C. Chen,* National Tsing Hua University, Taiwan, R.O.C.*; H.H. Cheng, C.H. Kuan,* National Taiwan University, Taiwan, R.O.C.*; L.J. Chen,* National Tsing Hua University, Taiwan, R.O.C.

Recently, the use of the low temperature Si (LT-Si) buffer layer to achieve dislocation-free SiGe films was found to be effective to share the mismatch strain in epilayers. However, the mechanism of strain relaxation in a LT-Si buffer layer has not been well understood. In the present work, the growth of 300-nm-thick Si@sub0.7@Ge@sub0.3@ films with a LT-Si buffer layer grown at 550°C~350°C and with thickness of 50nm~250nm have been carried out by molecular-beam epitaxy. The SiGe films were characterized by transmission electron microscopy (TEM), double-axis x-ray diffraction (DAXRD), atomic force microscopy (AFM) and photoluminescence (PL). From DAXRD measurement, Si@sub0.7@Ge@sub0.3@ films with a 100-nm-thick LT-Si buffer layer grown at different temperatures were found to be fully relaxed (100%). However, Si@sub0.7@Ge@sub0.3@ films became partially relaxed with increased thickness of LT-Si buffer layers. From cross-section TEM (XTEM) observation, the microstructures of LT-Si buffer layers

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[1] **Morton S. Traum Award Finalist**

change with deposition temperature and thickness of LT-Si layers. XTEM images showed that the distribution of dislocations formed in the LT-Si buffer layer is correlated with the degree of relaxation. The strain relaxation mechanism is explained in terms of the compliant effect of LT-Si buffer. A novel method based on this mechanism using a thin Ge layer interposed below the LT-Si buffer layer for Si@sub0.7@Ge@sub0.3@ growth is demonstrated. The interposed Ge layer plays a critical role in leading the misfit dislocations to transverse along the LT-Si/Si interface. Controlling misfit dislocations in LT-Si buffers was achieved. The interposed Ge layer was expected to promote the relaxation of the top SiGe films.

4:00pm **SC-TuA7 Heteroepitaxy of Highly Mismatched Systems and the Role of Coincidence Lattice***, **K.H. Ploog**,* Paul Drude Institute for Solid State Electronics, Germany **INVITED**

While till mid 1980 a good lattice match of substrate and constituent layers in most semiconductor heterostructures was considered to be mandatory for successful device operation, this constraint has since become more relaxed. Today not only semiconductor materials with considerable lattice mismatch are explored in devices, but also heterostructures combining materials very dissimilar in structure, bonding, and chemical properties play an ever increasing role in the development of novel device concepts. In the heteroepitaxy of such highly mismatched systems, the existence of a "coincidence" lattice at the interface often leads to a unique epitaxial alignment and misfit accommodation in the early stages of epitaxy. This structural coincidence between the adjacent lattices helps to generate a low-energy interface. Using functional selforganized molecular beam epitaxy (MBE), even the epitaxy of metastable phases (like cubic GaN-on-GaAs), of M-plane oriented GaN[GaN(1-100) on g-LiAlO2(100)], and of layers with a symmetry different from the substrate (like hexagonal MnAs on cubic GaAs) can be obtained and the resulting nanostructures at the respective interface can be controlled in a reproducible manner. The M-plane group-III nitride heterostructures are of great importance for highly efficient blue/UV light emitters, and ferromagnetic MnAs on GaAs heterostructures are paving the way to spin-electronics operating at room temperature.

4:40pm **SC-TuA9 Nanoscale Dislocation Patterning in PbTe/PbSe (001) Lattice-mismatched Heteroepitaxy***, G. Springholz, **K. Wiesauer**,* University of Linz, Austria

Molecular beam epitaxy of PbTe on 5.2% lattice-mismatched PbSe (100) is studied using scanning tunneling microscopy. It is found that at a critical thickness of 0.8 monolayers, pure edge type misfit dislocations are formed at the layer/substrate interface. In the STM images these misfit dislocations appear as dark lines that run over the epitaxial surface along the four-fold directions. From atomically resolved lattice images, the dislocation Burgers vector is found to be ½ parallel to the interface. This unusual misfit dislocation configuration is explained by the fact that the dislocation are formed by climb rather than glide processes. From detailed investigations of the early relaxation stages, we find that all misfit dislocations are all injected from monolayer step edges on the surface, which greatly reduces the nucleation barrier of dislocation half loops. As the layer thickness increases, the dislocation density drastically increases and a nearly perfect quadratic grid of dislocations with an average spacing of 10 nm is formed, indicating that at 10 ML more than 90% of the misfit strain is relaxed. In addition, the course of strain relaxation is found to be in well agreement with the Frank-van-der-Merwe model. This surprising result is explained by the reduction of the dislocation nucleation barrier by the edge injection mechanism. The remarkable uniformity of the dislocation array is evidenced by the appearance of satellite peaks in the FFT power spectra of the STM images due to the dislocation superstructure. From a statistical analysis we find a variation of the lateral dislocation spacing of only 12%, which is better than the typical size uniformity of self-assembled quantum dots. Thus, these structures could serve as templates for the deposition of self-organized ordered nanostructures.

5:00pm **SC-TuA10 STM-Controlled Epitaxy of Cobalt-Semiconductor Compounds***, **I. Goldfarb**,* Tel Aviv University, Israel*; G.A.D. Briggs,* Oxford University, UK

Metal-semiconductor compounds play a key role in micro- and optoelectronic devices, mostly as contacts and interconnects. At present, the most popular are the silicides of Ti, and even more so of Co (due to its suitability for self aligned process). However both CoSi@sub 2@ and TiSi@sub 2@ are usually used in a form of polycrystalline thin films. While monocrystalline epitaxial growth of TiSi@sub 2@ on silicon is impeded by its large lattice mismatch between them, it could have been expected for the CoSi@sub 2@ in view of the latter's low mismatch with silicon. Obviously, monocrystalline contacts with improved electrical characteristics are highly desirable. Yet, CoSi@sub 2@ does not grow on silicon as a moncrystalline two-dimensional layer, at least not on the Si(001) surface, where CoSi@sub 2@ forms misoriented three-dimensional islands. CoGe@sub 2@ is another interesting metal-semiconductor compound that can be used, for example, as contacts to SiGe alloys and GaAs. CoGe@sub 2@ forms three-dimensional islands on Ge/Si(001), which are very similar to the CoSi@sub 2@ ones on Si(001). In this work we investigate the mechanisms of CoSi@sub 2@ and CoGe@sub 2@ growth by carefully-controlled e-beam evaporation of Co onto Si(001) substrates, as monitored in situ, from the very initial submonolayer stages, by scanning tunneling microscopy (STM) and reflection high-energy electron diffraction (RHEED). In order to affect the resultant epilayer morphologies, we use flat and vicinal surfaces, and two different ways of synthesis: reactive deposition (where Co is deposited onto hot substrate), and solid-phase reaction (where Co is deposited at lower, or room temperature). We attempt to account for the observed morphological differences of the epilayers by correlating them with the above-mentioned parametric differences.

5:20pm **SC-TuA11 Electron-beam Patterning of Cobalt Fluoride on 10-nm Length Scale***, **M. Malac**, Y. Zhu, M. Schofield,* Brookhaven National Laboratory

Electron-beam modification of a precursor material can be utilized to fabricate metallic structures on single-digit nanometer dimensions. Whereas, reliable fabrication of magnetic nanostructures is essential for study of fundamental processes in magnetism, cobalt fluoride (CoF2) precursor is a candidate for such fabrication of magnetic (cobalt) nanostructures. We have studied in situ electron beam patterning of CoF2 using a JEOL 3000F transmission electron microscope. The microscope is equipped with a Gatan Image Filter allowing for electron-energy-loss chemical analysis, and equipped for electron holography for mapping of magnetic fields. Our results on electron beam (<10 nm probe) modification of cobalt fluoride show that electron dose typically of 900 C/cm2 is needed for complete removal of fluorine at temperature 570 K. However, cobalt particles about 3 nm in diameter start to form at electron doses on the order of 200 C/cm2. Nucleation of cobalt particles initiates at the grain boundaries of the CoF2 precursor. The Co particles grow during exposure resulting, after complete exposure, in structures composed of separated, faceted cobalt particles typically 5 - 15 nm in size. The cobalt particles are either c-axis parallel or perpendicular to the substrate plane. Elevated sample temperature during exposure was necessary to eliminate buildup of microscope-related contamination. Cooling the sample to liquid nitrogen temperature during exposure also resulted in elimination of microscope contamination, but the resulting cobalt structures were composed of individual, separated particles. We believe that the non-continuous nature of the final cobalt structures stems from the surface energetics of high surface energy metal (cobalt) on low surface energy substrate (amorphous carbon). A real-time high-resolution TEM movie of the exposure process will be presented to provide insight to the exposure process.

## Surface Science
## Room 122 - Session SS+SC-WeM
## Adsorption on Semiconductor and Metal Oxide Surfaces

**Moderator:** R.J. Lad, University of Maine

8:20am **SS+SC-WeM1 Empirical Density Functionals and the Adsorption of Organic Molecules on Si(100)***, **M.A. Phillips**, N.A. Besley, P.M.W. Gill, P. Moriarty, P.H. Beton,* The University of Nottingham, UK

Density Functional Theory (DFT) has been used in the study of the adsorption of organic molecules such as ethene and ethyne for a number of years. Typically, for semiconductor surfaces, DFT methods are used in conjunction with a cluster model of the substrate.@footnote 1@ However, the computational expense of DFT calculations implies an upper limit on the size of the substrate model, and thus on the size of adsorbate molecule. As such, the study of larger adsorbates requires some reduction in computational expense, often leading to the use of parameterised semi-empirical methods. Unfortunately, such methods do not give good agreement with experiment for many semiconducting elements: another approach is required for these materials. The Empirical Density Functional, EDF1, has been shown to give very good agreement with values of atomisation energy, ionisation potential and proton affinity for the majority of species included in the G2 experimental data set.@footnote 2@ Furthermore, this functional does not require the evaluation of 'exact exchange' contributions, and is therefore significantly less computationally expensive than 'hybrid' functionals. However, the success of EDF1 in the determination of any other physio-chemical properties, in particular adsorption geometry, adsorption energy and vibrational structure, has never been tested. Here, we present the results from a density functional study of the adsorption of organic molecules on the Si(100) surface using EDF1, and discuss their validity through comparison to experimental measurements and results from equivalent calculations using the well known functional, B3LYP. We also compare the computational expense when using EDF1 in these calculations to that when B3LYP is used. @FootnoteText@ @footnote 1@ R. Konecný and D. J. Doren, Surf. Sci. 417 (1998), 169-188. @footnote 2@ R. D. Adamson, P. M. W. Gill and J. A. Pople, Chem. Phys. Lett. 284 (1998), 6-11.

8:40am **SS+SC-WeM2 Scanning Tunneling Microscope Investigation of Adsorption of Titanium Atoms on Si(111)-7x7 Surface***, **H.F. Hsu**, M.C. Lu,* National Tsing Hua University, Taiwan, R.O.C.*; H.-L. Hsiao,* Tunghai University, Taiwan, R.O.C., Taiwan*; L.J. Chen,* National Tsing Hua University, Taiwan, R.O.C.

C54-TiSi@sub 2@ has been the primary silicide for contact application in ULSI devices. The initial stages of interfacial reactions of Ti thin films on silicon are of both scientific and the technological interests. The strong reactivity of Ti with Si was manifested by the interatomic mixing at room temperature. The atomic scale studies of initial Ti-Si reactions at very low coverage have been scarce. In particular, it is not clear whether Ti atoms react with the Si substrate from the very beginning of deposition or the formation of a silicide-like compound starts at some critical coverage. In the present study, an atomic-scale characterization of room temperature titanium adsorption on the Si(111)-7x7 surface has been investigated. Preferential adsorption of Ti atoms on the Si center adatom sites at very low coverage was found. At higher coverage, a peculiar contrast feature is observed. The observed feature is attributed to the charge redistribution caused by the adsorption of more than one Ti atoms on this subunit cell. At very low Ti coverage (~0.007 ML), some of the Si adatom sites appear to be brighter in both filled-state and empty-state STM images. The contract behavior is likely to be due to the adsorption of Ti atoms on the Si adatom sites. It was found that Ti atoms adsorb preferentially on top of the Si center adatoms and, to a less extent, on top of the Si corner adatoms. Upon further deposition of Ti, two center adatoms and corresponding corner adatom become darker and the center of these three adatoms become brighter. The observed change in the apparent height is caused by the redistribution of charge near the Si adatom sites. The result indicates that more than one Ti atoms were adsorbed on a triangular subunit cell.

9:00am **SS+SC-WeM3 High-Resolution Core-Level Study of the Initial Stage of Oxygen Adsorption on a Si(111)-(7x7) Surface***, **K. Sakamoto**, H.M. Zhang, R.I.G. Uhrberg,* Linköping University, Sweden

As motivated by the technological importance of thin silicon oxide films in semiconductor devices, the initial stage of oxygen adsorption on silicon surfaces has been a topic of experimental and theoretical investigations. Among the various reports on oxygen adsorption, Si 2p core-level studies have played crucial roles in elucidating the structures of the SiO@sub 2@/Si interfaces. However, very few Si 2p studies are available for the initial stage of oxygen adsorption on a Si(111)-(7x7) surface. In this paper, we present a high-resolution Si 2p core-level photoemission study of submonolayer oxygen adsorption on the (7x7) surface. The photoemission measurements were performed at beamline 311 at the MAX-II synchrotron radiation facility in Lund, Sweden. The clean (7x7) surface was exposed to 0.1-20 L of oxygen at 120 K, which correspond to coverages below 1 ML. Significant intensity of the Si 2p component due to the Si@super 2+@ species is observed already at 0.3 L, and the component due to the Si@super 3+@ species is clearly observed at a dosage higher than 1.0 L. These results indicate that more than two oxygen atoms adsorb to one Si atom even at a very low coverage. After annealing the oxygen adsorbed sample at 600 K, the Si 2p component due to the Si@super 2+@ species shows a shift of 0.4 eV to the higher binding energy side. This result suggests different atomic configurations for the Si@super 2+@ species at 120 K and after annealing the sample at 600 K. We will also present detailed studies of the dosage- and temperature-dependent intensities of the Si 2p components due to the suboxide species.

9:20am **SS+SC-WeM4 First-Principles Theory of Finite-Temperature Adsorbate Ordering in Ba/Si(111)-"3x2"***, **S.C. Erwin**, C.S. Hellberg,* Naval Research Laboratory

Alkali metal adsorbates induce a 3x1 reconstruction of Si(111) widely believed to be a "honeycomb-chain channel" structure. This model is based on a true Si=Si double bond in the surface layer, which at 1/3 ML coverage leads to the elimination of all dangling bonds and thus keeps the fundamental gap free of surface states. Alkaline-earth adsorbates also appear to induce 3x1 (as well as higher-order) reconstructions, yet despite the extra electron the resulting surfaces remain fully gapped---an apparent contradiction to the one-electron band picture. Lee et al. recently suggested that for alkaline-earth adsorbates the coverage is in fact 1/6 ML, and showed that a 3x2 honeycomb-chain channel model is indeed fully gapped.@footnte 1@ We use density-functional methods first to confirm that the model of Lee et al. is indeed energetically preferred at low coverages. Second, we predict that structurally related 5x2 and 2x1 reconstructions will appear---if they are not preempted---at higher coverages. Finally, we propose an explanation for why the 1/6 ML phase appears 3x2 in STM but 3x1 in LEED: namely, that at moderate temperatures the adsorbates will exhibit only short-range order, due the near energetic degeneracy of H3 and T4 adsorption sites. To demonstrate this, we extract from our density-functional calculations the adsorbate-substrate and adsorbate-adsorbate interactions, and based on these carry out classical Monte Carlo simulations to explore the detailed temperature dependence of adsorbate ordering. @FootnoteText@@footnte 1@G. Lee, D. Shin, H. Kim, J. Koo, and S. Hong, Bull. Amer. Phys. Soc. 46 (2001).

10:00am **SS+SC-WeM6 Adsorption Induced Deflection and Frequency Changes in a Silicon Nitride Cantilever due to Ca@super 2+@ Ions***, **S. Cherian**, A. Mehta, T.G. Thundat,* Oak Ridge National Laboratory

Cantilever based micromechanical sensors exploit changes in surface stress due to interactions between the analyte species and cantilever surface. Charged groups on the cantilever surface play a significant role in binding induced deflection of the micro-cantilever. The deflection and frequency response of triangular silicon nitride cantilevers when exposed to calcium chloride solution was investigated in a flow system. The silicon nitride cantilever used was 200µm long and 20µm wide. Calcium chloride solutions of increasing concentrations were injected sequentially into the flow cell and the cantilever response measured. The fundamental resonance frequency of the cantilever shifted to lower values with increasing solution concentrations. The deflections due to interaction with the CaCl@sub 2@ were towards the gold side. The concentration versus deflection curve followed a Langmuir adsorption isotherm. The cantilever response is attributed to chemisorption of calcium ions onto the silicon nitride side. To verify this a calcium binding protein, calmodulin, was used. A cantilever that was exposed to CaCl@sub 2@ solution was subsequently exposed to calmodulin. Calmodulin binding to Ca @super 2+@ ions on the cantilever surface resulted in a deflection. This deflection was significantly different from that observed when calmodulin was exposed onto a fresh cantilever. These observations were further confirmed by fluorescent measurements using a fluorescently tagged calmodulin. These results demonstrate that consideration of ionic interactions of charged species in the medium with cantilever surfaces is critical in interpreting deflection data of cantilever based sensors. This also suggests the importance of passivating one of the surfaces in order to make the deflection of the functionalized cantilever specific to the species of interest.

10:20am **SS+SC-WeM7 Adsorption of NO and NO@sub 2@ on Barium Oxide: Surface Nitrition and Nitration***, P.J. Schmitz, R.J. Baird,* Ford Motor Company*; **M. Miletic**, J.L. Gland,* University of Michigan

Alkaline earth oxides surfaces are known to trap NOx species by chemisorption even under excess oxygen conditions typical of lean burn engines exhaust. These oxides, particularly barium oxide, have been proposed as active components in cyclic automotive NOx abatement strategies because of their ability to store and release NOx under rich/lean exhaust cycling. However, molecular understanding of the adsorption and reactions of NO, and NO2 on alkaline earth oxide surfaces remains incomplete. A series of XPS and temperature programmed studies of NO and NO2 adsorption and reaction on model barium oxide thin films prepared in-situ are reported here. These experiments indicate that charge transfer and reactive chemisorption play an important role even during low temperature adsorption on barium oxide surfaces. Nitrite and nitrate species form preferentially on reactive adsorption sites and can be reactively desorbed in the 400 to 600 K temperature range. The coverage of the precursor molecular species plays an unexpected role both in reactive adsorption and desorption on barium oxide surfaces. These results are discussed in terms of recent DFT calculations which highlight the importance of reactive configurations, charge transfer, and surface oxidation/reduction processes.

10:40am **SS+SC-WeM8 Electronegative Adsorbates on TiO@sub 2@: Reducing Effects of S and Cl***, **E.L.D. Hebenstreit**[1], W. Hebenstreit,* Tulane University*; H. Geisler,* Xavier University of Louisiana*; C.A. Ventrice, Jr.,* University of New Orleans*; D.A. Hite, P.T. Sprunger,* Louisiana State University*; U. Diebold,* Tulane University

TiO@sub 2@(110) is a well-studied model catalyst with an abundance of technical applications. Sulfur and chlorine are common impurities in many catalytic systems which poison catalytic reactions. The adsorption of molecular S and Cl on TiO@sub 2@(110)(1 x 1) has been studied with scanning tunneling microscopy (STM), x-ray and ultraviolet photoelectron spectroscopy (XPS, UPS), and low energy electron diffraction (LEED). At room temperature both adsorbates bind dissociatively to 5-fold coordinated Ti atoms and oxygen vacancies. At elevated temperatures (120°C - 440°C), S and Cl replace surface oxygen atoms. S forms different types of superstructures in dependence on coverage and adsorption temperature. No long-range ordering was found in the a dsorbed layer for Cl. Both adsorbates reduce the surface but S leads to a stronger oxygen depletion than Cl. In photoemission experiments, adsorption of either S or Cl at elevated temperatures cause additional emission at the high binding energy side of t he valence band and increases emission from the defect state. Adsorption of S leads to band gap states which fill the band gap completely. Evidence was found that the reduction state of TiO@sub 2@ crystals strongly affects the surface coverage of S and Cl at elevated temperatures. The rate of the site exchange of the adsobates between a weakly bound precursor state on Ti and the replacement of oxygen is kinetically limited by the arrival of diffusing bulk defects at the surface.

11:00am **SS+SC-WeM9 Electronic and Chemical Properties of Ce@sub 0.8@Zr@sub 0.2@O@sub 2@(111) Surfaces: Photoemission, XANES, Density Functional, and NO@sub 2@ Adsorption Studies***, **G. Liu**, J.A. Rodriguez, J. Hrbek, J. Dvorak,* Brookhaven National Laboratory*; C.H.F. Peden,* Pacific Northwest National Laboratory

Synchrotron-based photoemission,conventional XPS, XANES, and first-principles density functional (DF) calculations were used to study the electronic properties of a Ce@sub 0.8@Zr@sub 0.2@O@sub 2@ mixed-metal oxide. The results of DF calculations show that the band gap in bulk Ce@sub 0.8@Zr@sub 0.2@O@sub 2@ is ~ 0.6 eV smaller than in bulk CeO@sub 2@, with the Zr atoms in the mixed-metal oxide showing smaller positive charges than the cations in ZrO@sub 2@ or CeO@sub 2@. When present in a lattice of CeO@sub 2@, the Zr atoms are forced to adopt larger metal-O distances than in ZrO@sub 2@, leading to a reduction in the oxidation state of this element. Due to non-equivalent Zr-O distances, at least three different types of oxygen atoms are found in the Ce@sub 0.8@Zr@sub 0.2@O@sub 2@ system. O K-edge XANES spectra for a series of Ce@sub 1-x@Zr@sub x@O@sub 2@ (x=0, 0.1, 0.2, 0.3, 1) compounds show a distinctive line shape for the mixed-metal oxides that can not be attributed to a sum of CeO@sub 2@ and ZrO@sub 2@ features, supporting the idea that the O atoms in Ce@sub 1-x@Zr@sub x@O@sub 2@ are in a special chemical environment. XPS Ce 3d spectra show the presence of Ce@super 3+@ cations which may be related to the relative stability of oxygen vacancy defects upon incorporation of zirconia into ceria. The interaction of NO@sub 2@ gas with Ce@sub 0.8@Zr@sub 0.2@O@sub 2-x@(111), CeO@sub 2-x@(111), and Zr(Y)O@sub 2-x@(111) reduced surfaces was examined. Ne@super +@ ion sputtering was used to generate substantial concentrations of Ce@super 3+@, Zr@super 2+@ and Zr0 centers on the oxide surfaces. On CeO@sub 2-x@(111), NO@sub 3@, NO@sub 2@ and N were seen upon adsorption of NO@sub 2@. In contrast, only NO@sub 2@ and N were detected after adsorption of NO@sub 2@ on Ce@sub 0.8@Zr@sub 0.2@O@sub 2-x@(111) and Zr(Y)O@sub 2-x@(111). Adsorption of NO@sub 2@ induced an increase in the oxidation state of the metal cations (Ce@super 3+@ to Ce@super 4+@; Zr0 to Zr@super 2+@).

11:20am **SS+SC-WeM10 Probing Chemical and Topological Heterogeneity of Carbonaceous Surfaces via Temperature Programmed Desorption of Simple Molecules from Model Carbonaceous Surfaces***, **J. Kwon**, R. Vidic, E. Borguet,* University of Pittsburgh

Carbonaceous surfaces find applications in fields ranging from tribology to environmental remediation to catalysis. These surfaces are generally characterized by varying extent of chemical and topological heterogeneity that affects key elementary processe s such as adsorption and desorption. Temperature programmed desorption of model adsorbents (propane and acetone), representative of polar and non-polar organic compounds, was used to investigate the role of surface chemical and topological heterogeneity on the physical and chemical properties of model carbonaceous surfaces (air cleaved and plasma oxidized highly oriented pyrolytic graphite - HOPG). We observed that hydrogen and oxygen containing functional groups, which tend to block available adsorption sites, exist on air cleaved and plasma oxidized HOPG. Thermal treatment leads to removal of these groups and to over an order of magnitude increase in adsorption capacity. Thermal treatment (> 900 oC) of carbonaceous surfaces appears essential for maximum accessibility to adsorption sites. The surface defects induced by plasma oxidation yield greater surface area available for adsorption and higher energy sites. This novel approach promises a better understanding of chemically and topologically heterogeneous nanoporous carbons used in practical applications.

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[1] **Morton S. Traum Award Finalist**

## Semiconductors
## Room 111 - Session SC+SS+EL-WeA
## Chemistry of Semiconductor Etching & Cleaning

**Moderator:** G. McGuire, MCNC

2:00pm **SC+SS+EL-WeA1 The Chemistry of Anisotropic Silicon Etching: Tackling an Old Problem with New Tricks*, M.A. Hines,*** Cornell University **INVITED**

Aqueous bases, such as KOH, TMAH, and NH@sub 4@F, are the most important class of industrial silicon etchants. The popularity of these etchants is driven in large part by their extreme anisotropy (i.e. their high face-specificity). Relatively little is known about the chemical origins of etchant anisotropy, though. The problem is simple. On an atomic scale, an anisotropic etchant must be highly defect selective, but the study of surface defect reactivity is notoriously difficult. In this talk, I will discuss two new approaches to studying these reactions. On an atomic scale, I will show how defect reactivity can be quantified using a combination of scanning tunneling microscopy (STM) experiments and atomistic kinetic Monte Carlo simulations. This combination yields very detailed information about site-specific reactivity. To complement these rather time-consuming studies, I will also describe a new technique, which uses microfabricated test patterns, to rapidly assay the reactivity of 180 silicon surfaces simultaneously. We use this technique to perform orientation-resolved chemical kinetics experiments. I will show that the orientation-dependence provides additional insights into chemical reactivity. New phenomena, such as orientation-dependent morphological transitions, will also be described.

2:40pm **SC+SS+EL-WeA3 In situ Infrared Spectroscopy of Wet Chemical Etching of Si and InP with Electrochemical Control*, O. Pluchery,*** *S.B. Christman, Y.J. Chabal,* Agere Systems

The fabrication of Integrated-Circuits requires many different steps, including growth or etching. Since device performance strongly depends on surface preparation and control at each step, we have developed in situ Fourier transform infrared (FTIR) spectroscopy using multiple internal reflections to monitor the nature of interfaces. At the heart of high speed silicon technology is the growth of ultra thin oxide layer on top of the Si substrate. We monitor here the structure of such thermally grown oxides by sequential etching in dilute HF. The analysis of the LO and TO vibrational phonon modes of the oxide at 1070 and 1270 cm@super -1@ respectively shows that the etching mechanism exhibits two kinetic regimes depending on whether the HF flow wets the surface in a static or dynamic way. For static wetting, the LO absorption of the oxide undergoes a dramatic distortion that can be related to the unusual nature of the diffuse layer in the vicinity of the oxide surface. The etching mechanism depends in effect on the competition between diffusion and kinetics in this layer. In contrast to silicon, the passivating oxides of InP substrates are rather intricate. We examine here InP wafers that are covered by a thin oxide typical of "epi-ready" wafers offered by vendors. Analysis of the FTIR spectra shows a coexistence of several phases, such In@sub 2@O@sub 3@ (850 cm@super -1@) and InPO@sub 4@ at higher frequencies along with mixed oxide phases at intermediate frequencies. These oxides can also be removed by etching in HCl (10 wt%). This leaves a clean but very reactive InP surface that quickly attracts contaminants so that in situ analysis is highly desirable. In addition to the in-situ spectroscopy, we have devised an electrochemical control of the surface that makes it possible to further modify the composition of the adlayer as well as the diffuse layer.

3:00pm **SC+SS+EL-WeA4 Atomic Hydrogen Etching in Hot Wire Chemical Vapor Deposition System of Silicon Thin Films*, O. Srivannavit,*** University of Michigan

Atomic hydrogen generated by the filament in Hot Wire Chemical Vapor Deposition System plays an important role in depositing of thin films. It is believed that the etching process by atomic hydrogen taking place during the deposition process is one of key mechanism to obtain high quality thin films. In order to see a clear effect of interaction of atomic hydrogen with the growth surface, we focused only on the etching process in this system. We used amorphous and crystalline silicon as the substrate and then monitored its etching rate. The etching rate increases with increases of filament temperature due to increasing amount of atomic hydrogen generated on the filament. When substrate temperature increases, the etching rate decreases. We believe this is due to the decrease of the surface coverage of hydrogen with the increase of substrate temperature. The etching rate increases initially with pressure increase and then remains constant with further pressure increase. This phenomenon indicates that there is the competition between the increase in the amount of the atomic hydrogen generated and decrease in the diffusion coefficient of atomic hydrogen to the etching surface when pressure increases. The etching rate increases in the order of amorphous Si > poly-Si > crystalline silicon. This effect plays a key role in the selective deposition in this system.@footnote 1@ In addition, we found that there is preferential crystalline orientation etching (111) < (110) < (100) which can be used to explain the crystalline orientation during deposition of poly-Si films in this system.@footnote 2@ This preferential etching among amorphous phase and crystalline phase with the different orientation can be explained by the amount of dangling bonds in the silicon films. @FootnoteText@ @footnote 1@ S. Yu, E. Gulari and J. Kanicki, Appl.Phys. Lett., 68, 2681 (1996) @footnote 2@ S. Yu, S. Deshpande, E. Gulari and J. Kanicki, Mat. Res. Soc. Symp. Proc., 377, 69 (1995).

3:20pm **SC+SS+EL-WeA5 Single Ion Impact Effects on Semiconductor and Insulator Surfaces Induced by Slow, Very Highly Charged Ions*, T. Schenkel,*** Lawrence Berkeley National Laboratory*; A.V. Hamza, J.W. McDonald, D.H. Schneider, A. Kraemer, A. Persaud,* Lawrence Livermore National Laboratory

The interaction of slow (<5 keV/u), very highly charged ions, such as Xe@super 44+@ and Au@super 69+@, with solid surfaces is dominated by the deposition of potential energy, rather then the kinetic energy of the ions.@footnote 1,2@ For Au@super 69+@, the sum of the binding energies of the electrons that were removed when forming the ion is 170 keV. This energy is deposited into a nanometer scale area within about 10 fs when an Au@super 69+@ ion impinges on a surface.@footnote 3@ In our presentation we will report on the characterization of undoped silicon after exposure to low doses (~10E11 cm@super -2@) slow, highly charged ions. We recently observed strong photoluminescence at ~565 nm from irradiated silicon surfaces.@footnote 4@ Possible microscopic mechanisms for this effect will be discussed. We will compare atomic force microscopy data from surface defects induced by single ion impacts on mica, self-assembled monolayers and silicon in light of model descriptions of the materials response to the impact of slow, highly charged ions. Acknowledgements: This work is supported by the Director, Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098. Part of this work was performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Laboratory under contract No. W-7405-ENG-48. @FootnoteText@@footnote 1@T. Schenkel et al, Prog. Surf. Sci. 61, 23 (1999) @footnote 2@T. Schenkel, et al., Phys. Rev. Lett. 80, 4325 (1998) @footnote 3@M. Hattass, et al., Phys. Rev. Lett. 82, 4795 (1999) @footnote 4@M. W. Newman, et al., submitted for publication.

3:40pm **SC+SS+EL-WeA6 Ex Situ Removal of Carbon and Oxygen from a Gallium Nitride (0001) Surface*, F. Machuca,*** *Z. Liu, Y Sun, R.F.W. Pease, W.E. Spicer,* Stanford University*; P. Pianetta,* SSRL and Stanford University

We report on a chemical cleaning study of gallium nitride (GaN) using synchrotron radiation to probe the electronic structure of the semiconductor surface and the adsorbed impurities. We study sulfuric peroxide and sulfuric water chemistries for carbon and oxygen removal using the surface sensitive core level information using XPS. We report that a sulfuric peroxide wet treatment followed by a vacuum anneal at 700C reduces C and O concentrations to a few percent of a monolayer. Moreover, this is the first study achieving an atomically clean GaN surface well below the decomposition temperature by 200C. This is a direct result of a weaker form of carbon being chemisorbed to the GaN surface after the peroxide treatment and that is subsequently thermally desorbed. The chemical form is predominantly an oxide of carbon. Whereas the sulfuric water treatment leaves a residual refractive carbon on the surface of GaN in the form of hydrocarbons. These hydrocarbons persist up to the maximum annealing temperature of 740C tested. We also show that by treating the GaN surface with an aggressive oxidizing chemistry like sulfuric peroxide, there is only near monolayer coverages of oxygen. This is direct evidence for the existence of a suboxide on the GaN surface and demonstrates GaN (0001) is not an active surface for bulk oxidation. We also test the effectiveness of the annealing ambient during the thermal desorption portion of the cleaning by comparing vacuum to ammonia annealing. Our findings indicate ammonia is ineffective in aiding thermal desorption of C and O at temperatures at or below 740C, contrary to other reports. Lastly, we offer evidence for a novel oxynitride species on the GaN surface.

4:00pm **SC+SS+EL-WeA7 The Study of InP(100) Chemical Cleaning by Synchrotron Radiation Photoemission Spectroscopy***, **Y Sun**, F. Machuca, Z. Liu,* Stanford University*; P. Pianetta,* Stanford Synchrotron Radiation Lab*; W.E. Spicer,* Stanford University

The activation process for GaAs negative electron affinity (NEA) photoemitters has been studied extensively. However, the surface chemistry of other NEA materials such as InP is sufficiently different from that of GaAs that additional study is warranted on all aspects of the process starting from the initial surface cleaning to the final activation step. This work will concentrate on the preactivation clean in which the the surface species will be quantified using photoelectron spectroscopy. The goal of this work is to develop clean starting surface that will be used in subsequent activation studies. The cleaning process has three steps, the first two taking place in an argon purged glove bag attached to the load lock of the vacuum system to eliminate atmospheric contamination. Synchrotron radiation is used for the photoemission in order to obtain the necessary surface sensitivity and resolution for the In 4d, P 2p, C 1s and O 1s core levels as well as the valence band. In our most effective cleaning process, the InP is first etched in 4:1:100 H@sub 2@SO@sub 4@:H@sub 2@O@sub 2@:H@sub 2@O and results in a surface with 0.5-1 monolayers of In and P oxides and 0.5-1 ML of C contamination. Note that this is in contrast with GaAs in which this same etching step leaves elemental As and Ga suboxide and thus only requires a subsequent heat treatment to achieve a clean surface. For InP, a second oxide etching step is therefore required. This can either use a 9% HCl or a 1:1 H@sub 2@SO@sub 4@:H@sub 2@O solution both of which result in a hydrophobic surface with 0.3 ML of elemental P, 0.1 ML of C and complete removal of both the P and In oxides,. The lack of any significant amounts of S or Cl on the surface leads us to postulate that this surface is P terminated. Finally, a 360°C anneal in UHV gives a stoichiometric InP surface with no elemental P and only 0.05 ML C. These surfaces are now suitable for similar detailed studies of the full NEA activation process.

4:20pm **SC+SS+EL-WeA8 Ion Irradiation Induced Spontaneous Nanoscale Corrugation on Silicate Glasses***, **C.C. Umbach,*** Cornell University*; R.L. Headrick,* Cornell High Energy Synchrotron Source*; K.-C. Chang, J.M. Blakely,* Cornell University

Grazing incidence x-ray scattering was used to determine the temperature and ion-energy dependence of nanoscale corrugations that form on an amorphous SiO@sub 2@ surface eroded by Ar@super +@ ions. The corrugations have wavelengths between 20 and 200 nm with amplitudes of 1 nm. The corrugation wavelength @lambda@@super *@ shows a nearly linear dependence on ion energy for ion energies between 0.5 and 2 keV. Between room temperature and ~300° C, @lambda@@super *@ depends weakly on temperature and above ~300° it shows an Arrhenius-like increase. Ion-assisted viscous relaxation in a thin surface layer is shown to be the dominant smoothing process during erosion;the rate of viscous smoothing scales as (@lambda@@super *@)@super -4@. Similar ion-induced corrugations have also been observed on aluminoborosilicate glasses.

## Electronics
## Room 124 - Session EL-ThM
## Quantum Electronics

**Moderator:** C.R. Abernathy, University of Florida

8:20am **EL-ThM1 Fabrication of a Silicon-based Solid State Quantum Computer***, R.G. Clark,* ***M.Y. Simmons****, A.S. Dzurak, A.R. Hamilton, S. Prawer, D.N. Jamieson, G. Milburn,* University of New South Wales, Australia **INVITED**

The fabrication of a scalable silicon-based quantum computer, in which the qubits are nuclear spin states of single phosphorus atoms embedded in isotopically pure silicon registered to surface control gates@footnote 1@, is a significant technological challenge. The Australian program is approaching this in two ways. In our 'bottom up' program the embedded phosphorus array is fabricated using advanced STM lithography techniques followed by Si MBE overgrowth. In our 'top down' strategy, a detailed process has been developed in which single phosphorus atoms are implanted (with on-chip verification) self-aligned to the surface control gates and fast single electron transistor readout devices. The fabrication pathways each have their list of associated problems. An outline will be given of the practical issues that have to be overcome, together with a view on how this might be achieved including progress to date. In our bottom-up program we have recently reported@footnote 2@ that it is possible to fabricate an atomically-precise linear array of single phosphorus bearing molecules on a silicon surface with the required dimensions for the QC. Our recent work has focused on the next step of implementing strategies for incorporating the P atoms substitutionally into the silicon surface with enhanced bonding and without disturbing the P array prior to encapsulation by subsequent silicon overgrowth. Our strategy in the top down program is to concentrate on fabricating the simplest few-qubit test structures that will enable us to access the critical physics. However we have approached this from the viewpoint of developing a reliable, reproduceable process which, for linear phosphorus arrays, can then be readily scaled up to multi-qubit devices. An overview will be given of key details of the top down fabrication scheme and measurements on the first test structures. @FootnoteText@ @footnote 1@ B.E.Kane, Nature 393, 133 (1998) @footnote 2@ J.L. O 'Brien, S.R. Schofield, M.Y. Simmons, R.G. Clark, A.S. Dzurak et al, Phys. Rev. B Rapid Communications (in press): cond-mat/0104569 (2001)

9:00am **EL-ThM3 Ratchets, Heat Pumps and Maxwell's Demon: Quantum Transport in the Non-linear Regime***,* ***H. Linke,*** Univ. of Oregon, Eugene*; T.E. Humphrey,* Univ. of New South Wales, Australia*; P.E. Lindelof,* Niels-Bohr Inst., Denmark*; A. Lofgren,* Lund Univ., Sweden*; R. Newbury,* Univ. of New South Wales, Australia*; P. Omling, W.D. Sheng,* Lund Univ., Sweden*; A.O. Sushkov,* Univ. of New South Wales, Australia*; A. Svensson,* Lund Univ., Sweden*; R.P. Taylor,* Univ. of Oregon, Eugene*; H.Q. Xu,* Lund Univ., Sweden **INVITED**

Ratchets are non-equilibrium systems in which directed particle motion is generated using spatial or temporal asymmetry, in the absence of time-averaged macroscopic forces or gradients. After introducing general examples for ratchets and their application s, an overview will be given on a series of recent experiments on so-called quantum ratchets for electrons. These devices are based on GaAs/AlGaAs heterostructures containing a two-dimensional electron gas. The non-linear response of a spatially asymmetri c nanostructure (such as a triangular quantum dot) to an applied voltage is used to partially rectify a symmetric AC voltage. The required non-linear behaviour is generated using quantum effects, such as electron interference or tunneling through an asymm etric energy barrier. A particularly interesting observation is that the direction of the current generated in tunneling ratchets depends on energy, that is, the net flow of electrons at low energy is in a direction opposite to that of electrons at highe r energy. This observation implies that quantum ratchets perform an energy-sorting task similar to that assigned to Maxwell's demon - that is, they may act as heat pumps or even as heat engines. We will discuss the properties of such quantum heat pumps, focusing the discussion on the thermodynamic limits to their efficiency.

9:40am **EL-ThM5 Two Dimensional Electronic Properties of a Disordered Three Dimensional Conductor in the Extreme Quantum Limit***,* ***D. Haude,*** *M. Morgenstern, I. Meinel, R. Wiesendanger,* Hamburg University, Germany

Scanning tunneling spectroscopy images of n-InAs(110)are recorded in magnetic fields corresponding to the extreme quantum limit. From the results it is concluded that the appearence of the so called Hall dip in magnetotransport corresponds to an appearance of a contrast pattern in the local density of states. The energy and magnetic field dependence of the contrast pattern is very similar to drift states usually expected in two dimensional systems exhibiting the quantum Hall effect. The appearance of a pseudogap at the Fermi level evidences that localization is involved in the change of the local density of states. From the results a simplified but straightforward explanation of the Hall dip controversially discussed since 1956 can be given.

10:00am **EL-ThM6 First-principles Study of Conduction Channels of Atomic Wires***, N. Kobayashi,* National Institute of Advanced Industrial Science and Technology (AIST), Japan*; M. Aono,* Osaka University, Japan*;* ***M. Tsukada,*** University of Tokyo, Japan

Electron transport through nanoscale structures has been investigated from the viewpoint of nanoscale physics and technology. A number of studies have been performed for the transport of atomic wires and molecular bridges. One of the theoretical approaches to the transport is analysis of individual conduction channels. We report an analysis of the conduction channels of atom wires using the density functional theory with nonlocal pseudopotentials. Electronic states are calculated using the Green function technique, and are decomposed into individual channel components using the eigenchannel decomposition. We elucidate the channel transmission, the channel local density of states, and the channel current density, and clarify the characteristics of the channel for material kind. Furthermore, we show how the channels open or close for finite bias voltage, and discuss the I-V characteristics.

10:20am **EL-ThM7 Quantum Transport through One Dimensional Aluminum Wires***,* ***I.P. Batra,*** *P. Sen, S. Ciraci,* University of Illinois at Chicago

Quantum conductance and quantized Hall resistance in narrow channels have been well understood by using the two-dimensional electron gas (2DEG), a model system which has been realized in semiconductor heterojunctions. An essential property of the 2DEG is its ability to produce a constriction of width comparable to the Fermi wavelength, a property not shared by even thin metal films. But the advent of scanning tunneling microscopy (STM) has enabled scientists to fabricate wires of "atomic" dimensions. This has led to an explosion of interest in the quantum transport properties of nanostructures. Here we consider the specific case of a one dimensional (1D) wire consisting of Aluminum atoms. First we have to find the optimal structural arrangement of the 1D system. This was done using the first-principles density functional method combined with molecular dynamics. It is found that aluminum can form stable zigzag structures similar to those found for Au. In addition, we find, other novel structures, which have not been reported for any other material. We present our understanding of the bonding as derived from charge density analysis for aluminum wires. With the calculated atomic and electronic structure in hand we proceed to discuss the quantum ballistic transport through these nanowires. Our calculations are based on channel capacity arguments that can be motivated using the Heisenberg's uncertainty principle. Our results are compared with the numerical calculations by Lang, who has performed careful analysis of conductance as a function of Al nanowire length in atomic domain. We finally comment on the thermal conductance and Wiedemann-Franz law in the nano-domain.

10:40am **EL-ThM8 Probing a One Dimensional Conductor Confined Below a Charged Step Edge***,* ***Chr. Meyer****, M. Morgenstern, J. Klijn, R. Wiesendanger,* Hamburg University, Germany

Although one dimensional conductors exhibit unique properties, spatially resolved investigations are still rare. On InAs(110) we found a special type of charged step edge inducing a one dimensional electron system (1DES) below that step edge. We investigated this quantum wire with scanning tunneling spectroscopy (STS) over a length of 800 nm in various magnetic fields between 0 T and 6 T. The STS-curves on the step edge show two subbands of the 1DES with ground state energies of -66 meV for the first and -20 meV for the second subband giving an electron density of 1.2x10@super 8@/cm. Spatially resolved images of the local density of states (LDOS) reveal that the first and second subband have a width of 20 nm and 50 nm respectively. Along the step edge the LDOS of the 1DES shows an energy dependent fluctuation length in the range from 15 nm to 70 nm corresponding to the dispersion of InAs. We suggest that electron scattering on impurities in the quantum wire is responsible for the observed fluctuations in the LDOS. We compare our measurements with theoretical calculations of a random field disordered 1DES, that predict a broadening of the ideal 1D DOS.

## Semiconductors
## Room 111 - Session SC+SS+EL-ThM
### Interaction of Hydrogen and Organics with Silicon

**Moderator:** C.B. Musgrave, Stanford University

8:20am **SC+SS+EL-ThM1 Prepairing-dependent Desorption Kinetics of Hydrogen from Si(100)-2x1***, **H. Nakazawa**, M. Suemitsu,* Tohoku University, Japan

The reason why H@sub 2@ desorption from Si(100) surface shows a first-order desorption kinetics has been a controversial issue for more than a decade, and various desorption models have been proposed accordingly. Although most of the models assume prepairing of surface hydrogen atoms at a dimer as a precursor state, few attempts have ever been made to confirm its role in the desorption kinetics. We here show that the reaction order for the H@sub 2@ desorption from Si(100) can be varied by changing the hydrogenating gas and the thermal condition of the hydrogenation and that its behavior is systematically interpreted as a change of fractional coverage of paired hydrogen atoms. Three hydrogenating gases (atomic hydrogen (H), silane, and disilane) and three thermal conditions (room-temperature adsorption (RT), high-temperature adsorption (HT), and post-annealing (PA)) were tested. The desorption kinetics was analyzed by the peak position, the spectral shape, and their coverage dependence of the temperature-programmed desorption (TPD) spectra. As a result, the desorption kinetic order increased as H < disilane < silane and RT < HT < PA. To investigate the microscopic detail, we developed a set of rate equations for desorption with a fractional coverage of unpaired hydrogen atoms being chosen as a key parameter, which described the whole variation of the TPD spectra quantitatively. Using the obtained parameter, we argue the dependence on the hydrogenating gas in terms of different arrangements of surface H atoms. The dependence on the thermal condition is explained by a selective desorption from paired hydrogen atoms as well as the dissociation of paired hydrogen atoms during thermal treatments.

8:40am **SC+SS+EL-ThM2 In situ Measurements of the Stability of H terminated Si Surfaces and Kinetics of Oxide Regrowth in Ambient***, **V. Fomenko**, D. Bodlaki, E. Borguet,* University of Pittsburgh

The passivation of semiconductor surfaces is key to the operation of semiconductor devices. HF treatment removes native and deposited oxides from silicon. The resulting H-terminated surface is technologically and fundamentally important, and has been subject of a number of experimental and theoretical studies. H termination on Si surfaces has been considered to a stable in air at least for semiconductor wafer processing time scales. However, there is some disagreement as to the timescale of stability. In part this depends on the experimental probes. Using SHG, ellipsometry,contact angle, STM and AFM we have investigated the stability of the surface in ambient and under laser irradiation. in-situ second harmonic generation (SHG) experiments probe the oxide regrowth on hydrogen terminated Si(111) surfaces via SHG rotational anisotropy that is sensitive to hydrogen termination via changes the nonlinear optical response of the interface, both in the magnitude and shape of the SHG rotational anisotropy patterns. In addition, laser induced oxidation of H passivated Si(111) surfaces can be induced with intense ultrashort near IR laser pulses.

9:00am **SC+SS+EL-ThM3 Hydrogen and Si(001): Adsorption/Desorption Pathways and the "Barrier Puzzle"***, **F.M. Zimmermann**,* Rutgers University **INVITED**

Although dissociative adsorption of molecular hydrogen on Si(100) is thermodynamically favored by an adsorption energy of almost 2 eV, the sticking probability is immeasurably small (less than 10@super -11@) at room temperature, indicating the presence of a large energy barrier to adsorption. An adsorption barrier is expected to manifest itself in desorption as well by imparting hyperthermal amounts of kinetic energy to the desorbing molecules. Surprisingly, however, H@sub 2@ molecules associatively desorbing from Si(001) show no signs in their translational or rotational kinetic energy distributions of having traversed such a barrier, in apparent contradiction with microscopic reversibility. We have obtained experimental and theoretical results resolving this long-standing puzzle. Using surface second harmonic generation as a sensitive coverage probe, we observed that the dissociative sticking probability increases markedly with hydrogen coverage, and decreases with exposure pressure. Both dependencies are very unusual and impose severe constraints on the adsorption mechanism. By combining detailed measurements of the adsorption and desorption kinetics with statistical mechanical modeling and ab initio calculations, we arrived at a quantitative, mechanistic description of adsorption/desorption consistent with all observations and providing a natural explanation of the barrier puzzle. The model involves two distinct reaction pathways. At intermediate to high hydrogen coverages, thermal adsorption and desorption are dominated by an adsorption-barrier free, autocatalytic pathway, while a non-autocatalytic, bare-dimer pathway with a ~0.7 eV adsorption barrier dominates at very low coverages. Fitted model parameters are in quantitative agreement with density functional theory calculations.

9:40am **SC+SS+EL-ThM5 Noncontact AFM Study for Hydrogen Termination on Silicon Surfaces***, **Y. Sugawara**, S. Morita,* Osaka University, Japan **INVITED**

In order to most effectively apply the noncontact atomic force microscopy (AFM) using frequency modulation (FM) technique as a science tool in a variety of fields such as surface science, it is very important to understand fully the imaging mechanisms of the noncontact AFM on various samples. The imaging mechanism has been investigated on a chemically reactive surface such as semiconductor surface and an insensitive surface such as pure metal surface and layered material surface. However, there is no report of a comparative study between a reactive surface and an insensitive surface using same tip. For instance, Si(100)2x1:H monohydride surface is that a Si(100)2x1 reconstructed surface is terminated by a hydrogen atom, and do not newly reconstruct as metal deposited semiconductor surface, and the surface structure hardly change. Thus, Si(100)2x1:H monohydride surface is one of most useful surface for a model system to investigate the imaging mechanism, experimentally and theoretically. However, there is no report for noncontact AFM imaging on Si(100)2x1:H monohydride surface, and whether the interaction between a very small atom as hydrogen and a tip apex is observable with noncontact AFM do not have been clarified. In the present experiments, we compared the noncontact AFM images obtained for the Si(100)2x1 reconstructed surface with that for Si(100)2x1:H monohydride surface to investigate the role of chemical reactivity on the surface. It is found that the distance between bright spots is increased by the hydrogen termination. On Si(100)2x1 reconstructed surface, the noncontact AFM atomically resolved the dangling bonds localized outside the silicon dimer with a clear contrast. On the other hand, on Si(100)2x1:H monohydride surface, the noncontact AFM atomically resolved the individual hydrogen atoms on top most layer.

10:20am **SC+SS+EL-ThM7 Making Organic Molecules on Cu(100) and GaAs(100)***, **N.K. Singh**, N. Paris, P. Gatland,* The University of New South Wales, Australia

Alkyl coupling reactions, to form longer chain hydrocarbons, form the basis of many catalysed industrial processes. Surface studies carried out to date to understand the mechanisms by which carbon-carbon bonds form during the coupling process have been restricted to reactions of alkyl halides on coinage metal surfaces. Our recent investigations have shown that GaAs(100), a compound semiconductor, is also capable of catalysing alkyl coupling reactions, which had not been realised previously. Coupling products form irrespective of whether the alkyl groups are derived from alkanethiols or alkyl halides. However, on GaAs(100) the respective higher alkenes form, whereas it is known higher alkanes form on coinage metals. In this paper the surface reactions of a select group of alkanethiols (propanethiol, 1,1,1-trifluoroethanethiol) and alkyl halides (iodoethane, 2-iodo-1,1,1-trifluoroethane) on GaAs(100) and Cu(100), studied by thermal desorption and X-ray photoelectron spectroscopies, will be presented in order to establish the trend in the product mixtures on the two surfaces. We will show that both surfaces exhibit disproportionation and coupling reactions. Disproportionation reactions of the adsorbed alkyl fragments form the corresponding gaseous alkene, alkane and hydrogen. The coupling reactions however on the two surfaces differ. So for example, on Cu(100) CF@sub 3@CH@sub 2@I forms CF@sub 3@CH@sub 2@CH@sub 2@CF@sub 3@ as the coupling product while on GaAs(100) it forms CF@sub 2@=CHCH@sub 2@CF@sub 3@, the corresponding alkene. In the case of coupling reactions of CF@sub 3@CH@sub 2@SH, on Cu(100) CF@sub 3@CH@sub 2@CH@sub 2@CH@sub 3@ is formed while on GaAs(100) , CF@sub 2@=CHCH@sub 2@CH@sub 3@ is formed. These products are inconsistent with the products formed by CF@sub 3@CH@sub 2@I reactions. We will discuss the mechanisms by which these coupling reactions occur, and postulate reasons for the differences in the observed product mixtures on GaAs(100) and Cu(100).

10:40am **SC+SS+EL-ThM8 Adsorption and Thermal Decomposition of Iodoethane on Si(100)-2x1: Kinetically-Favored Adsorbate Ordering***, **A.V. Teplyakov**, K.M. Bulanin, A.G. Shah,* University of Delaware

The adsorption and chemical transformation of iodoethane were studied on a Si(100)-2x1 surface using multiple-internal reflection Fourier-transform infrared spectroscopy (MIR-FTIR). Although ethyl groups are stable on the Si(100)-2x1 surface at room temperature, thermal annealing studies suggest the formation of ethylene, a major hydrocarbon reaction product, accompanied by the loss of hydrogen, which is left on the surface until the temperature of recombinative desorption is reached. Adsorption of iodoethane on Si(100), followed by annealing to 570 K, leaves only hydrogen and iodine on the surface. MIR-FTIR spectroscopy shows that hydrogen is bound in several different types of site at temperatures between 295 K and 570 K. Annealing to higher temperatures produces a distribution dominated by a single hydrogen configuration. First-principles theory and polarization-dependent infrared spectra are consistent with the identification of this configuration as a dimer occupied by one hydrogen and one iodine atom. Calculations show that this configuration is not thermodynamically favored relative to other possible configurations. The observed ordering is attributed to kinetics, a consequence of slow pairing of iodine atoms.

11:00am **SC+SS+EL-ThM9 Are Silicon and Germanium Surfaces Chemically Similar? Reactions of Amines***, **C. Mui**[1], G.T. Wang, J.H. Han, C.B. Musgrave, S.F. Bent,* Stanford University

The organic chemistry at silicon and germanium surfaces has been studied in the past, and the chemical similarity between the two materials is often exploited. In this study, we will present an example in which the surface chemistry of silicon and germanium are notably different. We have used surface infrared spectroscopy and temperature programmed desorption to investigate the chemistry of amines at the Si(100)-2x1 and the Ge(100)-2x1 surfaces. We find that surface reaction of methylamine and dimethylamine on the Si(100)-2x1 surface results in facile N-H dissociation, whereas molecular adsorption occurs on the Ge(100)-2x1 surface. We also show that molecular adsorption of amines on both the Si(100)-2x1 and the Ge(100)-2x1 surfaces occurs through the formation of surface dative bonds which are stable at room temperature. Quantum chemistry calculations are used to explain the observed reactivity difference between the two surfaces. We find that N-H dissociation of dimethylamine is kinetically favored compared to N-CH3 cleavage on both surfaces. However, while N-H dissociation on the Si(100)-2x1 surface is unactivated, the overall activation energy for N-H cleavage on the Ge(100)-2x1 surface is above the vacuum level, explaining the lack of reactivity on the Ge(100)-2x1 surface. We will also discuss our theoretical approach for modeling reactions at semiconductor surfaces, including the effect of surface cluster models and basis sets.

11:20am **SC+SS+EL-ThM10 The Influence of Conjugation in Attachment of @pi@-Electron Containing Organic Molecules to the Si(001) Surface: Acrylonitrile vs. Allyl Cyanide***, **M.P. Schwartz**, S.K. Coulter, R.J. Hamers,* University of Wisconsin-Madison

Organic chemists have developed methods for controlling chemical reactions of complex molecules by defining a broad and detailed set of rules for reactivity. Controlling electron density within a molecule through the use of electron donating or withdrawing groups is a very important way in which to influence product distributions. While a wide variety of unsaturated organic molecules can be tethered to the Si(001) surface, little is known about the role of conjugation of @pi@-electrons in influencing product distribution. In this study, we have investigated the attachment of acrylonitrile (CH2=CH-CN) and allyl cyanide (CH2=CH-CH2-CN) to the Si(001) surface to determine how conjugation of an electron withdrawing group to a vinyl group influences the final surface products. X-ray photoelectron spectroscopy (XPS) and Fourier transform infrared spectroscopy (FTIR) measurements show that the attachment chemistry differs significantly for these two molecules. Allyl cyanide adsorbs primarily through the vinyl group while acrylonitrile attaches predominantly via the cyano group. Acetonitrile and benzonitrile were also studied to help determine the nature of the final surface products. The role of conjugation in determining product distributions for attachment of allyl cyanide and acrylonitrile to the Si(001) surface will be discussed.

11:40am **SC+SS+EL-ThM11 Scanning Tunneling Microscopy of a Conjugated {C}3-oligomer on Si(100)***, **B. Grandidier**,* ISEN, France*; C. Krzeminski, J.P. Nys, C. Delerue, D. Stievenard,* IEMN/ISEN, France*; C. Martineau, P. Blanchard, J. Roncali,* IMMO, France

Scanning tunneling microscopy (STM) has been used to study the adsorption of a {C}3 p-conjugated oligomer on the Si(100) surface. The symmetry of the molecule is resolved with the STM and different conformations are observed. As the oligomer is made up of vinyl groups and aromatic constituents, which are all known to react with the Si(100) surface through cycloaddition reactions, ab initio calculations are performed to determine the occupied molecular orbitals of the free and covalently bound oligomers. The results are compared with the occupied state STM images to characterize the adsorption state of the different conformations.

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[1] **Morton S. Traum Award Finalist**

## Electronics
## Room 124 - Session EL-ThA
### In-Situ Semiconductor Characterization

**Moderator:** D.E. Aspnes, North Carolina State University

2:00pm **EL-ThA1 In-situ Analysis, Monitoring and Control of III-V-Semiconductor Epitaxial Growth***, **W. Richter**,* TU Berlin, Germany **INVITED**
Epitaxial growth of semiconductor structures requires control of the growth process on the atomic scale. This, however, is difficult to achieve by just controlling macroscopic growth parameters like partial pressures (fluxes) and temperatures. It is thus desirable to have in real time microscopic information from the growing surface for a direct analysis and conseqently control on the ongoing growth process. Optical probes offer in this respect important advantages: they are in general non invasive, they can be fast in obtaining the needed information and finally they can be applied in all growth environments (vacuum or gasphase based growth methods). The "optical" disadvantage of having a low spatial resolution can be overcome quite often by extra "calibration" measurements with high resolution spatial probes like STM, AFM, LEED. I will discuss first the analysis of reconstructed surfaces by reflectance anisotropy (RAS). Simultaneous measurements in MBE and MOVPE together with theoretical calculations allow to correlate optical spectra with surface reconstructions. Based on these basic data it is possible to describe adsorption and desorption processes of the basic constituents (Group III and V elements). Moreover, growth in dependence of partial pressure and temperature can be described via different modes in a flux - temperature phase diagram, allowing thus to define the surface growth status nearly independent of the special epitaxial equipment. Monitoring and control of device growth seem to be now possible.

2:40pm **EL-ThA3 Direct Numerical Inversion of Real-time Ellipsometric Data for Monitoring and Control of Optical Filter Deposition***, D. Kouznetsov, A. Hofrichter, **B. Drevillon**,* Ecole Polytechnique CNRS, France
In situ ellipsometry is well known to be one of the most sensitive, non-disturbing tools for controlling and monitoring the growth of thin films. However the rapid advances in ellipsometric instrumentation, especially the increasing real time spectroscopic capabilities of state of art ellipsometers necessitate the development of new algorithms for an optimal assessment of the available information. In this work we apply a new direct numerical inversion algorithm for the real-time reconstruction of homogeneous and inhomogeneous refractive index profiles for the monitoring and the control of optical thin film depositions. The algorithm is based on a second order Taylor decomposition of the coefficients of the Abeles matrices of the newly grown layer. The variation of the real-time spectroscopic ellipsometry data are expressed as polynomial functions depending on the dielectric constant and the thickness of the newly grown layer. This allows a direct inversion of the ellipsometric signal and assures the high speed of the algorithm. Typical inversion times are 150 ms for 16 wavelength with a typical precision of 0.02 for the refractive index and less than 2% error in the reconstructed thickness. The algorithm is successfully applied for the real-time material characterization of transparent and weakly absorbant silicon oxynitrides deposited by plasma enhanced chemical vapor deposition. The complete process space can thus be explored in one single run. Combined with traditional ellipsometric control algorithm this method allows to grow multilayer and gradient optical coatings with high accuracy in respect to initial design.

3:00pm **EL-ThA4 Integrated Multiwavelength Parallel-processing Rotating-compensator Ellipsometer/Reflectance-difference Spectrometer for Real-time Measurement and Control of OMCVD Growth***, **K. Flock**, M. Ebert, K.A. Bell, D.E. Aspnes,* North Carolina State University
Previous research has underlined the importance of real-time diagnostics for epitaxial growth of semiconductor materials and structures. We describe an optical system integrated with a modified rotating-sample commercial organometallic chemical vapor deposition (OMCVD) reactor that combines the functions of spectroscopic ellipsometry (SE) and reflectance-difference spectroscopy (RDS) in a single optical path to return information about growth rates, compositions, and film thicknesses (SE) and surface chemistry (RDS). The system is essentially a rotating-compensator ellipsometer for increased diagnostic power relative to rotating-polarizer or rotating-analyzer designs, with the rotation rate of the compensator synchronized to that of the sample. Synchronization reduces noise in the SE data by eliminating random optical-anisotropy contributions and also allows us to measure the non-normal-incidence RD spectrum directly. The original sample spindle was replaced with a design that allows sample runout to be adjusted dynamically to provide additional improvements in signal-to-noise ratios. A 1024-element photodiode array detector with a 0.2 m spectrograph provides a spectral range of 240 to 840 nm. Software designed to optimize both real-time response and repetition rate permits complete spectra to be obtained at a 6 Hz rate with a 400 MHz computer. Using a prototype rotating-polarizer system we demonstrated sample-driven closed-loop feedback control of a graded-composition InGaP structure grown on GaAs, where the composition was varied parabolically with thickness. During the growth of this structure it was necessary to reduce the flow through the trimethylindium by about half, which the RD data indicate is due to a change of incorporation efficiency due to an observed change of surface reconstruction.

3:20pm **EL-ThA5 In-situ Monitoring of Ag Film Growth on Si(111)7x7 Surface by Optical Second Harmonic Generation***, **H. Hirayama**, T. Kawata, K. Takayanagi,* Tokyo Institute of Technology, Japan
A growth of Ag films on the Si(111)7x7 surface was monitored by optical second harmonic generation (SHG). Ag-coverage dependent intensity oscillation was observed in p-polarized SHG signals with 1.20,1.30 and 1.40 eV pump photon energy. As has been reported recently by Pedersen et al, the SHG intensity oscillated with the Ag coverage. However, on the contrary to the previous report, the first peak in the oscillations was observed at 3ML for all the pump energy. The peak position was independent on the pump energy. Meanwhile, the subsequent peaks shifted toward lower coverage with the increase in the pump photon energy. A detailed comparison of the SHG intensity and AFM images of the Ag film grown on the Si(111) substrate showed that many three-dimensional Ag islands nucleated at the coverage for the first peak. The surface morphology changed to be two-dimensional smooth one at the coverage for the subsequent peaks. The AFM images and the SHG spectrum taken at the coverages of the peaks showed that the first peak in the SHG intensity oscillation corresponded to the local plasmon resonance with the 3D Ag island formation. The subsequent peaks were caused by the transitions with the quantized electronic states confined in the thin, flat Ag films. The characteristic transitions between the electronic states localized at the Ag/Si(111)7x7, 1x1 and @sr@3x@sr@3 interfaces were also detected as resonant peaks in the s-polarized SHG spectrum with the excitation photon energy ranged from 1.05 to 1.70eV.

4:00pm **EL-ThA7 RHEED Intensity Oscillation during Thermal Oxidation on Si(001) Surface with O@sub 2@***, **Y. Takakuwa**, F. Ishida,* Tohoku University, Japan
Auger electron spectroscopy combined with reflection high energy electron diffraction (RHEED-AES) was applied to investigate the surface reaction dynamics during thermal oxidation on Si(001)2x1 surface with O@sub 2@. In the RHEED-AES measurement, O KLL Auger electrons excited by a grazing-incident electron beam for RHEED observation were detected, enabling to observe simultaneously the SiO@sub 2@ coverage and surface morphology. In the temperature region of two-dimensional growth of SiO@sub 2@ islands at 630~800°C as confirmed by the time evolution of O KLL Auger electron intensity, an oscillatory behavior in RHEED half-order spot intensity was observed, indicating that etching of the surface occured between SiO@sub 2@ islands. The etching rate obtained by the oscillation period was 0.039 ML/s at an O@sub 2@ pressure of 2x10@super -7@ Torr independently of the temperature and SiO@sub 2@ coverage, and increased in proportion to the O@sub 2@ pressure, suggesting that the etching reaction was rate-limited by O@sub 2@ supply. Since part of adsorbed oxygen atoms is consumed for nucleation and two-dimensional growth of SiO@sub 2@ islands in this temperature region, the assigned rate-limiting reaction means that the etching reaction takes place not only through SiO desorption but also through SiO@sub 2@ growth, that is, incorporation of Si atoms into SiO@sub 2@ islands. The fraction of the amount of incorporated Si atoms into SiO@sub 2@ islands to that of etched Si atoms will be discussed against SiO@sub 2@ coverage.

5:00pm **EL-ThA10 SR-TXRF for the Investigation of the Deposition Mechanism of Trace Cu Impurities on Si Wafer Surfaces***, **K. Baur**,* Stanford Synchrotron Radiation Laboratory*; T. Homma, J. Tsukano,* Waseda University, Japan*; M. Watanabe,* Komatsu Electronic Metals, Japan*; A. Singh, S. Brennan, P. Pianetta,* Stanford Synchrotron Radiation Laboratory
Total Reflection X-ray Fluorescence (TXRF) spectroscopy using synchrotron radiation is one of the most powerful techniques for trace impurity analysis on Si wafer surfaces. In addition, among the more sensitive techniques, it is the only one that is non-destructive. We present the status of the

transition metal analysis activity at the Stanford Synchrotron Radiation Labororatory (SSRL) which has matured to a point where a facility exists at which semiconductor companies are able to perform industrially relevant measurements at state of the art detection limits. This facility features clean wafer handling and automated data acquisition making routine analytical measurements possible. The best sensitivity demonstrated to date is 3.4 E7 atoms/cm2 for a 5000 second count time corresponding to 7.6 E7 atoms/cm2 for a standard 1000 second count time. This is more than a factor of 100 better than what can be achieved with conventional TXRF systems. A new development at SSRL is the investigation of the deposition mechanisms of trace metal impurities during a wet cleaning process on Si wafer surfaces. This is considered to be influenced by the oxidation conditions at the silicon wafer surface. This study requires high surface sensitivity and renders Synchrotron Radiation TXRF the technique of choice. We will present our results on the deposition mechanism of Cu trace impurities on Si wafers immersed into ultra pure water, focussing on the correlation between the deposited Cu concentration and the amount of dissolved oxygen present in the ultra pure water.

## Semiconductors
## Room 111 - Session SC+SS-ThA
## Semiconductor Surface Structure

**Moderator:** R.M. Tromp, IBM T.J. Watson Research Center

2:00pm **SC+SS-ThA1 Direct Surface Structural Determination using Correlated Thermal Diffuse Scattering***, **T. Abukawa,*** Tohoku University, Japan **INVITED**

Since the atomic vibration is strongly correlated among neighbor atoms or within very short-range in crystal, the short-range coherency in electron diffraction may survive even if the long-range coherency is destroyed by thermal vibration. The short-range coherency causes broad structures in the thermal diffuse scattering (TDS). The broad diffraction structures due to short range coherency were indeed observed for a Si(001) surface when medium energy electron diffraction was measured at medium scattering angles.@footnote 1@ The broad features were observed as very simple oscillations of diffracted electron intensity. These features have been termed correlated thermal diffuse scattering (CTDS).@footnote 1@ Since CTDS is well interpreted as kinematical diffraction among nearest neighbor atoms composing the crystal, the three-dimensional Patterson function can be obtained by simple Fourier transformation of a three-dimensional CTDS pattern. When a medium electron beam is incident at a grazing angle, the surface sensitivity of CTDS is enhanced, and the building blocks of surfaces, i.e. the lengths and the orientations of all the surface related nearest-neighbor bonds, can be directly obtained from the Patterson function analysis. The application of Patterson function analysis of CTDS will be demonstrated for the surface structures of Si(001)2x1,@footnote 2@ Si(111)@sr@3x@sr@3-In@footnote 3@ and Si(111)4x1-In. @FootnoteText@ @footnote 1@ T. Abukawa, C.M. Wei, T. Hanano, and S. Kono, Phys. Rev. Lett. 82, 335 (1999). @footnote 2@ T. Abukawa, C.M. Wei, K. Yoshimura and S. Kono, Phys. Rev. B62, 16069 (2000). @footnote 3@ T. Abukawa, K. Yoshimura and S. Kono, Surf. Rev. Lett.7, 547 (2000).

2:40pm **SC+SS-ThA3 Atomic Structures of the of InP (111) Surface***, **C.H. Li,** D.C. Law,* University of California, Los Angeles*; L. Li,* University of Wisconsin, Milwaukee*; R.F. Hicks,* University of California, Los Angeles

The atomic structure of the indium-terminated InP (111), prepared by metalorganic vapor-phase epitaxy (MOVPE), has been characterized by scanning tunneling microscopy (STM), low energy electron diffraction (LEED), and x-ray photoemission spectroscopy (XPS). Three reconstructions are observed depending on the MOVPE process conditions and temperature of annealing in vacuum after growth: these are the (rt3xrt3), (2x2) and (1x1). The (rt3xrt3) reconstruction is the most interesting of these and consists of one ad-atom per unit cell resting on a full layer of indium atoms. This structure is stabilized by the incorporation of oxygen atoms, which are gettered from the MOVPE environment by the indium-rich surface. At the meeting, the atomic structure of each InP (111) reconstruction will be described and compared to those observed on the gallium-rich GaAs (111) and GaN (0001) surfaces.

3:00pm **SC+SS-ThA4 Surface Stress and the Morphology of Si(111) near Tc***, **J.B. Hannon,** J. Tersoff, R.M. Tromp,* IBM Research Division

It is well known that surface stress can strongly influence the structure and chemical composition of surfaces. Despite significant theoretical progress, few quantitative experimental investigations have been reported. One reason for this is the long-range of elastic interactions at surfaces. To quantitatively determine the influence of surface stress, the structure of the surface over micron-scale distances must be precisely known. In this talk I describe low-energy electron microscopy measurements of Si(111) surface structure near the 7x7 to 1x1 transition temperature (Tc = 1135 K), where phase coexistence is observed. We find that the equilibrium domain geometry is determined by a competition between the free energy difference between the phases, which favors a single phase, and elastic relaxation at the phase boundaries, which favors phase coexistence.@footnote 1@ Elastic relaxation occurs because of the difference in surface stress between the two phases. For Si(111), the stress difference has been measured by Twesten and Gibson.@footnote 2@ In equilibrium, the force on each phase boundary vanishes. We use this fact to determine the free energy difference between phases, and phase boundary creation energy, from the measured domain configurations. In equilibrium, each phase boundary gives rise to an independent equation relating the free energy difference, the boundary creation energy, and the stress difference. By measuring domain configurations as a function of temperature, we determine the temperature dependence of the free energy difference between phases near Tc. Our measurements correspond to an entropy difference between the phases of only 0.01 kB per 1x1 unit cell, a surprisingly small value given the fact that the 7x7 structure has long-range order and the 1x1 phase does not. These results indicate that the degree of disorder in the two phases is similar. @FootnoteText@ @footnote 1@J.B. Hannon, et al., PRL, in press @footnote 2@PRB 50, 17628 (1994).

3:20pm **SC+SS-ThA5 Origin of the Wide Si(7 7 17) Domain Parasitic on Si(5 5 12) Surface***, **S.H. Cho,** J. Zhang, J.M. Seo,* Chonbuk National University, Korea

Recently the high-index and single-domain Si(5 5 12) has attracted much attention due to its potential application as a template for one dimensional nanowire fabrication. However, another high-index and single-domain (7 7 17) plane has not been reported yet, although they have similar plane directions of only 0.3 degree off and commonly consist of (2 2 5) and (3 3 7) sections [i.e., (5 5 12)=2x(3 3 7)+(2 2 5) and (7 7 17)= (3 3 7)+(2 2 5)]. From the recent STM investigation on Si(5 5 12), we have detected the wide Si(7 7 17) domains parasitic on Si(5 5 12). Most of wide (7 7 17) domains appear in the terrace adjacent to the step parallel to (-1 1 0) row direction. In a single terrace, the (7 7 17) domain extends to a few hundreds Angstrom from the step, then transforms to (5 5 12). Some (7 7 17) domains are also detected from the bent surface without steps. These wide and pure (7 7 17) domains, appearing near the step or on the bent surfaces, are experiencing the compressed stresses, and these excessive stresses replace the compressed stress originating from a (3 3 7) section in (5 5 12). Therefore, the extra (3 3 7) section is not required in a (5 5 12) plane under such stresses, which results in (7 7 17) domain until such local compressed stresses are released.

3:40pm **SC+SS-ThA6 First-Principles Study of Thermal Fluctuation of Si(111)@sr@3 X @sr@3 - Ag Surface Appeared in Non contact AFM Images***, **M. Tsukada,** N. Sasaki, S. Watanabe,* University of Tokyo, Japan

Until recently ''Honeycomb-Chained-Triangle (HCT)'' model for the atomic structure of Si(111) @sr@3 X @sr@3 -Ag surface (referred to @sr@3 -Ag surface hereafter) seemed to be accepted. However, a new structural model called ''InEquivalent-Triangle (IET)'' model was proposed by Aizawa et al.@footnote 1@ based on the first-principles calculation as well as the low temperature STM. The IET model is energetically more favorable than the HCT model by about 0.1 eV per @sr@3 X @sr@3 unit cell. In IET model, a mirror plane symmetry is broken and the inequivalent Ag triangles are located in the unit cell. In the present work, we calculated NC-AFM images of IET structure based on a density functional theory. In simulating two-dimensional NC-AFM images, we used a "Fourier expansion method". In this method, the two-dimensional symmetry of the tip-surface system is considered. The thermal averaged images of the fluctuating two different phases of IET structures are calculated in the following way. Namely, at each scanning position of the tip over the surface, the frequency shift is calculated from the force-curve which is obtained from the canonical weighted average of the both phases of IET. The simulated theoretical images reproduces fairly well the experimental observation at room temperature. Therefore our result confirms that the room temperature apparent HCT structure is the thermal fluctuated structures of the two phases of IET. The effect of the tip apex structure on AFM images is also discussed together with the thermal fluctuation. @FootnoteText@ @footnote 1@ H.Aizawa, M.Tsukada, N.Sato and S.Hasegawa, Surf. Sci. 429, L509 (1999).

4:40pm **SC+SS-ThA9 Adsorption of C@sub 2@H@sub 2@ on Si(100) - New High Resolution Core-level Photoemission and Photoelectron Diffraction Results***, M. Kittel,* ***M. Polcik****, J.-T. Hoeft, D.I. Sayago,* Fritz-Haber-Institut der MPG, Germany*; R.L. Toomes, D.P. Woodruff,* University of Warwick, UK

The adsorption of acetylene and ethylene on Si(100) has been subject of a large number of experimental and theoretical studies. Most theoretical studies have favoured a 'di-@sigma@' bonding character for both species, in which the C-C axis lies parallel to the Si dimers with the molecules symmetrically placed atop the dimers. Two independent experimental scanned-energy mode photoelectron diffraction (PhD) studies of the structure of the ethylene adsorption system have provided confirmation of this idea,@footnote 1,2@ but in the case of acetylene adsorption, one such study@footnote 3@ found this atop dimer configuration, but another found a totally different site between two dimers@footnote 2@. In an attempt to resolve this discrepancy we have carried out further experimental studies of the Si(100)/acetylene system at different temperatures and coverages, using high-resolution C 1s photoemission and C 1s PhD. Our new measurements confirm the dominance of the aligned atop-dimer geometry under all conditions studied. We find no direct evidence for a second species, except under conditions associated with fragmentation of the molecular adlayer by the incident soft X-ray beam, although the PhD data could be reconciled with some fractional occupation of other lower-symmetry sites which may contribute only very weak PhD modulations. @FootnoteText@ @footnote 1@ P.Baumgärtel et al, New.J.Phys 1 (1999) 20.1 @footnote 2@ S.H.Xu et al., Phys. Rev. Lett. 84, 939 (2000) @footnote 3@ R. Terborg et al., Phys.Rev.B 61, 16697 (2000).

5:00pm **SC+SS-ThA10 The Effect of an As-flux on the Surface Structure During the Growth of Si on GaAs(001) c(4x4)***,* ***T.A.R. Müller***[1]*, B.D. Schultz,* University of Minnesota*; H.H. Farrell,* Idaho National Engineering and Environmental Laboratory*; A. Franciosi,* Universita' di Trieste, Italy and Univ. of Minnesota*; C.J. Palmstrom,* University of Minnesota

Despite the experimental discovery that two atomic monolayers of Si co-deposited with an As-flux are effective in decreasing the barrier height in the Al/Si/GaAs system by 0.5eV, the detailed interfacial atomic structures have yet to be determined. The present work focuses on understanding the evolution of the structure within the first few atomic monolayers caused by the deposition of Si with and without an As-flux on the GaAs(001) c(4x4) surface by MBE. In-situ Reflection High Energy Electron and Low Energy Electron Diffraction, work function measurements, X-ray photoelectron and Auger electron spectroscopies and Scanning Tunneling Microscopy have been used to determine the properties and composition of the surface as a function of Si coverage. For the co-deposition of Si with As, the measured work function increases up to a Si-coverage of 0.5 ML and the intensity ratio of the Ga and As 3d photoemission peaks decreases. However, for Si deposited at pressures <10@super -10@ mbar, the work function shows variations of <50meV from the starting surface and the XPS peak intensity ratio increases for a coverage of 0.5 ML. Atomistic models consistent with electron counting, surface symmetry, work function and composition changes will be presented.

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[1] **Morton S. Traum Award Finalist**

## Electronics
## Room 131 - Session EL+SE+TF-FrM
## Laser Processing of Surfaces

8:20am **EL+SE+TF-FrM1 Laser Creation of 3D Micro- and Nano-objects: Processing, Properties and Applications**, ***M.J. Stuke**, M. Koch,* Max-Planck-Institut f. Biophys. Chemie, Germany*; A. Moore,* University of the Pacific*; K. Mueller,* Max-Planck-Institut f. Biophys. Chemie, Germany*; G. Padeletti,* CNR Monterotondo*; K. Williams,* Max-Planck-Institut f. Biophys. Chemie, Germany*; G. Fuhr,* Humboldt University, Germany **INVITED**

Recent results obtained by VUV laser ablation of organic fibers and by laser direct write of 3D microelectrode structures will be described with special emphasis on: (1) creation of a cage on a tip for touch-free trapping, handling and transfer of NEUTRAL objects in solution. Video sequences will give direct evidence for the new possibilities (2) ultraprecise machining of spider fibers, an ultrastrong material.

9:00am **EL+SE+TF-FrM3 Excimer Laser Surface Treatment for Aluminum Carbide Growth**, ***F. Fariaut,*** GREMI, France

The excimer laser process reported is developed to enhance the mechanical and chemical properties of aluminum alloys. It would be interesting to use aluminum alloys in the automotive industry widely because of their low density, corrosion resistance and good workability. The motor weight can be reduced by replacing usual materials such as iron-steel by light alloys treated to increase their wear resistance. Ceramic materials generally exhibit great strength, resistance to wear and oxidation. The use of laser beams allows surface treatment to be located at the parts strongly exposed to wear and friction. The surface undergoes a transformation leading to an increase in hardness without changing the dimensions of the piece, thus avoiding no remachining after treatment. The laser process is especially suitable for environment protection as there is no pollution by chemical solvent or emanation. An excimer laser beam is focused onto the alloy surface in a cell containing 1 bar propylene gas. A vapor plasma expands from the surface and shock wave dissociates and ionizes the ambient gas. It is assumed that carbon from plasma in contact with the surface penetrates in depth. Thus it is necessary to work with a sufficient laser fluence to create the plasma, but this fluence must be limited to prevent laser-induced surface roughness. The carbon concentration profiles are determined from RBS and SEM coupled to EDX analysis. Crystalline quality is evidenced by XRD technique. TEM gives the in-depth microstructure. Fretting coefficient measurements exhibit a lowering for some experimental conditions. The polycrystalline cemented layer obtained is several micrometers thick and composed of a pure composition (columnar microstructure) top layer (200-500nm thick) standing on a diffusion layer (grains). This layer allows a significant decrease in the fretting coefficient.

9:20am **EL+SE+TF-FrM4 Laser Surface Treatment for Corrosion Prevention**, ***C. Georges**, N. Semmar, C. Boulmer-Leborgne,* GREMI, France*; C. Perrin, D. Simon,* CERI, France

The materials used in electrical contact applications are constitued of a copper alloy (brass or bronze) covered with nickel coating (diffusion barrier) and with a gold coating. There are some porosities in the nickel and gold layers which induced corrosion of the underlying layers. To modify structure of gold coating, some laser surface treatments have been undertaken. An excimer laser is used as the photon absorption coefficient is larger in UV range and because the laser beam homogeneity is available for a surface treatment. The purpose of this surface treatment is to suppress the porosities of the gold layer which are responsible of the corrosion pits and to smooth the surface as the roughness bothers a correct electrical contact. The effects of the laser treatment are studied according to different surface parameters (roughness and composition of the substrate, thickness and composition of the gold coating). The laser beam parameter influence on surface melting is simulated by numerical code. Tests of corrosion are carried out in the humid synthetic air containing low contents of pollutants (NO2, SO2 and Cl2). The technique used to control these effects are : optical microscopy, SEM, grazing X-rays and ESCA. One dimension heat conduction is resolved to simulate the temperature time evolution and the melted depth as a function of the laser parameters (laser fluence, pulse time duration). This modelling helps to the understanding of mechanisms for laser interaction with the connector surface and will allows to determine the laser type to use for this appication.

9:40am **EL+SE+TF-FrM5 Laser Processing Opportunities with a High Average Power Free Electron Laser**, ***H.F. Dylla**, S.V. Benson, J. Boyce, G. Biallas, D. Douglas, G.R. Neil, R. Evans, A. Grippo, J. Guebeli, K. Jordan,* Jefferson Lab*; M.J. Kelley,* Jefferson Lab and College of William and Mary*; R. Li, L. Merminga, J. Preble, M. Shinn, T. Siggins, R.W. Walker, G.P. Williams, B. Yunn,* Jefferson Lab

A kilowatt class free electron laser has been operational at Jefferson Lab since 1999. The associated user facility laboratories are being used for laser-materials studies that take advantage of the FEL's high average power, broad tunability and sub-picosecond pulse structure. The presently operating FEL delivers kilowatt level powers over the mid-infrared (3-7 microns). Recently, the device has extended operation through the visible (at the 100 watt level) and the UV (at the 10 watt level) through harmonic generation. A major upgrade is currently under way that will increase the power level in the IR to 10 kW and extend kilowatt operation through 300 nm in the UV. FEL users involved in materials processing have demonstrated unique applications involving: pulsed laser deposition, laser nitriding, laser production of carbon nanotubes, laser ablation and laser micromachining.-This work supported by the Office of Naval Research, the Commonwealth of Virginia, DOE Contract DE-AC05-84ER40150, and the Laser Processing Consortium.

## Semiconductors
## Room 111 - Session SC+SS-FrM
## Growth and Epitaxy of Semiconductors

**Moderator:** A.A. Baski, Virginia Commonwealth University

8:40am **SC+SS-FrM2 STM Observations of the Initial Growth Process of Ge on Si(105) Surfaces: the Stability of Ge/Si(105) Surfaces**, ***Y. Fujikawa,*** University of Wisconsin-Madison*; T. Sakurai,* Tohoku University, Japan*; M.G. Lagally,* University of Wisconsin-Madison

The mechanism of the formation of self-organized SiGe quantum dots on the Si(100) surface has been intensively investigated because of the technological importance of achieving uniform size and high order in the dots. Although it has been demonstrated that the strain created by the lattice mismatch between Ge and Si plays an important role in the transition to 3D island growth and in 3D island ordering, there still is no satisfactory explanation of SiGe(105) facet formation, which creates the regular shape of the SiGe islands. We have used STM to observe the surface structures formed when Ge is deposited on Si(105) surfaces, in order to clarify the coverage dependence of the stability of the (105) surface. When the Ge coverage is greater than 0.5 ML, a p(2x1) reconstructed stable surface is observed, as previously reported.@footnote 1@ At a coverage of ~ 0.5 ML or less, we observe formation of a p(4x1) structure over parts of the surface. The transformation to a p(4x1) structure is complete at 0.04 ML coverage. Decreasing the Ge coverage to 0.02 ML results in roughening of the Si(105) surface. During the transition from the p(2x1) to the p(4x1) structure, a significant change in surface morphology is observed. At coverages of 0.2 ML or less, the formation of the topmost layer tends to start from upper-step edges, while it starts from lower-step edges for coverages above 0.2 ML. As a result, defect arrays are frequently observed at the lower-step edges when the coverage is 0.2 ML or less, due to the incomplete formation of the topmost layer at the lower-step edges. This result clearly indicates the presence of increased strain on the Ge/Si(105) surface as the coverage of Ge is reduced. Ge thus stabilizes the surface. This work is partially supported by NSF and by the Ministry of Education, Culture, Sports, Science and Technology, Japan. @FootnoteText@ @footnote 1@ Tomitori et al., Surf. Sci. 301 (1994) 214.

9:00am **SC+SS-FrM3 Modulated Semiconductor Structures Studied by In Situ Scanning Tunneling Microscopy**, ***C.A. Pearson**, C. Dorin, Y. Chen, J. Mirecki Millunchick, B.G. Orr,* University of Michigan-Flint

Semiconductor structures known to exhibit compositional modulation are compared to similar structures that do not exhibit compositional modulation using in situ scanning tunneling microscopy. The structures are grown by molecular beam epitaxy on InP(001) following the growth of a lattice matched InGaAs buffer layer. InAs/GaAs and InAs/AlAs short period superlattices (SPSs) can be classified as having either rough or smooth interfaces. Rough interface SPSs exhibit compositional modulation. The buffer layer and smooth interface SPSs are structures that do not exhibit compositional modulation. Images of these structures are characterized by long wavelength surface undulations. This contrasts significantly from images of modulated structures, which show both long and short wavelength surface undulations. Another distinction is that the lattice planes on the modulated structures appear much more dendritic due to the short wavelength undulations. The relationship between the morphology of the buffer layer and the resulting SPS structure is discerned through these comparisons. Segregation of species is identified as well using scanning tunneling spectroscopy. Results from proximal probe experiments will increase the atomistic understanding of surface roughness and its role in compositional modulation.

9:20am **SC+SS-FrM4 Scandium Gallium Nitride Alloys and ScN/GaN Heterostructures Grown by Molecular Beam Epitaxy***, **A.R. Smith**, H.A.H. Al-Brithen, D.C. Ingram,* Ohio University

Scandium nitride is an interesting transitional metal nitride semiconductor with a simple crystal structure (rocksalt). Part of the interest in ScN is as a lower bandgap material (Eg = 2.1 eV) which can be combined with GaN to form novel heterostructures or alloys. In particular, GaN has a lattice constant close to ScN (both about 4.5Å ); it may therefore be possible to form an alloy with band gap in the range 2.1-3.4 eV. However, since ScN is rocksalt while GaN is zincblende or wurtzite, it is not clear that a simple alloy or interface can be formed. We have first investigated the growth of pure ScN on magnesium oxide (001) substrates by molecular beam epitaxy (MBE) using a RF-plasma source and a scandium effusion cell. The Sc/N flux ratio was found to be critical in determining the structural, optical, and electronic properties of the grown epitaxial layers. Under N-rich conditions, the growth is epitaxial, and we find atomically smooth terraces separated by steps having height a/2. Films grown N-rich are stoichiometric and transparent with a direct optical transition at 2.15 eV; further efforts are underway to experimentally verify the theoretically predicted indirect transition near 1 eV. We have begun to investigate the growth of GaN/ScN(001). First, we grew ScN(001) at growth temperature 850°C; next, we initiated GaN growth at reduced substrate temperature 550°C under Ga-rich conditions. After several minutes, the growth temperature was increased to 750°C, and the Ga flux was reduced but still maintaining Ga rich conditions. Reflection High Energy Electron Diffraction (RHEED) showed a pattern consistent with cubic GaN(001). X-ray diffraction showed only one peak beside the MgO substrate peak revealing that the GaN film is cubic having the same (002) orientation as the ScN(001) layer. A Sc-Ga-N layer was also grown on MgO(001) with growth temperature at 850°C. Structural and optical properties will be presented.

9:40am **SC+SS-FrM5 Formation and Decay Processes of Silicon Mounds on Si(111) Surfaces***, **A. Ichimiya**, K. Hayashi,* Nagoya University, Japan*; E.D. Williams, T.L. Einstein,* University of Maryland*; M. Uwaha,* Nagoya University, Japan **INVITED**

Two types of isolated single silicon pyramids on the Si(111) surfaces between 700K and 800K have been produced using an STM tip. Pyramids of 75% are normal stacking at the interface between the pyramid and the substrate (called type U). For pyramids of 25% which are in the twin relation of the type U pyramids, there is a stacking fault at the interface (called type F). The pyramids have certain facets just after the creation. Indices of main facets of the mounds on the Si(111) surface are {311}, and small facets are {221} for the type U and {331} for the type F. Just after the production, the pyramid begins to decompose. During the decay of the type U pyramid, the facets of the pyramid transform into multi-bilayer steps. Finally the mound becomes a bilayer mound (2D) with a truncated triangle shape. The longer edges of the 2D mounds are along the unfaulted halves of the DAS structure of the substrate, while these edges are the shorter one of the pyramid. The decay process of the type F pyramid is layer-by-layer without step bunching. Decay rates of the type F pyramids are about 3 times larger than those of the type U due to the stacking. The energy state of the type F pyramids is about 0.06eV higher than that of the type U. We have measured height evolution of the pyramids during decay, and found that the height decay is due to the power law , t@super 1/4@, where t is the decay time. Such the simple law is predicted by Israeli and Kandel@footnote 1@ for infinite cone decay. It should be noted that such the simple law is in very good agreement with the experimental results of silicon pyramid decay. The results are explained by attachment-detachment limited processes at step edges. The measured decay rates are in very good agreement with decay rates which are evaluated from those of 2D mounds.@footnote 2@ @FootnoteText@ @footnote 1@ N. Israeli and D. Kandel, Phys. Rev. Lett. 80, 556 (1998. @footnote 2@ A. Ichimiya, Y. Tanaka and K. Ishiyama, Phys. Rev. Lett. 76, 4721 (1996).

10:20am **SC+SS-FrM7 Role of Surface Steps in the Arrangement of Silicon Nano-dots on Vicinal Si(111) Surfaces: STM Investigation***, **J.S. Ha**, K.-H. Park, Y.-J. Ko, K. Park,* ETRI, Republic of Korea

Regular array of nano-structures such as dots and wires can be obtained by elaborate control of chemical reactions on stepped surfaces. In this work, we have investigated the role of surface steps in the arrangement of silicon nano-dots on vicinal Si(111) surfaces by scanning tunneling microscopy(STM). Nanometer sized silicon nitride islands were formed on a vicinal Si(111) surface, which was 1@super o@ off toward [112] direction, via thermal nitridation using N@sub 2@ gas. On the nitrided surface, oxygen gas was dosed at 700 @super o@C to induce a local selective etching of silicon using silicon nitride islands as masks. The resultant surface showed one-dimensional arrangement of silicon nano-dots along the step edges of the silicon surface. The lateral size of the dot in the direction perpendicular to the step edges was restricted to the terrace width of the stepped Si(111) surface. Preferential growth of silicon nitride islands on the edges of single height steps is considered to be responsible for the arrangement of silicon nano-dots along the step edges of the 1 @super o@ off vicinal Si(111) surface. Furthermore, comparative STM studies to investigate the role of surface steps, which were done on Si(111) surfaces with miscut angles of 0.1@super o@ and 4@super o@ off toward [110] direction, will be also discussed.

10:40am **SC+SS-FrM8 Thermal Growth of High-density Silicon Quantum Dots on SiO@sub 2@/Si(001) with Submonolayer Silicon Adatom Predeposition***, **J.G. Ekerdt**, J.H. Zhu, W.T. Leach,* University of Texas at Austin

A nonthermal method to facilitate nucleation and subsequent thermal chemical vapor deposition of Si quantum dots on SiO@sub 2@/Si(100) with high density and uniform size is demonstrated. Submonolayers (0.12 to 0.02 ML) of Si adatoms are predeposited on a room temperature to 825 K SiO@sub 2@/Si(001) substrate by cracking disilane on a high-temperature filament in a UHV chamber at pressures on the order of 10@super -7@ Torr. The quantum dots are grown at 825 K with a disilane pressure of 2x10@super -6@super Torr. The Si quantum dot density is increased and size distribution is narrowed by predeposition of Si adatoms when compared to thermal growth on bare SiO@sub 2@/Si(100). The dot density and size is controlled by the amount of Si adatom predeposition; 9.5x10@super 11@ cm@super -2@ density and 5.5 nm size are demonstrated on SiO@sub 2@/Si(001). A surface kinetic model is also presented that accounts for dot nucleation, adatom formation during growth, diffusion of adatoms to growing dots and epitaxial growth of dots. The method provides an effective way to control the nucleation, and consequently the growth, of quantum dots on dielectric surfaces.

11:00am **SC+SS-FrM9 Nucleationless Island Formation in SiGe/Si(100) Heteroepitaxy***, **P. Zahl**, P.W. Sutter,* Colorado School of Mines

The self-assembly of quantum dot (QD) islands in lattice-mismatched heteroepitaxy has been studied extensively. One of the objectives of recent research is the creation of long-range ordered arrays of QDs of uniform size, a major technological milestone that would pave the way for application of these nanostructures in electronic and optoelectronic devices. The formation of epitaxial QD islands is generally assumed to involve nucleation, a statistical process that would severely impede QD organization. Our recent observations by low-energy electron microscopy, however, have demonstrated that QD islands in heteroepitaxial systems such as SiGe/Si(100) can self-assemble in a coninuous process that avoids nucleation.@footnote 1@ With the observed nucleationless islanding, perfect periodic arrays of uniform QD islands may form spontaneously under suitable growth conditions or may be induced by weakly invasive growth modifiers that enhance existing ordering forces. We present a systematic study of the evolution of SiGe QD islands on Si(100) by combining growth with in-situ scanning tunneling microscopy. Our microscopic observations are analyzed to detect island interaction mechanisms that may act as driving forces for spontaneous spatial ordering in the nucleationless islanding process. First results on the use of growth modifiers to enhance or induce long-range order will be presented. @FootnoteText@ @footnote 1@ P. Sutter and M. G. Lagally; Phys. Rev. Lett., 84(20):4637-4640, 2000.

11:20am **SC+SS-FrM10 Electronic Structure of a Heteroepitaxially-Passivated Si(111) Surface: GaSe-terminated Si(111)***, **M.A. Olmstead,*** University of Washington*; R. Rudolf, C. Pettenkofer,* Hahn-Meitner Inst., Germany*; A.A. Bostwick, J.A. Adams,* University of Washington*; E. Rotenberg,* Advanced Light Source, Berkeley*; F.S. Ohuchi,* University of Washington*; R. Fritsche, A. Klein, W. Jaegermann,* Tech. Univ. Darmstadt, Germany

Dissimilar materials heteroepitaxy often results in an interface reaction that passivates substrate dangling bonds. This forms a low energy surface that promotes islanded, rather than laminar, growth of the subsequent overlayer. GaSe-terminated Si(111) is an example of such a stable, low-diffusion barrier surface with no states in the Si band gap; it may serve as an ideal substrate for quantum dot growth on Si(111). We have performed detailed studies of the electronic and atomic structure of GaSe-terminated Si(111) using energy-dependent and angle-resolved valence band and core-level photoemission spectroscopy. The surface termination consists of a Ga layer bonded to the top-most Si atoms and a Se layer on top with each Se atom bonded to three Ga. Our photoelectron diffraction results show the Ga and Se atomic arrangement is identical to that of a half-sheet of the layered semiconductor GaSe. The surface thus contains no dangling bonds, but has fully-occupied lone-pair states similar to As-terminated Si(111). The observed dispersion of the energy bands is very close to those of a GaSe single crystal and is interpreted in terms of tight binding energy states. The dominance of the GaSe-derived states over those of Si-derived states is obvious and is different from As-terminated Si.

11:40am **SC+SS-FrM11 Surface Reaction Study of TaN Growth from MOCVD Precursors on Cu(111)***, J.-B. Wu,* National Chiao-Tung University, Taiwan*; **Y.W. Yang,*** Synchrotron Radiation Research Center, Taiwan*; Y.-F. Lin, H.-T. Chiu,* National Chiao-Tung University, Taiwan

Understanding the reaction pathway followed by MOCVD precursors during thin film growth is a scientifically challenging problem. Transition metal nitride films, due to their wide applications in semiconductor processing, e.g., in areas like diffusion barrier materials, have been extensively studied. However, the knowledge about detailed surface nitride chemistry has been relatively scarce. Here, we report on surface reaction studies of TaN CVD precursors carried out by using high-resolution XPS, TDS, and NEXAFS techniques. The precursors studied include some custom-synthesized compounds (@supert@BuN)Ta(NEt@sub2@)@sub3@ and (@supert@BuN)Ta(NEtMe)@sub3@ that are characterized by the presence of absence of @beta@-methyl groups and by whether singly or doubly-bonded nitrogen being attached to a Ta atom. The @beta@-methyl group is known to influence the decomposition pathway of amido group, which in turn can determine the amount of carbon being incorporated into the films. XPS data show that the formation of nitride species starts at surface temperatures higher than 500 K and, as the reaction proceeds, graphic carbons are incorporated into TaN species and significant Ta oxides are formed due to favorable exothermicity. During the course of surface decomposition, multimass TDS data point to the evolution of hydrogen, hydrocarbon species, and possibly acetonitrile. Oxidation resistance and degree of carbon incorporation are found to vary with the precursors. Based on these results, possible reaction mechanisms and the effect of precursor are to be discussed.

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