Wednesday Morning, November 17, 2004

Surface Science
Room 210C - Session SS2-WeM
Semiconductor Surface and Interface Structure

Moderator: A.A. Baski, Virginia Commonwealth University

8:20am **SS2-WeM1 Atomic Structure Determination of @beta@-SiC(001)-(3x2): Experiment and Calculations***, A. Tejeda,* Universidad Autonoma de Madrid, Spain*; D. Dunham,* Northern Illinois Univ.*; F.J. Garcia de Abajo,* CSIC-UPV/EHU and DIPC, Spain*; J.D. Denlinger, E. Rotenberg,* Ernest Orlando Lawrence Berkeley National Lab*; **E.G. Michel,*** Univ. Autonoma de Madrid, Spain*; P. Soukiassian,* Commissariat a l'Energie Atomique and Northern Illinois Univ.

Silicon carbide is a IV-IV compound wide band-gap semiconductor with multiple technological applications. The structure of the Si-rich 3C-SiC(001)-(3x2) surface reconstruction is determined using soft x-ray photoelectron diffraction. Photoelectrons are detected along a full hemispherical sector for different photon energies. The experimental intensity modulations were compared in this work with the results of a suitable scattering formalism that simulates the measured PED by modeling the structure of the last atomic layers. A spherical-wave multiple-scattering cluster formalism was used to reproduce the data and discern the correct surface structure of Si-rich 3C-SiC(001)-(3x2), obtained from a systematic search between the models proposed in the literature. The favored model is a modified version of the two-adlayer asymmetric dimer model (TAADM). An R-factor analysis has been employed to refine this model. We determine the interlayer spacings of the last six atomic layers and find a corrugation of 0.25 Å for the atoms in the outermost dimer. Atoms in the layer underneath dimerize as well, with alternating long and short bond lengths. The long-and-short alternateness between dimer bond lengths explains the top dimmer asymmetry along one single direction. The dimerization takes place through lateral relaxation, without large vertical distortions. The third atomic layer is also dimerized, with a dimer bond length of 2.43 Å. We conclude our results, together with STM and GIXRD experiments, converge in a unifying model for the 3C-SiC(001)-(3x2) surface.

8:40am **SS2-WeM2 Identification of Si and Ge on the Hydrogen-Terminated Ge/Si(001) Surfaces for Observation of Intermixing***, **Y. Fujikawa,** A. Kuwano, M. Kawashima, Y. Yamada-Takamura, T. Nagao, T. Sakurai,* Tohoku University, Japan

Control of the local composition of SiGe films in an atomic level is of great technological importance for designing the SiGe nanodevices. Intermixing effect between Si and Ge is the key issue to achieve precise composition control at the surface layer. It has been known that hydrogen-rich condition at ~300 degree C induces segregation of Si to the surface layer on the Ge covered Si(001) surface, while Ge prefers to stay at the surface layer without hydrogen@footnote 1@. This result implies that the hydrogen-annealing treatment is a useful method to control the composition of SiGe surface layer. We investigated the hydrogen-terminated Ge/Si(001) surface using STM to find that Ge-H sites are imaged as brighter protrusions in comparison with Si-H sites under the empty-state imaging condition. This effect is similar to the case of Cl-terminated Ge/Si(001) surface, which was observed recently@footnote 2@. Si-H and Ge-H sites on the hydrogen-terminated Ge/Si(001) with a Ge coverage of 1.5 ML were resolved successfully using this empty-state imaging condition to study the atomic process of intermixing. Furthermore, it turned out that the Si segregation by the hydrogen-annealing produces significantly bright features beside the dimer-row vacancies (DVLs), in addition to the features coming from Ge-H and Si-H sites. This feature can be attributed to the broken rebonded structure inside the DVL, which contributes the re-adjustment of the surface strain which is modified by the Si segregation. @FootnoteText@ @footnote 1@ Rudkevich et al., Phys. Rev. Lett. 81, 3467 (1998).@footnote 2@ Lin et al., Phys. Rev. Lett. 90, 046102 (2003).

9:00am **SS2-WeM3 The Surface of Silicon-on-Insulator: Structure, Stress, and Three-Dimensional Nanocrystals***, **M. Lagally**,* University of Wisconsin-Madison **INVITED**

Future generations of silicon devices will require approaches beyond the conventional in terms of both fabrication and characterization. In particular, instead of bulk Si, most devices will use silicon-on-insulator (SOI) or variants, such as strained-Si-on-insulator (sSOI), SiGe-on-insulator (SGOI), Si-on sapphire (SOS), and so forth, where in all cases a very thin crystalline layer of Si or SiGe is bound to an oxide or other insulator. Whereas the potential technological value of these materials is without question, what roles do the vacuum-Si and oxide-Si interfaces play? Is there anything interesting that has not already been discovered in the many years in which Si surfaces have been studied? We describe some interesting behaviors. Most important is the presence of strain and the essential instability of the very thin crystalline layer (called the template layer) resting on an oxide. Under appropriate conditions the template layer can dewet, agglomerate, and self-organize into an array of Si nanocrystals. Using LEEM, we observe this process and, with the help of first-principles total-energy calculations, we provide a quantitative understanding of this pattern formation and show how addition of Ge affects the energies and hence the pattern. We have been able to image the surface of SOI with STM, providing insights into the surface structure. Growth of heteroepitaxial films on SOI brings with it unique defect generation mechanisms that are associated with the Si-oxide interface, and a bending of the template that is counterintuitive. We fabricate thin membranes and free-standing structures to investigate the effect of added uniaxial stress on adatom diffusion and the nucleation and coarsening of 2D and 3D structures on this surface. Aspects of the work are supported by NSF, DARPA, ONR, and DOE.

9:40am **SS2-WeM5 Si Epitaxial Growth on Br-Si(100): How Steric Repulsive Interactions Dictate Overlayer Development***, **G.J. Xu**[1], J.H. Weaver,* University of Illinois at Urbana-Champaign

Scanning tunneling microscopy results show the consequences of Si adatom deposition onto Br-saturated Si(100)-(2x1). Those adatoms undergo an exchange reaction with Br but they are immobile at room temperature. In the low coverage regime, annealing to 650 K leads to dimerization, limited ordering, and the formation of short Si chains. Adatom capture by those chains produces features of even and odd numbers of atoms. Annealing at 700 K eliminates the odd chains, but diffusion is highly constrained by Br site blocking. With increased Si coverage, there is further nucleation of chains and chain growth. The local patterning of the Si chains reveals the influence of the strong steric repulsive interactions of Br as out-of-phase structures were favored over in-phase structures around any given chain. Eventually, those interactions favor adlayer (3x2) patches rather than (2x1) islands. Second layer chains appear after the deposition of ~0.3 ML, with layer-2 nucleation at antiphase domain boundaries of layer-1. Bromine loss was observed, even at 650 K, and it is probably tied to the dynamics of atom exchange involved with Si diffusion on a saturated surface.

10:00am **SS2-WeM6 Vacancy Induced Nano-Wire Structure of Ga@sub 2@Se@sub 3@ on Si(100)***, **T. Ohta**, D.A. Schmidt, C.Y. Lu, Q. Yu, M.A. Olmstead, F.S. Ohuchi,* University of Washington

We report formation of nano-wire structure of gallium-selenide (Ga@sub 2@Se@sub 3@) grown on arsenic terminated silicon (Si) (100). Ga@sub 2@Se@sub 3@ crystallizes into a defected zinc-blende structure with every third of the Ga site vacant. Vacancies are necessary to maintain charge neutrality in the crystal, and are responsible for its highly anisotropic electrical and optical properties by ordering into line geometry. Scanning tunneling microscopy (STM) revealed that wire structure is two-unit-cell-wide with the separation between wires of about three-unit cell, and its direction is influenced by alternating symmetry of the initial substrate. We will discuss its atomic structure, evolution of its initial growth and the interface structure between Ga@sub 2@Se@sub 3@ and Si, based on our recent investigation using STM and core-level photoemission spectroscopy (PES). It is shown that the formation of the wire structure is strongly related to the ordering of structural vacancies, and we will present its growth model. This formation mechanism is unique to the prevalence of structural vacancies incorporated in Ga@sub 2@Se@sub 3@, unlike other nano-structure formation mechanisms driven by defects or strain, such as for InAs nanodots on GaAs or SiGe clusters on Si. This work is supported by NSF Grant DMR 0102427 and M. J. Murdock Charitable Trust. T. O. further acknowledges support from University Initiative Fund of the University of Washington, and D. A. S., UW-PNNL Joint Institute for Nanoscience research award.

10:20am **SS2-WeM7 STM Study of Silicon Surfaces at P-N Junctions Prepared by Low-Temperature Processing***, **T.-C. Shen,*** Utah State University*; J.S. Kline, J.R. Tucker,* University of Illinois at Urbana-Champaign

Dopant distribution at p-n junctions has been extensively studied by many techniques. Recent advance of electron devices further demands a thorough understanding and precise control of the dopant behavior at nanometer scale. Feenstra et al. pioneered the technique of cross-sectional

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

STM to image the p- and n-type GaAs interface. To examine planar p-n junctions in Si, conventional high temperature surface preparation in ultrahigh vacuum is not suitable due to enhanced dopant diffusion and desorption. In this presentation, we report some of our experimental findings based on a previously developed low-temperature surface preparation technique involving 300eV Ar ion sputtering and 600-700°C annealing. The B-doped substrates used in this work are either at an impurity level of 3x10@super 17@ cm@super -3@ or 1x10@super 19@cm@super -3@. N-type patterns are fabricated by implanting 40-50 keV As ions at a dose of 1x10@super 15@cm@super -2@ into the B-doped substrates. The atomically clean and flat surfaces prepared at low temperatures allow us to obtain atom-resolving images both in the As-implanted region and the B-doped substrate as well as their original interface. We observe for the first time that heavily B-doped substrates lead to c(4x4) patterns on the surface the same as the result of diborane exposure. When terminating the surface with H, we find that the dangling bonds in the As-region are much brighter than those on the substrate. More c(4x4) regions and less C and H-induced clustering are observed in the As region. Surface topography at different annealing conditions, the role of dopant atoms in the diffusion of other impurities and their electronic effect will be discussed. This work is supported by DARPA-QuIST program under ARO contract DAAD 19-01-1-0324.

10:40am **SS2-WeM8 Hydrogen Interaction with a Si(113)-3x2 Surface***, **M. Yoshimura**, K. Mamiya, K. Ueda,* Toyota Technological Institute, Japan

Since the Si(113) surface is thermally stable and has a low energy compared to that of the low-index surfaces such as Si(111) and Si(001), it is expected to a good substrate for epitaxy in semiconductor technology. The clean surface reconstructs into a 3 x 2 superstructure consisting of pentamers and adatoms, as was proposed by Dabrowski et al.@footnote 1@ Each 3 x 2 cells contain a subsurface interstitial located below one of the tetramers, which lowers the total surface energy. On the other hand, hydrogen termination is one of important techniques in the silicon-based device processes. However, hydrogen interaction with the Si(113) has been studied only by spectroscopic measurements such as electron energy loss spectroscopy (EELS)@footnote 2@. Here, we report ultrahigh vacuum scanning tunneling microscopy (UHV-STM) study of the atomic hydrogen adsorption onto the clean Si(113)-3 x 2 surface on an atomic scale. A Si(113) surface was cleaned by a conventional procedure and was exposed at room temperature to atomic hydrogen by cracking of hydrogen molecules using a hot tungsten filament. After 10 L exposure, the reduction in the density of states around Fermi level was confirmed by scanning tunneling spectroscopy (STS). STM images revealed clearly that some adatoms were missing and some pentamers changed their image contrast, probably due to hydrogen adsorption at the surface dangling bonds of the corresponding sites. The clustering was not observed up to this exposure level. Based on the results of STM/STS together with low-energy electron diffraction (LEED), we discuss the initial adsorption processes of atomic hydrogen on Si(113)-3x2 at an atomistic level. @FootnoteText@ @footnote 1@ J. Dabrowski et al., Phys. Rev. Lett. 73 (1994) 1660.@footnote 2@ K. Jacobi and U. Meyer, Surf. Sci. 284 (1993) 223.

11:00am **SS2-WeM9 Application of the Simplified Bond-Hyperpolarizability Model to Bulk Second- and Third-Harmonic Generation in Semiconductors***, **H.J. Peng**, E.J. Adles, D.E. Aspnes,* North Carolina State University

Application of nonlinear optical (NLO) spectroscopies to the analysis of surfaces and buried interfaces of crystalline semiconductors requires an understanding of the contributions from the second- and third-harmonic generation (SHG, THG) from the bulk. THG is particularly relevant because for reasons of macroscopic symmetry THG is the lowest NLO effect that can be used to study the surfaces and interfaces of (001)Si, which underlies integrated-circuits technology. We show that the simplified bond-hyperpolarizability (SBHM) model that we previously developed to analyze surface and interface contributions to second- and fourth-harmonic generation data for Si provides an accurate description of bulk THG of Si with no adjustable parameters beyond amplitude scaling. The SHG contribution, which is nominally forbidden in Si, can be evaluated from the known linear-optic response and, contrary to some speculation, is found to be negligible for this material. These results are expected to be applicable to other semiconductors as well, thereby simplifying the analysis of surfaces and interfaces by NLO techniques.

11:20am **SS2-WeM10 Second Harmonic Generation from Metallic Quantum Wells on Si(111) Surfaces***, **K. Pedersen**, T.G. Pedersen,* Aalborg University, Denmark*; P. Morgen,* SDU Odense University, Denmark

Optical second harmonic generation (SHG) from materials with bulk centrosymmetry such as metals and a number of elemental semiconductors is surface and interface sensitive due to the lack of electric dipole contributions to second-order nonlinearities in the bulk of such materials. Thin films on a substrate, having two dissimilar boundaries, are thus expected to be interesting objects for SHG studies. The buried interface can be reached even through 50 to 100 layers of metal but the interface signal appears coherently added to contributions from the free surface. Resonant electronic transitions that may appear in SHG spectroscopy can thus be localized either at the free surface or at the buried interface. Under proper growth conditions thin metallic films on semiconductors form crystalline layers showing sharp quantum well (QW) levels in photoemission spectroscopy. In SHG the discrete QW levels result in oscillating signals as the system passes through a series of resonant transitions between occupied and empty states for growing film thickness. In the present work electronic transitions at the buried interface are identified through the dispersion of quantum well resonances seen with SHG. Recordings of SHG from a wedge shaped Ag film (0-50 layers) grown on Si(111)7x7 surface show that resonances disperse toward lover thickness for growing photon energy. Shifts or breaks in dispersion curves appear when the phase of the interface signal changes at resonant electronic transitions. In addition to expected transitions near critical points of bulk Si an interface resonance is found between the two lowest critical points of bulk Si.

11:40am **SS2-WeM11 Spectroscopic Second Harmonic Generation on Hydrogenated Amorphous Silicon Surfaces and Interfaces***, **C.M. Leewis**, J.J.H. Gielis, I.M.P. Aarts, M.C.M. van de Sanden, W.M.M. Kessels,* Eindhoven University of Technology, The Netherlands

Optical Second Harmonic Generation (SHG) is applied on hydrogenated amorphous silicon (a-Si:H) films on fused silica substrates to investigate the presence of surface and buried interface dangling bonds. For amorphous material, e.g. a-Si:H, the SHG technique is surface-specific and therefore originates from both the film surface and the film-substrate interface. The origin of the second harmonic signal can be due to dangling bonds and strained bonds. In addition, optical interference effects can enhance the signal for certain wavelength-film thickness combinations. The technique is applied both ex situ, and in situ in a UHV setup on hot wire grown films. An incident polarization scan is performed for both p- and s-polarized SHG radiation while SHG is also measured while rotating the sample around the axis normal to the substrate. It has been established that the SHG can be described by the infinity-m symmetry class, which is in agreement with the amorphous nature of the material. In situ spectroscopic scans are performed with a probe photon energy in the range 1.0-1.6 eV for different polarizations. These scans are in agreement with ex situ scans on plasma deposited a-Si:H. The observed resonant peaks correspond possibly to surface and interface dangling bond states@footnote 1@. The presence of dangling bonds is investigated with real time measurements. These experiments during film growth have already shown that the SHG intensity increases instantly when growth is started, and gradually decreases during further growth. In addition, it is shown that the maximum SHG intensity increases for increasing substrate deposition temperatures in the range 520-720 K. The consequences for a possible surface and interface concentration of dangling bonds will be discussed. @FootnoteText@ @footnote 1@Pedersen et al., Phys. Rev. B 52, R2277 (1995).

Author Index

Bold page numbers indicate presenter

— A —
Aarts, I.M.P.: SS2-WeM11, 2
Adles, E.J.: SS2-WeM9, 2
Aspnes, D.E.: SS2-WeM9, 2
— D —
Denlinger, J.D.: SS2-WeM1, 1
Dunham, D.: SS2-WeM1, 1
— F —
Fujikawa, Y.: SS2-WeM2, **1**
— G —
Garcia de Abajo, F.J.: SS2-WeM1, 1
Gielis, J.J.H.: SS2-WeM11, 2
— K —
Kawashima, M.: SS2-WeM2, 1
Kessels, W.M.M.: SS2-WeM11, 2
Kline, J.S.: SS2-WeM7, 1
Kuwano, A.: SS2-WeM2, 1
— L —
Lagally, M.: SS2-WeM3, **1**
Leewis, C.M.: SS2-WeM11, **2**
Lu, C.Y.: SS2-WeM6, 1
— M —
Mamiya, K.: SS2-WeM8, 2
Michel, E.G.: SS2-WeM1, **1**
Morgen, P.: SS2-WeM10, 2
— N —
Nagao, T.: SS2-WeM2, 1
— O —
Ohta, T.: SS2-WeM6, **1**
Ohuchi, F.S.: SS2-WeM6, 1
Olmstead, M.A.: SS2-WeM6, 1
— P —
Pedersen, K.: SS2-WeM10, **2**
Pedersen, T.G.: SS2-WeM10, 2
Peng, H.J.: SS2-WeM9, **2**
— R —
Rotenberg, E.: SS2-WeM1, 1
— S —
Sakurai, T.: SS2-WeM2, 1
Schmidt, D.A.: SS2-WeM6, 1
Shen, T.-C.: SS2-WeM7, **1**
Soukiassian, P.: SS2-WeM1, 1
— T —
Tejeda, A.: SS2-WeM1, 1
Tucker, J.R.: SS2-WeM7, 1
— U —
Ueda, K.: SS2-WeM8, 2
— V —
van de Sanden, M.C.M.: SS2-WeM11, 2
— W —
Weaver, J.H.: SS2-WeM5, 1
— X —
Xu, G.J.: SS2-WeM5, **1**
— Y —
Yamada-Takamura, Y.: SS2-WeM2, 1
Yoshimura, M.: SS2-WeM8, **2**
Yu, Q.: SS2-WeM6, 1