

Thursday Morning, November 7, 2002

Surface Science

Room: C-110 - Session SS+EL-ThM

Structure of Semiconductor Surfaces & Interfaces

Moderator: C.J. Palmstrom, University of Minnesota

8:20am **SS+EL-ThM1 Strain Control of the Ge(105) Surface via Hydrogen Adsorption**, Y. Fujikawa, M. Kawashima, T. Nagao, T. Sakurai, Tohoku University, Japan, M.G. Lagally, University of Wisconsin-Madison

Controlling the size and shape of Ge quantum dots formed on the Si(001) substrate is of great technological importance for their potential application in future semiconductor devices. Surfactant effects on this system are regarded as a promising method to achieve the controlled growth of quantum dots. Among them, hydrogen adsorption, which has been studied intensively, is known to suppress the formation of Ge "huts", pyramidal nanocrystals bounded by four Ge{105} facets.¹ We have investigated hydrogen adsorption on a Ge(105) surface formed on a Si(105) substrate using STM to elucidate the role of surface strain on the stability of Ge(105) under hydrogen-adsorption conditions. The STM images of Ge(105) surfaces with adsorbed hydrogen atoms are understood based on the newly-established atomic structure of Ge(105).² We observe the stability of hydrogen-covered Ge(105) for different amounts of Ge initially deposited on the Si(105) surface. We find that hydrogen adsorption on Ge(105) surfaces formed from deposited amounts of Ge less than 1.5 ML makes the surface remarkably unstable and results in the formation of local defects. This fact indicates that hydrogen adsorption on Ge(105) increases the surface strain by arresting the strain-relief mechanism that would ordinarily occur on clean Ge(105) with the formation of sp²-hybridized dimers. Thus, the formation of Ge(105) will be unfavorable and suppressed in the presence of adsorbed hydrogen. This work is supported by NSF.

¹ Kahng et al., Phys. Rev. Lett. 80, 4931 (1998).

² Fujikawa et al., Phys. Rev. Lett. 88, 176101 (2001).

8:40am **SS+EL-ThM2 A LEEM Study of the Ge(001)-(2x1)-(1x1) Phase Transition; Domain Wall Proliferation and Dimer Break-up**, E. van Vroonhoven, H.J.W. Zandvliet, B. Poelsema, University of Twente, The Netherlands

The Ge(001) surface exhibits two phase transitions. At low temperatures it is c(4x2) reconstructed, evolving with increasing temperature into (2x1). The origin of the reconstruction is dimerization of the surface: the number of dangling bonds is reduced from two per surface atom, for a bulk terminated surface, to only one. In the c(4x2) phase the dimers are buckled in an anti-symmetric way; in the (2x1) phase the dimers rapidly switch between the two buckled orientations and appear symmetric. Due to the diamond structure of Ge, the dimer rows on neighboring terraces are rotated by 90°. At high temperature the (2x1) phase disappears and the (1x1) phase emerges. Two conflicting models have been proposed in literature. One model suggests that this phase transition is driven by vacancy pair creation and dimer break-up on the Ge(001) surface. The other claims that the phase transition involves (2x1) domain wall (step) proliferation rather than dimer break-up. Our results demonstrate that domain wall proliferation sets in around 950 K, leading to a complete loss of contrast in LEEM around 1050 K. The dimers, however, remain clearly visible up to about 1130 K. The dimer concentration is a strong function of the substrate temperature between 1030 and 1130 K. Our combined microscopy and diffraction data are only consistent with the first model. It is even possible for the first time to directly extract the free energy gain of dimerization, being 1.6 eV per pair. This value compares perfectly with calculations performed for silicon after scaling with the melting temperature. We estimate the temperature to be accurate with ± 25 K and thus the dimerization energy with ± 5%.

9:00am **SS+EL-ThM3 Encapsulation of SiGe Quantum Wells and Quantum Dots**, G.G. Jernigan, P.E. Thompson, US Naval Research Laboratory

Semiconductor device characteristics are dependent on the chemical and structural properties of the electrical interface. As such, we are interested in SiGe quantum wells and quantum dots grown in Si. Heterojunctions between Si / SiGe / Si are chemically smeared due to Ge segregation, but little is known about the structural nature of the heterojunctions. We will present an STM study of the encapsulation of a Si_{0.8}Ge_{0.2} alloy grown in Si at 500, 650, and 800 °C. Alloy deposition induces a rougher morphology than the initial Si surface. Intermixing of Ge from the alloy with the Si substrate is observed to happen immediately to produce a rough surface. The amount of intermixing increases with increasing growth temperature,

and at 800 °C the surface roughness exceeds the thickness of deposited alloy. After intermixing, Ge segregates out from the alloy, and the surface Ge leads to an island growth mechanism, which further increases the surface roughness. At 500, 650, and 800 °C the alloy surfaces obtain a steady-state value for surface roughness, which has been characterized as 2D planar, rippled, and huttled, respectively. Encapsulation of the alloy layer with Si attempts to restore a smooth morphology. At 800 °C where the height of the huts are ~40 nm, a 5 nm Si layer reduced the hut height to ~10 nm, and after 20 nm of Si, the huts are gone. Remnants of the underlying alloy morphology can still be seen on the surface in the form of square pits where material did not fill in between the huts. For lower growth temperatures, less Si is needed to reduce the surface roughness, and square pits are still observed from the underlying alloy. The square pits arise from Ge segregation modifying the S_A and S_B step-edge sticking coefficient of Si to produce equal sized S_A and S_B terraces. A structural model for the heterointerfaces based on the STM observations will be presented.

9:20am **SS+EL-ThM4 First Atomic-Resolution Ultrahigh Vacuum Scanning Tunneling Microscopy Study of GaSe/Si(111) Ultrathin Films**, T. Ohta, A. Klust, J.A. Adams, Q. Yu, M.A. Olmstead, F.S. Ohuchi, University of Washington

Gallium-selenide thin films deposited on Si(111) are of increasing interest for applications, both in their own right as optoelectronic structures, and as non-reactive, low surface energy, high band gap buffer layers for subsequent nanostructure formation. Gallium selenide crystallizes into two crystal structures, layered GaSe and cubic Ga₂Se₃ with bandgaps of 2.0 and 2.6eV, respectively. Crystal structure and stoichiometry of the deposited Ga_xSe_y can be controlled by the substrate temperature during deposition. We present the first atomic-resolution ultrahigh vacuum scanning probe microscopy study of GaSe/Si(111) ultrathin films. When GaSe thin films are deposited at substrate temperature 520°C, atomically flat surfaces consisting of a single molecular layer of GaSe with altered step structures of 7*7-Si(111) were observed. These surfaces have no dangling bonds to react with residual gases, or to provide nucleation sites for subsequent growth. We also observed occasional point defects causing long-range alterations of the local band bending, but no sharp states revealed by the tunneling spectroscopy. At lower substrate temperatures, Ga₂Se₃ multilayers with flat surface and triangle features with 3-4nm sides were formed. Height difference of the atomic steps suggests that the multilayers have a cubic structure. These triangles are likely associated with Ga or Se vacancies in the Ga₂Se₃.

This work was partially supported by the M. J. Murdock Charitable Trust and NSF Grant DMR 0102427.

9:40am **SS+EL-ThM5 Electronic and Structural Properties of Aluminum Selenide Ultrathin Film on Si(111)**, J.A. Adams, A.A. Bostwick, T. Ohta, A. Klust, University of Washington, E. Rotenberg, Advanced Light Source, F.S. Ohuchi, M.A. Olmstead, University of Washington

The wide band gaps of aluminum selenide and gallium selenide make them appealing candidates for blue-green opto-electronics, and they are closely lattice matched to silicon making them compatible in silicon-based structures and devices. However, very little is known about the properties of aluminum selenide heteroepitaxial films. Bulk aluminum selenide, a defected wurtzite structure, has a 3.1 eV band gap, and its hexagonal lattice constant is about 1.3% larger than Si(111). Unlike gallium selenide, which is stable in both layered GaSe and defected zincblende Ga₂Se₃ structures, layered AlSe has not been reported in either bulk or thin film form. We investigated varying thicknesses of ultrathin films of aluminum selenide grown epitaxially on Si(111) including sub-monolayer growth, a single bilayer, and the subsequent initial stages of growth on the bilayer. The AlSe/Si interface forms a bilayer structure similar to GaSe-terminated Si, although the temperatures for bilayer formation and for Se-evaporation from the film are higher for AlSe than for GaSe. The reactivity of the AlSe terminated Si(111) surface with both residual gases and for subsequent film growth is much higher than that of GaSe. Further deposition of aluminum selenide produces films that resemble the bulk stoichiometry Al₂Se₃. Electronic band-structure for AlSe/Si was investigated using angle resolved photoelectron spectroscopy (ARPES). Unlike GaSe/Si, the AlSe bilayer appears to have a true surface state. Si-Al bond lengths and Al-Se bond lengths were measured by energy dependent photoelectron diffraction (EDPD). Initial results indicate that the Al-Si bond is 8% larger than in Al/Si(111)-(√3x√3). Heterostructures of AlSe/GaSe on Si(111) will also be discussed. Funded by NSF Grant DMR-0102427.

10:00am **SS+EL-ThM6 Ga Surface Segregation in ErAs (100)/GaAs (100)**, *H.K. Jeong, T. Komesu, C.-S. Yang, P.A. Dowben*, University of Nebraska-Lincoln, *B.D. Schultz, C.J. Palmstrom*, University of Minnesota

Surface segregation has now been characterized by angle resolved x-ray photoemission for NiMnSb, a variety of perovskites, and a number of binary alloys. Using angle-resolved x-ray photoemission spectroscopy (ARXPS), the surface composition of the sample can be roughly established since the effective probing depth is shorter at large emission angles with respect to the surface normal. Epitaxial thin films of the rare earth pnictide ErAs(100) can be grown on GaAs(100), but at elevated temperatures the ErAs film degrades. Ga segregation through the ErAs to the surface has been identified by angle-resolved X-ray photoemission spectroscopy, following extensive annealing. The angle-resolved XPS data indicates that the segregation of Ga is extensive throughout the ErAs thin film and is not restricted just to the surface layer.

10:20am **SS+EL-ThM7 Absolute Orientation-Dependent TiN(001) Step Energies from Two-Dimensional Equilibrium Island Shape and Coarsening Measurements on Epitaxial TiN(001) Layers**, *S. Kodambaka, S.V. Khare, V. Petrova*, University of Illinois, *A. Vaillionis*, Stanford University, *I. Petrov, J.E. Greene*, University of Illinois

In situ high-temperature (1030-1185 K) scanning tunneling microscopy was used to determine the equilibrium shapes of two-dimensional TiN vacancy islands on atomically-smooth terraces of epitaxial TiN(001) layers. Inverse Legendre transformations of the equilibrium island shapes yield relative step energies as a function of step orientation within an orientation-independent scale factor λ , the equilibrium chemical potential of the island per unit TiN molecular area. We then use quantitative TiN(001) adatom island coarsening measurements to determine λ and, hence, absolute orientation-dependent step energies β and step stiffnesses β_0 . For $\langle 110 \rangle$ and $\langle 100 \rangle$ steps on TiN(001), we obtain: $\beta_{110} = 0.21 \pm 0.05$ eV/Å, $\beta_{100} = 0.25 \pm 0.05$ eV/Å, $\beta_{110} = 0.9 \pm 0.2$ eV/Å, and $\beta_{100} = 0.07 \pm 0.02$ eV/Å. From the β values, we calculate kink formation energies $\epsilon_{k10} = 0.40 \pm 0.2$ eV and $\epsilon_{k100} = 0.11 \pm 0.1$ eV based on the unrestricted terrace-step-kink model.

10:40am **SS+EL-ThM8 Scanning Force Microscopy Measurements on Ionic Crystals at Low Temperatures and Comparison to Atomistic Simulations**, *R. Hoffmann, M.A. Lantz*, University of Basel, Switzerland, *L.N. Kantorovich*, University College London, UK, *A. Baratoff, H.J. Hug*, University of Basel, Switzerland, *A.L. Shluger*, University College London, UK, *H.-J. Güntherodt*, University of Basel, Switzerland

Alkali halide surfaces were the first insulating materials to be imaged by scanning force microscopy (SFM) with true atomic resolution. Although atomic resolution images on alkali halides have been obtained by several groups, the tip-sample interaction above specific sites has so far been studied only theoretically.¹ Knowing this interaction force provides insight into atomic resolution image mechanisms and allows to study bonding interactions on a surface on the atomic scale. Recently, site-specific force-distance experiments have been performed for the first time at low temperatures on the Si(111) 7x7 surface.² Here we report similar measurements on the KBr (001) and the NaCl (001) surface in which we study the interaction forces and the imaging mechanism. The short-range forces have been calculated using atomistic simulations. The magnitude of the calculated forces agrees well with the experimental data, although for KBr the calculated corrugation is larger than the measured one even when the long-range forces are included. For NaCl also the corrugation is in good agreement to the experiment.

¹ L. N. Kantorovich et al. Surf. Sci. 445, 283 (2000)

² M. A. Lantz et al. Science 291, 2580 (2001)

11:00am **SS+EL-ThM9 Core-level Spectroscopy Study of the Clean c(4x2) and the Hydrogenated 2x1-H Phases on the 3C-SiC(001) Surface**, *L.S.O. Johansson, S.M. Widstrand, K.O. Magnusson, M.I. Larsson*, Karlstad University, Sweden, *H.W. Yeom*, Yonsei University, Korea, *S. Hara, S. Yoshida*, AIST, Japan

We report a core-level spectroscopy investigation of the clean Si-terminated 3C-SiC(001)-c(4x2) surface and the hydrogenated 3C-SiC(001)2x1-H surface. The 2x1-H surface was formed by exposing the clean c(4x2) surface to excited hydrogen gas. Desorption of the hydrogen at 900° C led to the restoration of the c(4x2) periodicity. Higher hydrogen exposures led to the formation of diffuse 1x1 and mixed 3x1/2x1 phases, as observed by low-energy electron diffraction (LEED). This behaviour is remarkably similar to hydrogen adsorption on the Si(001)2x1 surface. Si 2p core-level spectra from the clean c(4x2) surface displayed the characteristic surface peak shifted by 1.4 eV to lower binding energy, which in previous studies has been attributed to Si adatoms on top of a Si-terminated surface.^{1,2} The formation of the 2x1-H surface lead to dramatic changes in the Si 2p lineshape, where the main surface components now appeared closer to the

bulk peak. Detailed decompositions of the spectra are presented and are discussed in relation to the suggested structural models for the c(4x2) surface^{3,4} and to previous core-level studies.^{1,5}

¹ M.L. Shek, Surf. Sci. 349, 317 (1996).

² A. Catellani, G. Galli, and F. Gygi, Appl. Phys. Lett. 72, 1902 (1998).

³ P. Soukiassian, F. Semond, L. Douillard, A. Mayne, G. Dujardin, L. Pizzagalli, and C. Joachim, Phys. Rev. Lett. 78, 907 (1997).

⁴ W. Lu, P. KrÄger, J. Pollmann, Phys. Rev. Lett. 81, 2292 (1998).

⁵ V. Yu. Aristov, H. Enriquez, V. Derycke, P. Soukiassian, G. Le Lay, C. Grupp, and A. Taleb-Ibrahimi, Phys. Rev. B 60, 16553 (1999).

11:20am **SS+EL-ThM10 The Anomalous Effective Surface Debye Temperature of ErAs(100)**, *T. Komesu, H.K. Jeong, P.A. Dowben*, University of Nebraska-Lincoln, *B.D. Schultz, C.J. Palmstrom*, University of Minnesota

We have recently explored the surface electronic structure of ErAs(100), as well as the compositionally stability, but the vibrational modes are a key contribution to both electronic structure and compositional stability. Consistent with a surface electronic structure different from the bulk, here we show that the surface vibrational modes are different from the bulk from our estimates of surface and bulk Debye temperature using LEED (low energy electron diffraction) and XPS (X-ray photoemission spectroscopy). This could contribute to the very large temperatures dependence of transport effects across ErAs interfaces.

11:40am **SS+EL-ThM11 CRN Models of Covalent Amorphous Materials and Their Interfaces**, *D. Yu, G.S. Hwang*, The University of Texas at Austin

Understanding the structural properties of covalent amorphous (semiconductor and dielectric) materials and their interfaces as well as defect-dopant dynamics in the disordered systems is an outstanding problem of great importance for microelectronic and optoelectronic applications. Significant advances in Continuous Random Network (CRN) models have made it possible to generate the amorphous and interface structures that are in good agreement with experiments. This further allows us to address the behaviors of defects and dopants in the disordered structures. In this talk we will present our newly developed CRN models and some recent results on i) the diffusion and clustering dynamics of vacancies and self-interstitials in a-Si and the amorphous-crystalline interface, ii) the structures of a very thin amorphous SiO₂ layer and its interfaces with Si, and iii) thermal stability of Si/Ge nanoclusters in SiO₂.

Authors Index

Bold page numbers indicate the presenter

— A —

Adams, J.A.: SS+EL-ThM4, 1; SS+EL-ThM5, **1**

— B —

Baratoff, A.: SS+EL-ThM8, 2

Bostwick, A.A.: SS+EL-ThM5, 1

— D —

Dowben, P.A.: SS+EL-ThM10, 2; SS+EL-ThM6, 2

— F —

Fujikawa, Y.: SS+EL-ThM1, **1**

— G —

Greene, J.E.: SS+EL-ThM7, 2

Güntherodt, H.-J.: SS+EL-ThM8, 2

— H —

Hara, S.: SS+EL-ThM9, 2

Hoffmann, R.: SS+EL-ThM8, **2**

Hug, H.J.: SS+EL-ThM8, 2

Hwang, G.S.: SS+EL-ThM11, 2

— J —

Jeong, H.K.: SS+EL-ThM10, 2; SS+EL-ThM6, **2**

Jernigan, G.G.: SS+EL-ThM3, **1**

Johansson, L.S.O.: SS+EL-ThM9, **2**

— K —

Kantorovich, L.N.: SS+EL-ThM8, 2

Kawashima, M.: SS+EL-ThM1, 1

Khare, S.V.: SS+EL-ThM7, 2

Klust, A.: SS+EL-ThM4, 1; SS+EL-ThM5, 1

Kodambaka, S.: SS+EL-ThM7, **2**

Komesu, T.: SS+EL-ThM10, **2**; SS+EL-ThM6, 2

— L —

Lagally, M.G.: SS+EL-ThM1, 1

Lantz, M.A.: SS+EL-ThM8, 2

Larsson, M.I.: SS+EL-ThM9, 2

— M —

Magnusson, K.O.: SS+EL-ThM9, 2

— N —

Nagao, T.: SS+EL-ThM1, 1

— O —

Ohta, T.: SS+EL-ThM4, **1**; SS+EL-ThM5, 1

Ohuchi, F.S.: SS+EL-ThM4, 1; SS+EL-ThM5, 1

Olmstead, M.A.: SS+EL-ThM4, 1; SS+EL-ThM5,

1

— P —

Palmstrom, C.J.: SS+EL-ThM10, 2; SS+EL-ThM6,

2

Petrov, I.: SS+EL-ThM7, 2

Petrova, V.: SS+EL-ThM7, 2

Poelsema, B.: SS+EL-ThM2, **1**

— R —

Rotenberg, E.: SS+EL-ThM5, 1

— S —

Sakurai, T.: SS+EL-ThM1, 1

Schultz, B.D.: SS+EL-ThM10, 2; SS+EL-ThM6, 2

Shluger, A.L.: SS+EL-ThM8, 2

— T —

Thompson, P.E.: SS+EL-ThM3, 1

— V —

Vailionis, A.: SS+EL-ThM7, 2

van Vroonhoven, E.: SS+EL-ThM2, 1

— W —

Widstrand, S.M.: SS+EL-ThM9, 2

— Y —

Yang, C.-S.: SS+EL-ThM6, 2

Yeom, H.W.: SS+EL-ThM9, 2

Yoshida, S.: SS+EL-ThM9, 2

Yu, D.: SS+EL-ThM11, **2**

Yu, Q.: SS+EL-ThM4, 1

— Z —

Zandvliet, H.J.W.: SS+EL-ThM2, 1