Surface Science
Room 210 - Session SS3-ThM

Surface and Interface Structure II

Moderator: A.P. Baddorf, Oak Ridge National Laboratory

8:20am **SS3-ThM1 Polar Oxide Surfaces, *M. Gajdardziska-Josifovska,*** University of Wisconsin, Milwaukee **INVITED**

The stability of polar oxide surfaces has long been a problematic question in surface science. A bulk terminated polar surface has an infinite surface energy because alternating layers of oppositely charged ions produce a large dipole moment perpendicular to the surface. Such a singularity presents many interesting questions ranging from the fundamental "Can polar oxide surfaces exist?" via the mechanistic "How can they get stabilized?" to the applied "Would they have unique and useful surface and interface properties?". Both theory and experiment have provided several contrary answers to the first two questions, and the last is largely unexplored. In the seventies, the problem was considered closed with consensus between theory and experiment that polar oxide surfaces can not exist but must facet into neutral planes to gain finite surface energy. In the nineties the problem was reopened with experimental discoveries of reconstructed polar oxide surfaces and with theoretical predictions of clean reconstructed surfaces based on the idea of smallest neutral building blocks. At present, there is disagreement between the few proposed and solved polar oxide surface structures, and the reconstruction mechanism is under construction. An additional controversy surrounds the 1x1 structure of polar oxide surfaces. Classical electrostatic approaches predict that such structures can exist only by adsorption of charged species, OH being the currently favored termination, but quantum mechanical approaches predict two dimensional surface metalization of the clean 1x1 surface. I will review the present state of knowledge, with illustrations from our multi-technique experimental studies of the polar MgO and NiO (111) surfaces and their neutral (100) and (110) counterparts. Our data favors the reconstruction mechanism at high temperatures, and the OH adsorption mechanism at lower temperatures.

9:00am **SS3-ThM3 Helium Atom Scattering Study of the Surface Structure and Dynamics of in situ Cleaved MgO(001) Single Crystals@footnote 1@, *J.G. Skofronick,*** Florida State University*; G. Benedek,* Dipartimento di Fisica dell'Universita'*; G. Brusdeylins, D. Schmicker, S. Schmidt, V. Senz, J.P. Toennies, F. Traeger, R. Vollmer,* Max-Planck-Institute fuer Stroemungsforschung, Germany

A high resolution helium atom scattering study on the surface structure and dynamics of in situ cleaved MgO(001) single crystals, under ultra high vacuum conditions, in both high symmetry directions, has been performed. The Rayleigh modes were observed over most of the reduced surface Brillouin zone; these results agree with previous measurements and theory. Two new modes at and near the zone boundary for the and the high symmetry directions are observed at 40 meV and 36 meV, respectively. A weak half order reconstruction is observed in diffraction scans in the direction. A suggested mechanism for the latter is given. Refined bound state resonance information, giving the energy levels of the laterally averaged He+MgO(001) surface potential are included. @FootnoteText@ @footnote 1@ Supported in part (JGS) by DOE Grant No. DE-FG02-97ER45635.

9:20am **SS3-ThM4 Molecular Beam Epitaxy-Scanning Tunneling Microscopy of Wurtzite GaN Thin Films, *Q.Z. Xue,*** *Q.K. Xue, S. Kuwano, K.F. Kelly, S. Nakayama, I.S.T. Tsong, T. Sakurai,* Tohoku University, Japan*; T. Ohno,* National Research Institute of Metals, Japan

Gallium nitride has been known for their enormous potential applications for optoelectronics devices operating in the spectral range from blue to ultraviolet. As the present application depends critically on controlled heteroepitaxy of GaN thin films, complete knowledge of its growth behavior and fundamental physical properties is highly desired to optimize its film growth and device applications. GaN can crystallize into both hexagonal and cubic forms, depending on the substrates and the growth conditions. And the hexagonal GaN has a further freedom in its film polarity, which has direct influence on its surface structure and growth process. In the present work, a systematic investigation of the growth and the surface reconstructions of the wurtzite GaN have been in-situ performed using molecular beam epitaxy (MBE) combined with scanning tunneling microscopy (STM) system. A two-step method is developed to prepare the 6H-SiC substrate, and the Ga-polar GaN(0001) and N-polar thin films are grown by plasma-assisted-MBE on the Si-polar and C-polar 6H-SiC respectively. Through the post-growth Ga-deposition, distinctly different series of surface reconstructions have been obtained on the films for each polarity, that is, on GaN(0001) surface, 1x1, 2x2, 4x4, @sr@7x@sr@7, 5x5, 5@sr@3x2@sr@13, 10x10 and 1x1-Ga fluid are formed, while on GaN(000-1) surface, 2x4, 6x6, 2@sr@7x2@sr@7 are observed. All these phases are Ga-rich, and no ordered N-rich phase has been observed. Based on the atomically-resolved STM images and first principles total energy calculations, we will show that the structures of these phases can be understood under Ga-adatom scheme. Since many of them are not satisfied with electron counting which is popular for the conventional semiconductors, we will document that stability of these phases can be interpreted by Peierls or Mott-Hubbard metal-insulator transitions due to the many-body effects.

9:40am **SS3-ThM5 One-Dimensional Noble Metal Growth on Si(5 5 12), *A.A. Baski,*** *K.M. Jones, K.M. Saoud,* Virginia Commonwealth University **INVITED**

Metal-semiconductor systems that exhibit 1-D growth have lately been of interest, particularly those that form nanometer-scale metal rows on a semiconductor. The recently discovered surface of Si(5 5 12) forms a single-domain reconstruction composed of row-like structures.@footnote 1@ providing a unique template for the growth of 1-D nanostructures. Our recent scanning tunneling microscopy (STM) studies show that noble metals such as Ag and Au deposited onto Si(5 5 12) and annealed indeed form a wide variety of well-ordered overlayer rows.@footnote 2@ At coverages below 0.25 monolayers (ML), both metals grow as monatomic rows with an inter-row spacing of ~5 nm. These metal rows preferentially nucleate along the more reactive Si tetramer rows of the surface reconstruction, leading to their growth in a periodic array. Scanning tunneling spectroscopy (STS) data show that Ag wires have a finite density of states at zero volts, indicating metallic behavior. At higher coverages and annealing temperatures, the underlying Si reconstruction is removed and the growth behavior of Ag and Au diverges. Up to ~0.5 ML, Ag forms sawtooth rows which evolve with coverage to an extremely well-ordered array of stepped double rows. Surprisingly, this phase has a significant band gap (1.25 V) compared to the clean Si surface (0.5 V). At comparable coverages and annealing temperatures, Au growth is usually less ordered; however, significantly elevated temperatures (>500C) lead to the creation of well-ordered facet planes [e.g. (7 7 15) and (225)]. For all coverages and annealing temperatures studied here, deposits of Au and Ag form row-like morphologies on the Si(5 5 12) surface, indicating the utility of this high-index surface as a template for the growth of 1-D nanostructures. @FootnoteText@ @footnote 1@ A. A. Baski, S. C. Erwin, and L. J. Whitman, Science 269, 1556 (1995). @footnote 2@ H.H. Song, K.M. Jones, and A.A. Baski, J. Vac. Sci. Technol. A 17(4), 1696 (1999).

10:20am **SS3-ThM7 Stability and Nuclear Formation of Si(111)-7x7 Structure as Determined from Charge Redistribution in Surface Layers, *K. Miyake,*** *T. Kaikoh, Y.J. Li,* University of Tsukuba, Japan*; R. Morita, M. Yamashita,* Hokkaido University, Japan*; H. Shigekawa,* University of Tsukuba, Japan

Reconstruction of the Si(111) surface has been extensively studied by various experiments as well as theoretical considerations. And 7x7 structure has been concluded to be the most stable phase on the Si(111) surface in equilibrium condition. In fact, the 7x7 phase is completed on the well annealed surface, and phase transition between high-temperature "1x1" and 7x7 phases was directly observed around the critical temperature by using scanning tunneling microscopy (STM). The dimer-adatomstacking-fault (DAS) structure proposed by Takayanagi et al., @footnote 1@ which is compatible with the experimental and theoretical results, is widely accepted as the model for the Si(111)-7x7 reconstructed surface structure. And atomic arrangement of the DAS structure in the static form is now well established. However, since the DAS structure involves few surface layers and is very complicated, dynamics of the surface, mechanism for the formation and stabilizing processes of the structure, has not yet been completely clarified, and is still attracting considerable attention. By considering the charge transfer from adatoms to rest atoms, we can analyze the structure of the dimer and stacking-fault (DS) layers in the Si(111) dimer-adatomstacking-fault (DAS) structure in a subunit level. In comparison with the modified model of Vanderbilt, corner holes with the completed DS structure in the second layer, completed corner hole, was confirmed to play a key role not only in the mechanism to stabilize the DAS structure, but also in the formation process of it; formation of the completed corner hole works as a rate limiting process for the growth of the DAS structure.@footnote 2@ This mechanism was

shown to be quite consistent with the experimental results which had been obtained by STM on the quenched and HBO@SUB 2@ molecules irradiated Si(111) surface.@footnote 3@ Phase transition from Si(111)-7x7 to the B-induced @sr@3x@sr@3 structure, and the structure near the step edge was analyzed in detail. @FootnoteText@ @footnote 1@K. Takayanagi et al, J. Vac. Sci. Technol., A 3 (1985) 1502. @footnote 2@K. Miyake et al., Surf. Sci., 429 (1999) 260-273. @footnote 3@K. Miyake et al., Jpn. J. Appl. Phys., 38 (1999) 3841.

10:40am **SS3-ThM8 First Principles Study of Cross-sectional Surface Structure of III-V Heterostructures**, ***S.-G. Kim***, Vanderbilt University; *S.C. Erwin, B.Z. Nosho, L.J. Whitman,* Naval Research Laboratory

Heterostructures of III-V semiconductors form the basis for a variety of devices. The performance of these multilayer structures is extremely sensitive to the thickness of the layers and the nature of the interfaces between them. As the layers are made thinner, a microscopic understanding of interface structure and chemistry will become increasingly important for optimizing device performance. The challenge is how best to achieve a complete microscopic characterization. We demonstrate the power of combining density-functional theory with experimental data from cross-sectional scanning tunneling microscopy (XSTM). We use first-principles computational methods to interpret XSTM images that we have obtained from the (110) cleavage surface of 6.1-Å III-V heterostructures. We begin by determining theoretically the fully relaxed geometry of cleaved InAs/GaSb superlattices, using the local-density approximation (LDA) to density-functional theory. To understand the relative importance of electronic vs. structural effects in the STM topography, we generate simulated XSTM images over the cross-sectional surface and compare with our measured XSTM images. We also focus on the role played by the specific interface bond type (In-Sb vs. Ga-As bonds) and show, for example, that XSTM can indeed be used reliably to identify the interface bond type. Finally, we study in detail the thermodynamics of defect formation due to diffusion across the interface; these theoretical predictions compare very favorably with our XSTM studies, and form the basis for further studies of the impact of interfacial disorder on device performance.

11:00am **SS3-ThM9 Reflectance Difference Spectroscopy of Mixed Arsenic-Rich Phases of Gallium Arsenide (001)**, ***D.C. Law***, *M.J. Begarney,* University of California, Los Angeles; *L. Li,* University of Wisconsin, Milwaukee; *C.H. Li, Q. Fu, R.F. Hicks,* University of California, Los Angeles

The relationship between the reflectance difference spectra and the atomic structure of arsenic-rich reconstructions of GaAs (001) has been investigated. Scanning tunneling micrographs reveal that a complex roughening process occurs as the surface structure changes with decreasing arsenic coverage from 1.75 to 0.75 monolayers (ML). With the loss of 0.1 ML of As, small pits, one bilayer in depth and having the same c(4x4) reconstruction as the top layer, form in the terraces. At the same time, gallium atoms are liberated to the surface, disrupting the c(4x4) ordering. With further arsenic loss, (2x4) domains nucleate and grow on top of the c(4x4). This underlying layer gradually decomposes into a metastable (2xn) phase, and finally into the (2x4). In the reflectance difference spectra, negative peaks at 2.25 and 2.8 eV correlate with the c(4x4)-like arsenic dimers. However, the intensity of the latter feature strongly depends on the presence of adsorbates, such as alkyl groups and gallium adatoms. A positive peak at 3.25 eV appears to be related to the (2xn) structure. Finally, the intensity of the positive peak at 2.9 eV is shown to be proportional to the density of (2x4)-type dimers.

11:20am **SS3-ThM10 Dynamics of the Flip-Flop Motion of Single Buckled Dimers of Si(100)**, ***H. Kenji***, University of Tsukuba, Japan; *M. Ryuji, Y. Mikio,* University of Hokkaido, Japan; *H. Shigekawa,* University of Tsukuba, Japan

We report the direct observation of the flip-flop motion of single buckled dimers of Si(100) in real space by hovering the tunneling tip of scanning tunneling microscope over a pre-selected atom of the flip-flopping dimers and measuring the tunneling current. By this method, the complete time trace of the flip-flop motion of single dimers can be obtained, and from it, any desired properties of the dynamics can be deduced. Each dynamical flip-flop event (up to 200,000) was clearly resolved, and the time trace of the tunneling current shows that the flip-flop motion is a switching between two stable configurations. A statistical analysis of the autocorrelation function elucidates that the flop-flop motion is a stochastic process described by a two level system. The influence of the local environment on the dynamics of the flop-flop motion can be mapped out by executing the measurements on neighboring dimers. We found that the details of the dynamics of the flip-flop motion differ from dimer to dimer and from domain to domain. The activation energy of the flip-flop motion differs significantly (measured 32 meV, estimated 110~ meV) for dimers in different domains. http://dora.ims.tsukuba.ac.jp

11:40am **SS3-ThM11 Molecular Dynamics Simulations of Energetic Silicon Cluster Deposition on Graphite (0001)**, ***R. Neuendorf***, *R.E. Palmer,* The University of Birmingham, UK; *R. Smith,* Loughborough University, UK

Microcanonical Molecular Dynamics (MD) Simulations using classical interaction potentials@footnote 1@ have been employed to study the deposition of small Silicon clusters (3 to 55 atoms / cluster) onto a graphite (0001) surface. The clusters have been deposited with kinetic energies from 1 eV up to 100 eV per atom. We find that the deposition behaviour can be divided into four different regimes: i) wetting of the substrate for small clusters at low deposition energies leading to the creation of monolayer high isalnds ii) soft landing of larger clusters at low deposition energies iii) implantation of the clusters into the substrate at high deposition energies, leading to "hole drilling" as also found in the case of metal cluster deposition.@footnote 2@ iv) a regime of more complicated behaviour at intermediate deposition energies. @FootnoteText@@footnote 1@S. J. Carroll, S. G. Hall, R. E. Palmer and R. Smith, Phys. Rev. Lett. 81(17), 3715 (1998) @footnote 2@S. J. Carroll, P. D. Nellist, R. E. Palmer, S. Hobday and R. Smith, Phys. Rev. Lett. 84(12), 2654 (2000).

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