Surface Science
Room 327 - Session SS2-TuA

Surfaces and Interfaces of Semiconductors and Compound Materials

Moderator: A.A. Baski, Virginia Commonwealth University

2:00pm **SS2-TuA1 The Plasmons of ErAs (100)**, *H.K. Jeong[1], T. Komesu, P.A. Dowben,* University of Nebraska, Lincoln*; B.D. Schultz, C.J. Palmstrom,* University of Minnesota

Momentum resolved inelastic electron energy loss has been exploited to measure the surface and bulk plasmons of ErAs(100). The effects of the electronic band structure is seen in the weak plasmon dispersion. This is consistent with heavy mass of the states near the Fermi energy in the experimentally determined band structure. The ratio of bulk and surface plasmon energy is roughly . In both Hg@footnote 1@ and ErAs,@footnote 2,3@ there are indications that the surface is significantly less metallic in character than the bulk. The behavior of the surface plasmon is related to the metallicity of the surface,@footnote 1@ so as with mercury thin films,@footnote 4@ the band structure of ErAs@footnote 2@ should strongly influence the surface and bulk plasmons. While there are a number of studies of the plasmons of simple metals, there are only a few studies of plamons in 4f-5d systems, such as those undertaken from Hg thin films.@footnote 4@ @FootnoteText@ @footnote 1@P.A. Dowben, Surface Science Reports 40, 151 (2000) @footnote 2@H.K. Jeong, Takashi Komesu, P.A. Dowben, B.D. Schultz and C.J. Palmstrom, Physics Letters A 302, 217 (2002) @footnote 3@Takashi Komesu, Hae-Kyung Jeong, Jaewu Choi, C.N. Borca, P.A. Dowben, A.G. Petukhov, B.D. Schultz, and C.J. Palmstrom, Physical Review B 67, art. no. 035104 (2003) @footnote 4@B.-O. Kim, G. Lee. E.W. Plummer, P.A. Dowben and A. Liebsch, Phys. Rev. B 52, 6057 (1995) .

2:20pm **SS2-TuA2 Growth Characteristics of ErAs Interlayers in Metal/Ga@sub 1-x@Al@sub x@As Heterostructures**, *B.D. Schultz, J.L. Hilton,* University of Minnesota*; K. Lüdge,* Technische Universität Berlin, Germany*; C.J. Palmstrom,* University of Minnesota

Properties of thin-film metal contacts grown on GaAs substrates have long been explored for electronic device applications. For modern spintronic applications, control of the interfacial properties and the reactions between ferromagnetic metals and semiconductors is important for optimizing spin dependent transport across these interfaces. ErAs interlayers, as thin as 5ML, have been used as diffusion barriers to drastically reduce interfacial reactions between Fe@sub 1-x@Co@sub x@ and GaAs for growth temperatures up to 225°C. However, surface segregation of both Ga and As are observed during the Fe@sub 1-x@Co@sub x@ growth and are related to the growth characteristics of the ErAs interlayer. In-situ scanning tunneling microscopy (STM) studies of ErAs films grown by molecular beam epitaxy (MBE) at 535°C show that ErAs initially nucleates as 3-4 monolayer high islands embedded within, rather than on top of, the GaAs(100) surface. These islands grow laterally in size until a complete uniform film is formed, whereby additional growth occurs in a layer-by-layer mode. X-ray photoemission spectroscopy (XPS) reveals both the presence of Ga and As atoms on the ErAs surface following the formation of a continuous layer and the continued segregation of these atoms to the surface during growth. The excess As atoms dissociate from the ErAs surface upon post-growth anneals above 450°C, and STM images show additional ordering of the ErAs surface following these anneals. Growth of ErAs on AlAs(200Å)/GaAs(100) heterostructures eliminates the segregation of Ga to the ErAs surface and results in no surface segregation of Al atoms. This paper reports on the control of the growth modes and the surface composition of ErAs interlayers grown by MBE on Ga@sub 1-x@Al@sub x@As(100) surfaces as characterized in-situ by reflection high-energy electron diffraction (RHEED), low-energy electron diffraction (LEED), STM, and XPS. Supported by ONR, DARPA, and NSF.

2:40pm **SS2-TuA3 Some Tricks in Photoelectron Diffraction Experiments for Structural Investigations at Surfaces**, *J. Osterwalder,* University of Zuerich, Switzerland **INVITED**

A certain class of structural problems at surfaces is readily accessible to investigation by x-ray photoelectron diffraction (XPD). This is usually the case for surface and interface geometries where core levels of specific atoms can be singled out from the XPD spectrum that are located below the topmost atomic layer. Other atoms are thus placed in a forward scattering geometry, and their relative positions are exposed by the associated forward focussing peaks. Prominent examples for such geometries are multilayer epitaxial film growth or intermixing phenomena at interfaces. Yet, there are important structural problems where such forward scattering geometries are often absent, like the internal structure of a single monolayer film, the registry of the film with respect to the substrate, or the adsorption geometries of atomic adsorbates. Over the last several years, various tricks have been devised that expand the scope of XPD to this kind of problems: -(i) For O/Rh(111) it has been demonstrated that the weak backscattering off the substrate atoms can reveal the exact bonding site of the atomic adsorbate. Prerequisites are a high atomic number of the substrate material and low temperature. -(ii) For well ordered monolayer films, the internal film structure can be determined by measuring first and higher order diffraction fringes. This is exemplified by the system of hexagonal boron nitride (h-BN) on Ni(111) as well as several alkali monolayer systems on Al surfaces. -(iii) When a monolayer film is strictly commensurate with the substrate and well ordered, the film structure and registry can be extracted from XPD data of a substrate signal, measured with and without the monolayer present on the surface. The resulting difference data sets need to be compared to simulated data resulting from multiple scattering model calculations. Again, the case in point is h-BN on Ni(111).

3:20pm **SS2-TuA5 Synthesis and Characterization of an Ordered Ge Overlayer and Pt@sub 2@Ge Compound on Pt(100)**, *T. Matsumoto, M. Batzill, C. Ho, B.E. Koel,* University of Southern California

A c(2 x 2)-Ge overlayer and Pt@sub 2@Ge compound were formed by Ge deposition and annealing to 600 K on Pt(100) and characterized by Na@super +@-ALISS, XPD, LEED and STM. STM topographs and LEED patterns indicate a c(2 x 2) structure after 0.5-ML Ge deposition or 1.5-ML Ge deposition with annealing to 600 K. ALISS was used to unambiguously distinguish between the c(2 x 2) overlayer and surface alloy phases. This technique showed Ge-scattering angular peaks assigned to a large separation of Ge atoms along the [011] azimuth corresponding to a c(2 x 2)-Ge overlayer after 0.5-ML Ge deposition. Following 1.5-ML Ge deposition and annealing to 600 K, a new Ge-scattering angular peak appeared that was assigned to scattering from third-layer Ge atoms, however, no second-layer Ge scattering peak was observed. This structure is consistent with a body-centered tetragonal Pt@sub 2@Ge layer surface alloy which has alternating c(2 x 2) Ge-Pt and (1 x 1)-Pt(100) layers. XPD results also support this structural model. Annealing these surfaces to 900 and 1200 K resulted in partial dissolution of Ge atoms deeply into the bulk. XPS was also used to characterize the chemical nature of Ge and Pt at these surfaces.

3:40pm **SS2-TuA6 New Structural Model for Au/Si(111)5x2 from First Principles**, *S.C. Erwin,* Naval Research Laboratory

Gold induces quasi-1D reconstructions on several faces of silicon, including (111), (557), and (995). These systems have been widely studied for their unusual electronic properties, but the lack of any accepted structural model has hampered theoretical understanding and modeling of those properties. Here, a new structural model for Au/Si(111)5x2 is presented, based on first-principles density-functional calculations, which explains a number of experimentally observed features. The model is a variant of the "honeycomb-chain channel" now accepted as the structure of alkali-induced Si(111)3x1, but with Au atoms occupying top-layer Si positions to form a double chain structure. Energetically, the model is far more favorable than all previously published models. Moreover, the model explains the bright "protrusions" commonly observed in STM as single Si adatoms, which serve to stabilize the 5x2 reconstruction with respect to its 5x1 parent structure. The model also reproduces the "Y"-shaped features observed in STM far from the bright protrusions. Electronically, the predicted band structure is a combination of p-like cosine bands, consistent with angle-resolved photoemission measurements on the closely related Au/Si(557) surface.

4:00pm **SS2-TuA7 First Principles Study of the Stability of Ag Ultra-thin Films on III-V Substrates: An Interfacial Study**, *D.L. Irving, S.B. Sinnott,* University of Florida*; R.F. Wood,* Oak Ridge National Laboratory

Under normal deposition conditions, most metals grow on semiconducting and insulating substrates in either a Volmer-Weber or a Stranski-Krastinow fashion. However, recent experiments on Ag/GaAs(110) show that atomically flat Ag overlayers can be grown by use of a two-step deposition process. The final morphology of these films is not only dependent on the deposition temperature, but also on the amount of metal initially

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[1] Morton S. Traum Award Finalist

deposited. Quantum size effects have been proposed as the reason for the preferential stability of the metallic overlayer and a simple theory has been used to predict whether a material system will exhibit it. This study compares the adhesion energy trends predicted by this theory with those calculated by first principles density functional theory calculations. The first principles calculations are performed on both the Ag(111)/GaAs(110) and the Ag(111)/GaSb(110) interfacial systems. The results show how the stability and electronic structure of the Ag films changes as a function of film thickness.

4:20pm **SS2-TuA8 A Self-Assembled Two Dimensional Electron Gas: @sr@7x@sr@3 In on Si(111)**, *E. Rotenberg, H. Koh,* Lawrence Berkeley National Laboratory*; H.W. Yeom,* Yonsei University, Korea*; J. Schaefer,* University of Augsberg, Germany*; B. Krenzer, M. Rocha, S.D. Kevan,* University of Oregon

We present low-temperature, high-resolution photoemission measurements of the Fermi surface and bandstructure of single-domain @sr@7x@sr@3 Indium on Si(111). Electrons from both indium valence electrons and the silicon dangling bonds form a nearly free, two-dimensional electron gas (2DEG) on a pseudosquare lattice, which is almost completely decoupled from the underlying hexagonal silicon lattice at the Fermi level. Structural analysis with LEED and photoelectron diffraction is consistent with the pseudo-four-fold structure, and rule out both pseudo-six-fold as well as triple (120°-rotated) domains which were reported in previous studies. About half of the Si dangling bond electrons are donated directly to the 2DEG, while the remainder form three bands -- confined to relatively small regions of k-space -- which we associate with In/Si covalent bond formation. The mean free path of carriers in the 2DEG is found to be at least 500 Å along the interface.

4:40pm **SS2-TuA9 Buckling of Si and Ge(111)2x1 Surfaces**, *S. Nie, R.M. Feenstra,* Carnegie Mellon University*; J.Y. Lee, M.H. Kang,* Pohang University of Science and Technology, Korea

The structure of cleaved Si or Ge (111)2x1 surfaces is well established as consisting of @pi@-bonded chains.@footnote 1@ However, the buckling (i.e. tilt) of these chains has been the subject of recent interest, primarily because a determination of buckling will enable a better comparison between optical absorption data and recent quasi-particle calculations of the surface bandgap and optical response.@footnote 2@ Based on such a comparison it has been suggested that the sign of the buckling may be opposite on Si and Ge surfaces.@footnote 2@ Recent voltage-dependent scanning tunneling microscopy results support that interpretation,@footnote 3@ although that data were restricted to a narrow range of voltages and were performed only on Ge (not Si). In the present work we have performed detailed voltage-dependent STM imaging of both Si and Ge (111)2x1 surfaces, over a wide range of sample-tip voltages. The results are compared with first-principles theoretical predictions, for both positive and negative values of the buckling angle. We find that the wide range of voltages used in the study enables a definitive determination of buckling. Our results demonstrate that the sign of the buckling is indeed opposite on Si and Ge surface, in agreement with the prior work.@footnote 2@ We furthermore deduce from a comparison of the experimental and theoretical STM images a comprehensive view of the image contrast mechanism, incorporating energy-dependent contributions from each atoms in the unit cell. In particular, for empty states, the contrast shifts as the sample-tip voltage is increased from the lower atoms to the upper ones. @FootnoteText@@footnote 1@ K. C. Pandey, Phys. Rev. Lett. 47, 1913 (1981); 49, 223 (1982).@footnote 2@ M. Rohlfing, M. Palummo, G. Onida, and R. Del Sole, Phys. Rev. Lett. 85, 5440 (2000).@footnote 3@ R. M. Feenstra, G. Meyer, F. Moresco, and K. H. Rieder, Phys. Rev. B 64, 081306 (2001).

5:00pm **SS2-TuA10 Dimer Structure of the Si(001)2x1 Surface Observed below 10K by Scanning Tunneling Microscope**, *M. Ono, A. Kamoshida, E. Ishikawa, T. Eguchi, Y. Hasegawa,* The University of Tokyo, Japan

The dimer structure of the Si(001) surface has been discussed after recent low-temperature STM observations, which reported symmetric dimers at 5K. Various models to explain the observation contradictory to the previous reports, such as anomalous flip-flop dimer motion and new ground state induced by spin configuration, were proposed. To solve this issue, we studied it using an STM which can be operated under multiple extreme conditions of ultrahigh vacuum (>6x10@super -9@ Pa), low temperature (>2.8K), and high magnetic field (

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