NINETEENTH ANNUAL SYMPOSIUM

LABORATORY FOR SURFACE MODIFICATION

Thursday, March 3, 2005

9:00 a.m. to 5:00 p.m.

Rutgers, The State University of New Jersey

Fiber Optics Auditorium
Busch Campus
Piscataway, New Jersey
NINETEENTH ANNUAL SYMPOSIUM
LABORATORY FOR SURFACE MODIFICATION

8:15 Registration, coffee

8:45 Introductory Remarks

Professor Yves J. Chabal, Director of the Laboratory for Surface Modification
Professor David Madigan, Executive Vice Dean, Faculty of Arts and Sciences

I. Oxides and Interfaces

Chairperson, Charles Glashauser
Chair, Department of Physics and Astronomy

9:00 First-principles study of symmetry lowering and polarization in relaxed BaTiO$_3$/SrTiO$_3$ superlattices with in-plane expansion, K. Johnston, Dept. of Physics and Astronomy

9:15 Nanoscale smoothing and the analysis of interfacial charge and dipolar densities, M. H. Cohen, J. Junquera and K.M. Rabe, Dept. of Physics and Astronomy

9:30 Low temperature synthesis and cation ordering in nanostructured magnesium aluminate spinel, J.F. Al-Sharab$^1$, A. Singhal$^2$, G. Skandan$^2$, James Bentley$^3$, and F. Cosandey$^1$, $^1$Dept. of Ceramics and Materials Engineering, $^2$NEI, Corporation, 201 Circle Drive, Piscataway, NJ,08854, $^3$Oak Ridge National Laboratory, Metals and Ceramics Division, Oak Ridge, TN 37831

9:45 rf/microwave dielectric response of basrTiO$_3$ (60/40) thin films under anisotropic epitaxial misfit, W.K. Simon, E.K. Akdogan, A. Safari, Dept. of Ceramic and Materials Engineering

10:00 MOCVD growth and properties of high quality MgZnO films and nonotips, G. Saraf, H. Chen, J. Zhong, Y.Lu, Dept. of Electrical and Computer Engineering

10:15 – 10:45am Coffee Break and Poster Session
II. Nanoscale Surface Chemistry

Chairperson, Kathryn Uhrich
Department of Chemistry and Chemical Biology
Co-Director IGERT
Chair, Advisory Board, Polymerix Corp.

10:45  HIGHLIGHT PRESENTATION  - Molecular tripods: new sensitizers for semiconductor nanoparticles, Elena Galoppini, Chemistry Department, Rutgers, Newark

11:30  Passivation of germanium(100) substrate for high-k growth, S. Rivillon\textsuperscript{1} and Y. J. Chabal\textsuperscript{1,2}, \textsuperscript{1}Dept. of Chemistry and Chemical Biology, \textsuperscript{2}Dept. of Biomedical Engineering,

11:45  Dynamic and kinetic aspects of the adsorption of acrylonitrile on Si(001)-2×1, S. Rangan\textsuperscript{1}, S. Kubsky\textsuperscript{2}, J.-J. Gallet\textsuperscript{2}, F. Bournel\textsuperscript{2}, K. Le Guen\textsuperscript{2}, G. Dufour\textsuperscript{2}, F. Rocher\textsuperscript{2}, F. Sirotti\textsuperscript{3}, R. Funke\textsuperscript{4}, M. Keppe\textsuperscript{4}, G. Piaszenski\textsuperscript{4}, U. Köhler\textsuperscript{4}, \textsuperscript{1}Dept. of Chemistry and Chemical Biology, \textsuperscript{2}Laboratoire Chimie Physique Matière Rayonnement Université Pierre et Marie Curie, France, \textsuperscript{3}Laboratoire pour l'Utilisation du Rayonnement Electromagnétique, \textsuperscript{4}Experimentalphysik IV - AG Oberflächen, Ruhr-Universität Bochum Germany

12:00  AFM characterization of laminin micropatterns used to direct nerve cell growth, B.A. Langowski and K. E. Uhrich, Dept. Chemistry and Chemical Biology

12:15 - 1:45  -Lunch and Poster Session-
POSTER PAPERS

1. First-principles study of epitaxial perovskites, O. Dieguez, K.M. Rabe and D. Vanderbilt, Dept. of Physics and Astronomy

2. Polarization enhancement in two- and three-component ferroelectric superlattices, S. M. Nakhmanson, K. M. Rabe and D. Vanderbilt, Dept. of Physics and Astronomy

3. Structural and magnetic properties of SrRuO3 under epitaxial strain, A. T. Zayak1, K. M. Rabe1, X. Huang2 and J.B. Neaton3, 1Dept. of Physics and Astronomy, 2Department of Chemical Engineering and Materials Science, 3The Molecular Foundry, Material Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA

4. A novel mass spectrometer, A. V. Ermakov, B.J. Hinch, Dept. of Chemistry and Chemical Biology

5. Interaction of water vapor with the ruthenium (10-10) surface, T. Graber, B.V. Yakshinskay, T.E. Madey, Dept. of Physics and Astronomy


8. Surface and interface study of High-k material growth using in situ FTIR, Y. Wang, M.-T. Ho, L.Wielunski, L. Goncharova, T. Gustafsson and Y. Chabal, Dept. of Physics and Astronomy, Dept. of Chemistry and Chemical Biology, Dept. of Biomedical Engineering

9. Exact cluster size distribution in the one-dimensional Ising model and applications to hydrogen adsorption on Si(001)-2x1, M.B. Yilmaz and F. M. Zimmermann, Dept. of Physics and Astronomy


11. Surface and interfacial study of organic semiconductor field effect transistor for labelless DNA biosensor, M. Stickle1, Y. J. Chabal1, C. Roth, 1Dept. of Biomedical Engineering, 2Dept. of Chemistry and Chemical Biology

12. Structure and growth of (3-Aminopropyl) triethoxysilane and diethoxysilane self assembly on silicon(100), M. Li, A. Langner, S. Rivillon1, Y.J. Chabal1, 1Dept. of Chemistry and Chemical Biology, 2Dept. of Biomedical Engineering


15. Preparation of a novel heterogeneous titanocene catalyst for chiral reduction and asymmetric polymerization, A. Panarello, O. Vassylev and J. G. Khinast, Dept. of Chemical & Biochemical Engineering
III. Nanofabrication and Electronics

Chairperson, Stephen C. Danforth
Chair, Department of Ceramics and Materials Engineering

1:45 HIGHLIGHT PRESENTATION – Diblock copolymer self assembly for electronic device nanofabrication, Richard Ruiz, IBM T.J. Watson Research Center, Yorktown Heights, NY

2:30 Medium energy ion scattering study of epitaxial high-K films grown on Si, L. Goncharova¹, D. G. Stardoub¹, E. Garfunkel² and T. Gustafsson¹, "Dept. of Physics and Astronomy, Dept. of Chemistry and Chemical Biology

2:45 Interface band alignment in high-K gate stacks, E. Bersch¹, P. Hartlieb², S. Sayan, R. Bartynski¹, and E. Garfunkel², " Dept. of Physics and Astronomy, Dept. of Chemistry and Chemical Biology

3:00 A novel method to achieve high sensitivity for detection of low mass elements on Si using 2 MeV He RBS, L. Wielunski, Dept. of Physics and Astronomy

3:15 – 3:30pm ☕️ Coffee Break ☕️
IV. Electronic and Chemical Properties of Metal Surfaces

Chairperson, Theodore E. Madey
State of NJ Professor of Surface Science
Department of Physics and Astronomy (Laboratory for Surface Modification)

3:30  Electron-initiated dissociation of water layers on Ru(0001), N.S. Faradzhiev\textsuperscript{1}, T.E. Madey\textsuperscript{1}, K.L. Kostov\textsuperscript{2}, P. Feulner\textsuperscript{2} and D. Menzel\textsuperscript{2}, \textsuperscript{1}Dept. of Physics and Astronomy, \textsuperscript{2}Physik Department, TU München, Germany

3:45  Atomic structure of O/Ir(210) nanofacets, I. Ermanoski and T. E. Madey, Dept. of Physics and Astronomy

4:00  Occupied electronic states and CO adsorption on Ni/Cu(100) system, H. Yao, A. G. Danese and R.A. Bartynski, Dept. of Physics and Astronomy

4:15  A temperature dependent structural analysis of the C\textsubscript{2}N\textsubscript{2}/Cu(001) system using Helium Atom Scattering (HAS), I.G. Shuttleworth, E. Giflikli, A. Ernakov and B.J. Hinch, Dept. of Chemistry and Chemical Biology

4:30  Multiphonon helium atom-CN/Cu(001) surface scattering, E.Z. Giflikli, I.G. Shuttleworth, A.V. Ernakov, B.J. Hinch, Dept. of Chemistry and Chemical Biology

4:45  -End of Presentations/Talks; Laboratory Visits-
Abstracts for Talks

9:00  First-principles study of symmetry lowering and polarization in relaxed BaTiO$_3$/SrTiO$_3$ superlattices with in-plane expansion, K. Johnston, Dept. of Physics and Astronomy

The crystal structure and local spontaneous polarization of (BaTiO$_3$)$_m$(SrTiO$_3$)$_n$ superlattices is calculated using first-principles density functional theory. The in-plane lattice constant is constrained to be 1% larger than the SrTiO$_3$ substrate to model the relaxed superlattice structure observed in recent experiments. The symmetry is lowered to monoclinic space group $C_m$ allowing for polarization along the [110] and [001] directions. The polarization component in the [110] direction is found to develop only in the SrTiO$_3$ layers and falls to zero in the BaTiO$_3$ layers, whereas the polarization in the [001] direction is approximately uniform throughout the superlattice. These findings are consistent with recent experimental data and first-principles results for epitaxially strained BT and ST.

9:15  Nanoscale smoothing and the analysis of interfacial charge and dipolar densities, M. H. Cohen, J. Junquera and K.M. Rabe, Dept. of Physics and Astronomy

First-principles calculations on surfaces and interfaces provide a vast amount of information at the atomic level. Physically relevant charge and dipole densities to the interface are extracted via nanosmoothing procedures. We discuss the criteria for validity that these procedures should meet to leave the physical quantities unaffected. We have applied the model to compute directly the polarization charge density of a realistic ferroelectric capacitor.

9:30  Low temperature synthesis and cation ordering in nanostructured magnesium aluminate spinel, J.E. Al-Sharab$^1$, A. Singhal$^2$, G. Skandan$^3$, James Bentley$^3$, and F. Cosandey$^1$

$^1$Dept. of Ceramics and Materials Engineering, $^2$NEI, Corporation, 201 Circle Drive, Piscataway, NJ 08854, $^3$Oak Ridge National Laboratory, Metals and Ceramics Division, Oak Ridge, TN 37831

Nanostructured MgAl$_2$O$_4$ spinel has been synthesized at low temperatures by a direct conversion method from cubic $\gamma$-Al$_2$O$_3$. The MgAl$_2$O$_4$ spinel phase formation was analyzed by selected area electron diffraction (SAED) with direct comparison with simulated patterns. Phase chemistry and homogeneity of the nanostructured powders were investigated by spectrum imaging from either electron energy loss spectroscopy (EELS) or X-Ray energy dispersive spectroscopy (EDS). The degree of Mg and Al ordering in tetrahedral and octahedral sites has also been determined from combined simulations and relative diffraction intensity measurements.

9:45  rf/microwave dielectric response of BaSrTiO$_3$ (60/40) thin films under anisotropic epitaxial misfit, W.K. Simon, E.K. Akdogan, A. Safari, Dept. of Ceramic and Materials

BST (60/40) thin films were grown by PLD in the thickness range of 25 to 1200 nm. The complete residual strain tensor of the films was obtained, and the Matthew-Blakeslee critical films thickness were determined as 5 and 7 nm, respectively. At 10 GHz, variations in tunability from 27% to 54% due to changes in residual strain have been observed in the range 75-1200 nm and along the $<-110>$. A three-fold variation of relative permittivity (~500 to 150) and a substantial variation in tunability (54% to 34%) with in-plane crystallographic direction have been seen in the 600 nm thick film.
MOCVD growth and properties of high quality MgZnO films and nanotips, G. Saraf, H. Chen, J. Zhong, Y. Lu, Dept. of Electrical and Computer Engineering

ZnO and its ternary compound MgZn_{1-x}O are promising for photonics and electronics. MgZn_{1-x}O increases the direct energy bandgap of ZnO to 4.0 eV. MOCVD is used to grow MgZn_{1-x}O epitaxial films on R-Sapphire with ZnO as a buffer. We have also grown MgZnO nanotips on various substrates. The structural, electrical and optical properties are characterized.

HIGHLIGHT PRESENTATION – Molecular tripods: new sensitizers for semiconductor nanoparticles, Elena Galoppini, Chemistry Department, Rutgers, Newark

Passivation of germanium(100) substrate for high-k growth, S. Rivillon and Y. J. Chabal, Dept. of Chemistry and Chemical Biology, Dept. of Biomedical Engineering

Due to its high mobility carrier, germanium appears to be a promising semiconductor and controlling its surface chemistry is critical for the growth of high-k dielectrics. Using wet chemistry, we have investigated different methods for cleaning and passivating germanium (100) substrate and studied the resulting surfaces using infrared absorption spectroscopy.

Dynamic and kinetic aspects of the adsorption of acrylonitrile on Si(001)-2x1, S. Rangan, S. Kubsky, J.-J. Gallet, F. Bournel, K. Le Guen, G. Dufour, F. Rochet, F. Sirotti, R. Funke, M. Keppe, G. Piaszenski, U. Köhler, Dept. of Chemistry and Chemical Biology, Laboratoire Chimie Physique Matière Rayonnement Université Pierre et Marie Curie, France, Laboratoire pour l'Utilisation du Rayonnement Electromagnétique, Experimentalphysik IV-AG Oberflächen, Ruhr-Universität Bochum Germany

Using a combination of local (STM) and global, but chemically sensitive, probes (photoelectron and photoabsorption spectroscopies), we have examined how acrylonitrile (H_2C=CH-C≡N) reacts with the Si(001)-2×1 surface for coverages ranging from 10^{12} molecules/cm² to 10^{14} molecules/cm². At 300 K, in the very low coverage regime, only a cumulative-double-bond unit (C≡C=N) is formed. For coverages larger than 10^{13} molecules/cm², for which STM does not show ordered adsorption any more, adsorption kinetics are followed by real-time valence band photoemission and resonant Auger yield, associated with N 1s x-ray absorption spectroscopy (NEXAFS). Now three species (cyano-bonded, vinyl-bonded and cumulative-double-bond species) are detected.

AFM characterization of laminin micropatterns used to direct nerve cell growth, B.A. Langowski and K. E. Uhrich, Dept. Chemistry and Chemical Biology

Protein stripes used to direct Schwann cell attachment and outgrowth were microcontact printed onto poly(methyl methacrylate) (PMMA) substrates and analyzed by atomic force microscopy (AFM) to physically evaluate pattern dimensions, topography and homogeneity. The relation of protein stamping concentration and pattern height, as well as the role of pattern dimensions on cellular response will be discussed.
1:45 HIGHLIGHT PRESENTATION – Diblock copolymer self assembly for electronic device nanofabrication, Richard Ruiz, IBM T.J. Watson Research Center, Yorktown Heights, NY

Under suitable conditions, certain materials self organize into uniform nanometer scale domains with a degree of longer-range order, a spontaneous process known as self assembly. Self-organizing diblock copolymers offer particularly exciting possibilities for application to semiconductor electronics because the polymer materials can be implemented in the same manner as photoresists used in conventional lithography. Self assembly provides a low-cost, efficient means to engineer nanometer-scale structures over large silicon wafer areas. Our integration of this self assembly process with state-of-the-art semiconductor processing has enabled such device demonstrations as high-surface-area decoupling capacitors, nanocrystal FLASH memories, and suspended nanoporous membranes. Most self assembling materials lack any alignment capability, which has limited their application to devices which only require large numbers of uncorrelated nanometer-scale structures. More recently we have developed methods for self-aligning the 20nm size polymer domains to larger-scale patterns defined using conventional lithography. Our ability to precisely control the position of self-assembled nanometer-scale features opens many new possibilities for device applications.

2:30 Medium energy ion scattering study of epitaxial high-K films grown on Si, L. Goncharova1, D. G. Stardoub1, E. Garfunkel2 and T. Gustafsson1, 1Dept. of Physics and Astronomy, 2Dept. of Chemistry and Chemical Biology

Epitaxial oxide/Si heterostructures are of great interest as templates for the integration of functional materials with Si. We used MEIS depth profiling in combination with angular distribution analysis of scattered ions in channeling-blocking geometries to study composition and structure of thin epitaxial Sc2O3 and SrTiO3 films grown by MBE on Si. We found that for Sc2O3(111) on Si(111) the lattice mismatch was relived by a 60° rotation of the film with respect to the substrate. For SrTiO3/Si(001), the mobility of Ti and O species during re-crystallization anneal results in replacement of strontium silicide by a Ti-rich interfacial region. Our results show that such epitaxial oxides have truly excellent crystal perfection.

2:45 Interface band alignment in high-K gate stacks, E. Borsch1, P. Hartlieb2, S. Sayan, R. Bartyński1, and E. Garfunkel2, 1Dept. of Physics and Astronomy, 2Dept. of Chemistry and Chemical Biology

In order to successfully implement alternate high-K dielectric materials into MOS structures, the interface properties of MOS gate stacks must be better understood. We have measured the conduction and valence band densities of states for a variety MOS stacks using in situ using inverse photoemission (IPE) and photoemission spectroscopy (PES), respectively. Results obtained from clean and metallized (with Ru or Al) HfO2/Si, SiO2/Si and mixed silicate films will be presented.

3:00 A novel method to achieve high sensitivity for detection of low mass elements on Si using 2 MeV He RBS, L. Wielunski, Dept. of Physics and Astronomy

Typical RBS measurements provide very good sensitivity for detecting elements more massive than the main components of the sample (typically Si) and very low sensitivity for lower mass elements present in the surface layer (C, O). Glancing angle detection in combination with a channeling technique allows us to substantially reduce the typical background from the substrate, and permits high sensitivity detection of low mass elements on the surface of a more massive substrate (Si). Examples will be shown for C and O monolayer sensitivity detection on a Si substrate with an ultra-thin high-k ALD deposited HfO2 layer present. The physics and limitations of this approach will be discussed.
3:30 Electron-initiated dissociation of water layers on Ru(0001), N.S. Faradzhev, T.E. Madey, K.L. Kostov, P. Feulner and D. Menzel, Dept. of Physics and Astronomy, Physik Department, TU München, Germany

There is an active literature controversy concerning the thermal stability of H₂O and D₂O on the close-packed Ru(0001) surface: some claim that H₂O and D₂O are adsorbed as molecular layers, while others claim that the layers are partially dissociated. The published conclusions are based on electron or photon irradiation of the surface. We find that electron impact leads to partial dissociation of both H₂O and D₂O with extremely high cross section (~ 10⁻¹⁵ cm² at 90 eV). We conclude that previous reports have been influenced by partial dissociation induced by slow electrons.

3:45 Atomic structure of O/Ir(210) nanofacets, I. Ermanoski and T. E. Madey, Dept. of Physics and Astronomy

We report a study of faceting of the O/Ir(210) system using ultrahigh vacuum scanning tunneling microscopy (STM). Upon annealing, three-sided nano-pyramids are formed on the oxygen covered surface, and atomically resolved scans reveal smooth {311} facets and (110) facets that have a complicated superstructure on the atomic level. Our models based on truncated bulk iridium crystal properties show excellent agreement with experimentally observed surface atomic arrangements and distances.

4:00 Occupied electronic states and CO adsorption on Ni/Cu(100) system, H. Yao, A. G. Danese and R.A. Bartynski, Dept. of Physics and Astronomy

Quantum size effects in ultrathin metal films give rise to a wide array of new physical properties in the film. Cu-induced features seen in inverse photoemission (IPE) spectra of ultrathin Cu overlayers on the Ni/Cu (100) system exhibit an anomalous downward dispersion with increasing overlayer thickness. To investigate the origin of this phenomenon, we performed an IPE study of the Ni/Cu (100) and CO/Ni/Cu (100) systems as a function of Ni thickness. The IPE spectra from the Ni films exhibit very rich structure which is strongly modified by CO adsorption indicating that some features are associated with surface states of the Ni film, while others may be associated with the Cu/Ni interface. The results provide important clues to the anomalous behavior exhibited by Cu overlayers on this system.

4:15 A temperature dependent structural analysis of the C₂N₂/Cu(001) system using Helium Atom Scattering (HAS), L.G. Shuttleworth, E. Ciftlikli, A. Ermakov and B.J. Hinch, Dept. of Chemistry and Chemical Biology

The temperature dependence of the adsorption of cyanogen (C₂N₂) on Cu(001) has been studied using HAS. Adsorption at extremes of temperature (at a minimum of 170K and maximum 600K) produces a disordered surface, whereas adsorption across a zone in the middle of this region (240K-340K) results in an ordered c(10x6) surface. Thermal processing of this ordered surface produces an irreversible order-disorder transition. Hard-wall, single scattering simulations of the HAS experiment have provided some structural insights to the ordered phase.
4:30 Multi phonon helium atom-CN/Cu(001) surface scattering, E.Z. Ciftikli, I.G. Shuttleworth, A.V. Ermakov, B.J. Hinch, Dept. of Chemistry and Chemical Biology

C$_2$N$_2$ adsorption on Cu(001) is believed to be dissociative at ambient sample temperatures. Strong work function changes are suggestive of adsorbed CN$^-$ species. Angular resolved Helium Atom Scattering (HAS) scans, taken along the <110> azimuth and after stepwise dosing of the surface, show the development of a very broad, diffuse intensity background. Only in the later stages of dosing (>1.5 L), does growth of this diffuse feature slow as an ordered c(10x6) phase develops. Time of Flight (TOF) measurements indicate that the majority of the high coverage diffuse intensity is, in fact, inelastic and that the strong diffuse component is predominately due to multiphonon scattering. Careful analysis of the energy resolved and temperature dependent multiphonon scattering enables (a) the subtraction of multiphonon intensity, for elastic and single phonon analysis, and also (b) the determination of the form factor which is closely tied to the He-CN$^-$ interaction potential.
Abstracts for Posters

1. **First-principles study of epitaxial perovskites**, O. Dieguez, K.M. Rabe and D. V. Vanderbilt, Dept. of Physics and Astronomy

   We extend a first-principles method developed by King-Smith and Vanderbilt [Phys. Rev. B 49, 5828 (1994)] to investigate the properties of eight perovskites in epitaxial film form. These materials are BaTiO₃, SrTiO₃, CaTiO₃, KNbO₃, NaNbO₃, PbTiO₃, PbZrO₃, and BaZrO₃. For each film, we analyze what is its most stable phase for different values of the misfit strain that the substrate imposes on it. To help understand the results, we also introduce an external stress on each film and compute the phase diagram that results.


   Modern epitaxial engineering techniques allow for atomically thin layer-by-layer growth of perovskite-type oxides, yielding superlattices with compositionally abrupt interfaces and excellent ferroelectric behavior. We have performed ab initio studies of polarization-related properties of (CaTiO₃)ₙ(SrTiO₃)ₘ(BaTiO₃)ₚ superlattices pseudomorphically grown on SrTiO₃ substrate. Our results show that in systems containing layers of pseudomorphically strained BaTiO₃, polarization is increased compared to unstrained bulk-tetragonal BaTiO₃.

3. **Structural and magnetic properties of SrRuO₃ under epitaxial strain**, A. T. Zayak¹, K. M. Rabe¹, X. Huang² and J.B. Neaton³, ¹Dept. of Physics and Astronomy, ²Department of Chemical Engineering and Materials Science, ³The Molecular Foundry, Material Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA

   Using density functional theory we investigate structural and magnetic properties of SrRuO₃ single crystal under epitaxial strain. Calculations show that in thin film geometries SrRuO₃ undergoes significant structural modifications, strongly depending on the orbital ordering in the octahedral oxygen structure, whereby the magnetic and non-magnetic states of Ru⁴⁺ ion correspond to different structural parameters. Under very large epitaxial tensile strain the Ru⁴⁺ ion may change its spin configuration.

4. **A novel mass spectrometer**, A. V. Ermakov, B.J. Hinch, Dept. of Chemistry and Chemical Biology

   We have developed a novel mass spectrometer which has an entirely new basic principle – i.e. using an electrostatic ion trap. This mass spectrometer has an unlimited mass range, and is capable of achieving much higher sensitivity, better mass resolution, and much faster scan rates than the widely used (larger size and) more complicated quadrupole or magnetic sector mass spectrometers.

5. **Interaction of water vapor with the ruthenium (10-10) surface**, T. Graber, B.V. Yakshinskii, T.E. Madey, Dept. of Physics and Astronomy

   Ruthenium thin-film capping layers on multilayer reflecting optics are used for prototype extreme ultraviolet (EUV) lithography systems; Ru inhibits photon-induced mirror degradation. As part of a program to investigate mechanisms of mirror degradation, the interaction of H₂O and D₂O vapors with the atomically-rough Ru(10-10) surface is studied by TPD, XPS and LEIS. Evidence for both molecular and dissociative adsorption of water are found on this surface, but the desorption kinetics and binding energy of water depend appreciably on fractional monolayers of surface impurities.
6. Structure sensitivity in oxidation of CO and decomposition of NH\textsubscript{3} over Ir surfaces: relevance to environmental applications of Ir catalysts, W. Chen, I. Ermanoski and T.E. Madey, Dept. of Physics and Astronomy

We report on catalytic oxidation of CO and decomposition of NH\textsubscript{3} on clean planar Ir(210), and on clean nanoscale-faceted Ir(210) containing 3-sided pyramidal facets with both \{311\} and (110) faces. After annealing in oxygen to various temperatures \(\geq 600\text{K}\), facets with average sizes from 5nm to \(\sim 15\text{nm}\) are formed. The oxygen is removed by reaction with hydrogen at \(\sim 400\text{K}\), and the facets persist. Both planar and faceted surfaces are very active for the two reactions; both are structure sensitive on planar Ir(210) versus faceted Ir(210). Moreover, NH\textsubscript{3} decomposition exhibits size effects on the nanometer scale over faceted Ir(210) while no evidence is found for size effects in CO oxidation.

7. Faceting of O/Re (12\overline{3}1): a model system for catalytic studies, H. Wang, W. Chen, A.S. Y. Chan and T. E. Madey, Dept. of Physics and Astronomy

The adsorption of oxygen on Re (12\overline{3}1) has been studied by LEED, AES and STM. The atomically rough Re (12\overline{3}1) surface remains planar at room temperature after being exposed to oxygen. However, the O/Re (12\overline{3}1) surface undergoes drastic morphological changes to become completely faceted upon annealing at 700K or higher temperatures. With low oxygen coverages (~0.5ML), the facets form two-sided ridge-like structures that grow in size with annealing temperatures to maximum length >50nm. The two facets of the ridge are (1\overline{1}2\overline{1}) and (01 \overline{1} 0). When the oxygen coverage is about 1ML, the ridge-like structure is truncated by a third set of facets, identified as (10 \overline{1} 0). The faceted O/Re surfaces may be potential templates to grow ordered nanostructures, as well as candidates to study structural sensitivity in catalytic reactions.

8. Surface and interface study of High-k material growth using in situ FTIR, Y. Wang, M.-T. Ho, L.Wielunski, L. Goncharova, T. Gustafsson and Y. Chabal, Dept. of Physics and Astronomy, Dept. of Chemistry and Chemical Biology, Dept. of Biomedical Engineering

In this work, we report approaches to minimizing interfacial SiO\textsubscript{2} layer at Si/high-k dielectric interface. Using in situ infrared spectroscopy, we find that surface pre-functionalizations can effectively prevent silicon oxidation in HfO\textsubscript{2} ALD. Moreover, HfO\textsubscript{2} grows linearly on H- and nitride-terminated silicon. We have investigated the post deposition annealing effect on the structure of HfO\textsubscript{2} film.

9. Exact cluster size distribution in the one-dimensional Ising model and applications to hydrogen adsorption on Si(001)-2x1, M.B. Yilmaz and F. M. Zimmermann, Dept. of Physics and Astronomy

H\textsubscript{2} on Si(001)-2x1 is an extensively studied model system for understanding covalent bonding on semiconductor surfaces. It has been known for quite sometime that H atoms pair up on the dimers of Si(001)-2x1 surface and have a tendency to form one dimensional clusters along the dimer rows. In this study, we present the exact solution for the cluster size distribution in a one dimensional lattice gas model. Then we use this solution to determine the clustering energy of paired H atoms on the Si(001) surface. With the help of the solution we also present a model that explains the optical second harmonic generation efficiency of the Si(001) surface as a function of H\textsubscript{2} coverage.

We have used femtosecond pump-probe spectroscopy to observe the interaction of electron excitation and lattice vibration of LuMnO$_3$ in real time. Optical excitation at a sharp absorption peak at 800 nm corresponding to a Mn $d_{(x^2-y^2)\lambda\lambda\lambda}\rightarrow d_{(z^2)}$ transition served as the primary excitation step. Reflectivity changes as a function of delay time reveal electronic relaxation and coherent oscillations of several optical phonon modes. The interaction mechanisms of photons, electrons, and coherent phonons are discussed.

11. Surface and interfacial study of organic semiconductor field effect transistor for labelless DNA biosensor, M. Stickle$^1$, Y. J. Chabal$^{1,2}$, C. Roth$^3$, 1Dept. of Biomedical Engineering, 2Dept. of Chemistry and Chemical Biology

We are investigating the structure of thin organic semi-conductor films deposited via vacuum evaporation on an insulating layer (SiO$_2$) in order to optimize the charge transport. We use FTIR and X-ray diffraction to characterize the semiconducting organic thin film and to study orientation as well as bonds for the attachment and sensing of charged molecules.

12. Structure and growth of (3-Aminopropl) triethoxysilane and triethoxysilane self assembly on silicon(100), M. Li, A. Langner, S. Rivillon$^1$, Y.J. Chabal$^{1,2}$, 1Dept. of Chemistry and Chemical Biology, 2Dept. of Biomedical Engineering

Self-assembled monolayers (SAM) are of great interest because they provide a unique way to form well-ordered and oriented layers that are useful for many applications. We have systematically investigated the structure and growth dynamics of two silane molecules deposited on silicon dioxide surfaces using infra-red spectroscopy. We have found a reproducible way to form a single monolayer.


A novel surface acoustic wave (SAW) UV photodetector is fabricated using an epitaxial semiconductor/piezoelectric ZnO based multilayer structure on an r-plane sapphire substrate. The interaction of UV generated free carriers in the semiconducting ZnO layer with the electric field accompanying the propagating SAW in the piezoelectric ZnO layer results in a phase shift in the frequency domain, as a function of incident power density and wavelength. This integrated ZnO SAW optoelectronic device can be used as a passive remote wireless UV sensor.


Catalytic activity of some complexes of Pd (II) with N-containing ligands was studied. The ligands were metallated in homogeneous solution, or in the immobilized form. Immobilization of the ligands was carried out by the reaction of their functional groups with silanol groups of silica surface. Obtained catalysts displayed high activity in Suzuki coupling reaction. Effect of reaction conditions on the catalysts activity and selectivity was investigated.
Preparation of a novel heterogeneous titanocene catalyst for chiral reduction and asymmetric polymerization, A. Panarello, O. Vassylyev and J. G. Khinast, Dept. of Chemical & Biochemical Engineering

Chiral ansa-ethylene-bis(η-tetrahydroindenyl) Metal complexes, EBTHI-MX₂ complexes are highly active and selective catalysts for enantioselective reactions, including hydrogenations of olefins, ketones and imines, as well as various polymerization reactions. These catalytic complexes are homogeneous, and thus, do not possess the same advantages as heterogeneous catalysts, such as easy removal of the catalyst from the reaction mixture, catalyst recycling, prevention of metal leaching into the fine product, etc. While heterogeneous catalysts offer several advantages as described above, as of yet no heterogenized versions have been reported.

In this work we present the first successful strategy for heterogenizing EBTHI-MX₂ by introducing a carbon tether without disrupting the catalytic active site. This was accomplished by first introducing bromine to the EBI ligand followed by using the Suzuki Coupling reaction to introduce a wide variety of functional tethers in a simple and efficient five step synthesis. Due to the limited reactivity and ease in immobilizing, initial work focused using alkene tethers. Published procedures were used to introduce the active metal species. Lastly, employing a hydrosilylation methodology, the catalytic complex was immobilized onto a silica surface. Immobilization studies using the tethered ligand, helped determined optimal conditions for creating a uniform catalytic surface.