

Joint Meeting of the
Prairie Chapter of the **AVS** Science & Technology Society
& the **Illinois Chapter**
of the **Electrochemical Society**

7 October 2002, Monday

University of Illinois at Chicago
605 Chicago Circle Center
750 S. Halsted St.
Chicago, IL

Meeting Schedule

Time	Session A - Room 613	Session B - Room 713
	<i>Topic: Films for Tribology, X-Rays, and Magnetism</i> <i>Session Chair: David Schultz, UIC and Argonne</i>	<i>Topic: MEMS and Environmental Science</i> <i>Session Chair: Scott Shippy, UIC</i>
9:30 AM	Almila Yazicioglu, UIC: Fluid Transport and Phase Change in Carbon Nanotubes (#6)	Alan Feinerman, UIC: Compact Optical MEMS Actuators with Super Deformable Flexural Elements
9:50 AM	Kitty Lee, NWU: Synthesis and Tribological Studies of Nanolayers TiB ₂ /TiC Coatings for Possible Elevated Temperature Applications (#39)	Invited Talk Continued
10:10 AM	Joe Greene, UIUC: Microstructural and Surface Morphological Evolution at the Atomic Scale during Sputter Deposition of TiN	Jie Wu, Notre Dame U: An Inlaid Electroplated Copper Coil for Implanted and MEMS Applications (#14)
10:30 AM	Invited Talk Continued	Brian Davies, Bradley U, Dimerization of NO and Transformation to N ₂ O on Ge(100) (#12)
10:50 AM	Chian Liu, Argonne: Profile Coatings at the Advanced Photon Source (#7)	Peter Stair, NWU: Environmental Catalysis - Molecular Science and Potential Applications
11:10 AM	David Keavney, Argonne: Interface & Nanoscale Magnetism in Magnetoelectronic Devices Studies Using Synchrotron-Based Polarized X-ray Techniques (#23)	Invited Talk Continued
11:30 AM	*** Lunch & Vendor	Exhibit - Room 605 ***
	<i>Topic: Morphology and Microscopy</i> Rm 613 <i>Session Chair: John Noonan, Argonne</i>	<i>Topic: Surface Chemistry on Semiconductors</i> Rm 713 <i>Session Chair: David Schultz</i>
12:40 PM	Gopal Ready, IIT: An AFM Study of Living PC12 Cells (#36)	Robert Hamers, UW: Surface Science Meets Biology - Linking DNA with Group IV Semiconductors
1:00 PM	Nathan Guisinger, NWU: Atomic Level Characterization & Control of Free Radical Surface Chemistry Using Scanning Tunneling Microscopy (#22)	Invited Talk Continued
1:20 PM	Erick Fuoco, UIC: Controlling the Nanoscale Morphology and Chemistry of Organic Films by Polyatomic Ions (#40)	Reagan Kinser, NWU: Nanoscale Fabrication and Characterization of Chemically Modified Silicon Surfaces Using AFM in Liquids (#16)
1:40 PM	*** Coffee Break	- Room 605 ***
	<i>Topic: Vacuum Technology</i> Rm 613 <i>Session Chair: John Noonan, Argonne</i>	<i>Topic: Liquid Surfaces and Electrochemical Devices</i> <i>Session Chair: Gerry Zajac, BP</i> Rm 713
2:00 PM	Bruce Kendall, Elvac Laboratories: Ionization Gauge Measurements at Low Pressures (#5)	Mark Schlossman, UIC: Molecular Ordering at Liquid-Liquid Interfaces as Probed by X-ray Surface Scattering
2:20 PM	Invited Talk Continued	Invited Talk Continued
2:40 PM	Joe Gagliano, Argonne - Design of Roughing Pump System for APS RF Cavities	William Smyrl, U Minnesota: Portable Fuel Cells and Portable Batteries
3:00 PM	Phil Danielson, The Vacuum Lab - Fundamental of Vacuum Pumping	Invited Talk Continued
3:20 PM	Hans Luedi, Midwest Vacuum: Helium Leak Detection - Practical Applications, Tips & Ideas	Meeting of Chicago Section of Electrochemical Society
3:40 PM	*** Poster Session	- Room 605 ***
5:00 PM	*** Awards for Best	Posters - Room 605 ***

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Meeting Organization

Prairie Chapter of the AVS Science and Technology Society

Illinois Chapter of the Electrochemical Society

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Meeting Website: www.chem.uic.edu/avs/Prairiemeet02.html

Abstracts for Invited Talks

Microstructural and Surface Morphological Evolution at the Atomic Scale during Sputter Deposition of TiN: a HR-TEM, XRD, STM, and Modeling Study

Joe Greene

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Polycrystalline TiN and related transition-metal (TM) nitride thin films are typically deposited by magnetron sputter deposition and used as diffusion barriers in microelectronics as well as hard, wear, and corrosion resistant coatings in mechanical and optical applications. Since all cubic TM nitrides are highly anisotropic, control of preferred orientation is essential. We have used a combination of XRD, TEM, and HR-XTEM analyses to show that polycrystalline TiN layers grown by sputter deposition or reactive evaporation at low temperatures ($T_s < 450$ °C) exhibit competitive texture evolution with a columnar 111 "kinetically-limited" texture eventually becoming dominant. The columns are narrow and faceted with inter- and intracolumn porosity. Higher T_s or the use of high incident N_2^+/Ti flux ratios (> 5) with low N_2^+ energies (20 eV) in the magnetically-unbalanced magnetron mode result in non-competitive growth with a fully dense complete 002 orientation from the initial monolayer. The columns are broad-based with flat surfaces.

Kinetic Monte Carlo (KMC) modeling, assuming that the activation energy E_s for surface diffusion and the Ehrlich barrier E_b at descending step edges are larger on 111 than on 002, provides a qualitative understanding. Quantitative modeling requires a full set of surface and adatom transport activation energies: E_s , E_b , orientation-dependent step edge energies and stiffnesses, kink energies, and adatom formation energies. To obtain these parameters, we have grown single-crystal TiN(001) and TiN(111) layers on MgO(001) and $Al_2O_3(11\bar{2}0)$, respectively, at $T_s = 700-1050$ °C under conditions resulting in large (> 1500 Å) atomically-flat terraces. Partial TiN monolayers ($\theta_{TiN} = 0.1-0.8$ ML) were then deposited and *in-situ* high-temperature STM used to follow temperature-dependent coarsening and decay kinetics (Ostwald ripening) of 2D adatom and vacancy islands on flat terraces as well as temporal island shape fluctuations. From the results, combined with solutions of the Gibbs-Thompson and diffusion equations and a new theory of anisotropic shape fluctuations, we obtain the atomic transport parameters listed above which are then used as input into higher-level KMC and level-set models for predicting microstructural and surface morphological evolution as a function of growth parameters. The simulated and experimentally-determined microstructures and surface morphologies are in good agreement and provide detailed atomic scale understanding of complex surface interactions during reactive film growth.

Portable Fuel Cells and Portable Batteries

Professor William H. Smyrl
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Department of Chemical Engineering and Materials Science
Minneapolis, MN 55455

At the present time, there is a resurgence of interest in fuel cells after more than a decade of modest levels of research and development efforts. The increase of activity may be described around several types of fuel cells, but the interest here is in the compact fuel cell that was stimulated in its development by the Department of Defense. Attention was first attracted to it because it had a lower mass than the alternate electrochemical batteries. This theme of fuel cell vs battery is a continuing question for all small devices and applications, especially since the interest has now spread to portable electronic devices such as the cell phone, the laptop computer, portable digital assistants, and digital cameras. Most of the interest in the compact fuel cell is focused on the polymer electrolyte membrane system, and that will be the focus here. We have miniaturized methanol/oxygen fuel cells on silicon wafers and have shown that the performance approaches that for large state-of-the-art cells when scaled for size. Miniaturization and materials issues will be discussed in the seminar.

Environmental Catalysis: Molecular Science and Potential Applications

Peter C. Stair
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It is estimated that the annual release of byproducts (waste) into the environment from chemical manufacturing is 100 million tons. Clearly, improvements in 1) the efficiency and selectivity of chemical processes, 2) the treatment of chemical emissions, and 3) the understanding of chemical transformations in natural systems are required to significantly reduce the impact of this human activity on the environment. Catalysis is the essential process technology for the production of most chemicals and for the treatment of emissions in the United States. "Environmental Catalysis" is the name we have given to those catalytic processes associated with each of these areas. While there are many challenges and opportunities for contributions to catalytic science in each of these areas, catalytic oxidation is perhaps the greatest challenge but with the greatest potential. In this lecture the some of the challenges and the potential of catalytic oxidation will be discussed with particular attention to scientific issues under investigation in the Institute for Environmental Catalysis at Northwestern University.

Compact Optical MEMS Actuators with Super Deformable Flexural Elements

Alan Feinerman
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The Mesoscopic MEMS (MicroElectroMechanical Systems) technology developed at UIC allows the fabrication of structures not possible with conventional planar thin film patterning methods. These techniques enable the fabrication of an agile micro-mirror that can rapidly tip and tilt large angles in two independent directions with a small footprint on the substrate. The mirrors are also capable of piston motion, a third degree for freedom. The mirrors can be electrostatically actuated, and are tethered to the substrate with a drop of a conducting liquid. The drop is confined to a lithographically defined wetting area on the mirror and the substrate.

Molecular Ordering at Liquid-Liquid Interfaces as probed by X-ray Surface Scattering

Mark Schlossman
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Liquid-liquid interfaces play an important role in many chemical and biological systems in addition to being interesting model systems to study the statistical physics of interfaces and membranes. Water-oil interfaces are a model for the interaction of water with a hydrophobic molecular environment, important for protein folding and the formation of structures in complex fluids. Biological membranes exist at aqueous-aqueous interfaces and provide a dynamic platform for important cell processes. Recent advances in x-ray scattering measurements of liquid-liquid interfaces allow for the study of ordering and fluctuations in the molecular length scale. Several fundamental issues can be addressed, including (a) molecular ordering of solvents (bulk liquids) and surfactants at liquid-liquid interfaces, and the influence of the solvents on surfactant ordering, and (b) the existence of monolayer domains at these interfaces, the issue of domain equilibrium (creation and annihilation of domains), and phase transitions in these domain phases. Studies of water-oil interfaces that address these issues will be presented.

Ionization Gauge Measurements at Low Pressures

B. R. F. Kendall
Elvac Laboratories

Factors influencing the accuracy of ion gauge measurements at low pressures are reviewed. Hot-cathode gauges operating below 10 Torr may exhibit large errors resulting from electron-stimulated desorption, X-Ray effects, and thermal outgassing. Special hot-cathode gauges have been developed to minimize these problems. They include the extractor, modulated Bayard-Alpert and energy analyzing (Helmer) gauges. Unfortunately these have become increasingly rare (and expensive) in recent years. In cold-cathode gauges the main problems have been nonlinearities (especially below the magnetron knee), plasma instabilities, stray magnetic fields and delayed starting. Recent developments in several laboratories have progressively eliminated or reduced these problems, so that the latest-generation cold-cathode gauges are particularly well suited to low-pressure operation. Test results on modern magnetron, inverted magnetron and double-inverted-magnetron gauges will be presented.

Abstracts for Contributed Talks

Fluid Transport and Phase Change in Carbon Nanotubes

Almila G. Yazicioglu, Constantine M. Megaridis, and Özgür Aytekin

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Nevin Naguib, Haihui Ye, and Yury Gogotsi

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The study of carbon nanotubes has been rapidly progressing for the past decade. Fluid behavior in carbon nanotubes may be significantly different from that in conventional pipes, even microcapillaries. However, very few experimental studies have been reported on the behavior of fluids at the nanoscale¹. In this work, transmission electron microscopy (TEM) experiments are performed on carbon nanotubes filled with a multiphase aqueous fluid, whose components at room temperature are predicted to be 85.2% H₂O, 7.4% CO₂ and 7.4% CH₄ (mole) through thermodynamic equilibrium calculations². A recent study³ reported on the hydrothermal synthesis of multiwall carbon nanotubes with a high aspect ratio, high degree of graphitization and smooth internal walls. These nanotubes are rarely open-ended, while most of the closed-end nanotubes encapsulate a high-pressure multiphase aqueous fluid, displaying segregated liquid and gas inclusions with clearly defined interfaces⁴.

Dynamic fluid experiments were performed on fluid-filled carbon nanotubes via TEM using electron irradiation or a resistive heater stage to achieve gentle heating of the fluid contained inside the nanotubes. Phenomena such as thin meniscus evaporation, reversible liquid volume contraction/expansion, irreversible expansion/protrusion and precipitation, bubble formation, and thin film liquid transport with rates of the order 0.5 $\mu\text{m/s}$ have been observed and partially documented^{4,5}. Other experiments of transport of liquid from one side of a carbon nanotube to the other via evaporation and condensation demonstrated the feasibility of liquid transport in response to external thermal stimuli in pipes of <100 nm in diameters. Electron energy loss spectroscopy (EELS) analysis was also performed on a multiwall carbon nanotube with trapped aqueous fluid, which revealed that oxygen is present inside the nanotube, as well as on the inner and outer surface of the nanotube walls. This result further indicates that the surface of the carbon nanotube can adsorb oxygen, leading to the formation of functional groups, such as hydroxyl, which have been shown to transform the carbon nanotube surface to a hydrophilic one⁶.

Closed hydrothermal carbon nanotubes, having the ability to contain an aqueous fluid in the vacuum atmosphere of a TEM, seem to be very appropriate tools for fluid studies possibly approaching the continuum limit. It has been shown through high resolution TEM that the dense aqueous fluid wet the inner surface of the carbon nanotube, possibly due to the formation of oxygen-based groups, which render the carbon surface hydrophilic. Understanding fluid behavior at the nanoscale would facilitate the effective design and operation of future micro- and nanofluidic devices, such as drug delivery systems, biosensors, and micro heat pipes.

¹ Sobolev, V.D. *et al.*, J. Coll. Int. Sci. **222**, 2000; Bogomolov, V.N., Sov. Phys. Tech. Phys. **37**(1), 1992.

² Gogotsi, Y. *et al.*, Diam. Rel. Mat. **7**, 1998.

³ Gogotsi, Y. *et al.*, J. Mat. Res. **15**(12), 2000; Libera, J. and Y. Gogotsi, Carbon **39**(9), 2001.

⁴ Gogotsi, Y. *et al.*, Appl. Phys. Lett. **79**(7), 2001; Megaridis, C.M. *et al.*, Phys. of Fluids **14**(2), 2002.

⁵ Gogotsi, Y. *et al.*, MRS Symp. Proc., Boston, 2001.

⁶ Li, H. *et al.*, Ange. Chem. Int. Ed. **40**(9), 2001.

Synthesis and Tribological Studies of Nanolayered TiB₂/TiC Coatings for Possible Elevated Temperature Applications

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Multilayered coatings composed of 3 nm TiB₂ and various individual layer thicknesses of TiC were synthesized using non-reactive dual-cathode magnetron sputtering techniques with substrate rotation on silicon(001), M2 steel and WC cutting inserts. The two coating materials were chosen for their high hardnesses, melting temperatures, and immiscibility between different crystal structures. The goal of the research is to synthesize hard and chemically stable coatings that provide wear protection at high contact pressures and temperatures. Under appropriate deposition conditions, we obtained coatings with TiB₂(001) preferred orientation. Room-temperature hardness of these coatings approaches 70 GPa, far exceeding the rule-of-mixture value. Wear and durability tests using block-on-ring (at room temperature) and ball-on-disk (up to 250 C) configurations on coated M2 steels and C6 WC cutting inserts demonstrated the improved tribological performance of these coatings under unlubricated conditions compared with standard coatings such as TiN. Actual dry machining on coated C3 WC cutting inserts was performed. These results will be presented and discussed in terms of the coating's potential in dry machining and high-temperature tribological applications.

An Inlaid Electroplated Copper Coil for Implanted and MEMS Applications

Jie Wu and Gary H. Bernstein

Dept. of Electrical Engineering, Univ. of Notre Dame

A fabrication procedure was developed to electroplate metal microstructures of large dimensions within silicon substrates. This method circumvents the molding difficulties in microelectronic electroplating, relaxes the restrictions on mold topologies, and offers the potential for integration with circuits. The fabricated coils were used as the receiving coil of a loosely-coupled inductive link, which could be used extensively for applications in medical implants. Parasitic capacitance of integrated coils together with leakage inductance of inductive links causes system resonance, which is utilized to obtain extra voltage amplification at the output. The inductive link is capable of transmitting not only power, but also signals of particular waveforms by amplitude modulation. A comparison of system performance was made for thin film and electroplated coils. Electroplated coils yield better results in all cases. With an electroplated coil, higher output was obtained, and more power was delivered with better efficiency than from a thin film coil.

Dimerization of NO and transformation to N₂O on Ge(100)

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Temperature-programmed desorption studies of submonolayer coverages of nitric oxide (NO) on a Ge(100) (2x1) surface have determined the non-dissociative nature of the adsorption of NO on Ge(100) at 110 K. Subsequent electron bombardment results in electron-stimulated desorption of N₂O and N₂ at that temperature, without heating, which is attributed to the formation of NO dimers on the cold surface. This conclusion is supported by studies of adsorbed layers of N₂O, which is adsorbed at least partly non-dissociatively, and which yields little desorption of the parent N₂O molecule when bombarded with electrons.

Profile Coatings at the Advanced Photons Source*

Chian Liu

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We report a method of profile coating to achieve a certain selected thickness profile of a thin-film coating using dc magnetron sputtering. In profile coatings, the substrate is passed over a contoured mask at a constant speed to obtain a desired profile perpendicular to the substrate-moving direction. The shape of the contour depends on the desired profile and the thickness distribution directly above the gun at the substrate level. Four-inch-diameter Si wafers were coated through a 100-mm-long by 152-mm-wide aperture on the top of the shield-can. The thickness distribution was then obtained using a spectroscopic ellipsometer with computer-controlled X-Y stages. A model was developed to fit the measured thickness distribution. The relative thickness weightings are then obtained for the entire open area of the aperture. When the substrate is moving across the shield-can during a deposition, the film thickness is directly proportional to the length of the opening on the can along the moving direction. By equating the summation of relative weighting to the required relative thickness at the same position, the length of the opening at that position can be determined. By repeating the same process for the whole length of the required profile, a contour can be obtained for a desired thickness profile. The contoured mask is then placed very close (less than 1mm) to the substrate on the opening of the shield-can. The number of passes and the moving speed of the substrate are determined according to the required thickness and the growth rate calibration. This method of profile coating has been applied to coat laterally graded W/C multilayers for tunable x-ray double-monochromator and x-ray fluorescence detection applications. It has also been applied to coat gold on a cylindrical substrate to obtain an elliptical mirror for x-ray focusing applications. Test results for these applications will be presented.

* This work is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. W-31-109-ENG-38.

Interface and nanoscale magnetism in magnetoelectronic devices studied using synchrotron-based polarized x-ray techniques

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Applications incorporating magnetic materials into electronic devices, such as magnetic random access memory (MRAM), have increased the need for advanced characterization of layered and nanoscale magnetic structures. For example, MRAM elements typically consist of ferromagnet/insulator/ferromagnet tunnel junctions in which the barrier is formed via plasma oxidation of a metallic Al layer, with associated questions concerning the formation and structure of the barrier layer interface. Also, at very high densities, magnetostatic coupling between elements in patterned arrays are a concern. Magnetic circular dichroism, in combination with x-ray scattering and microscopy techniques, offers structural, chemical, and magnetic information with both layer specificity and lateral spatial resolution. The polarized x-ray facility at sector 4 of the Advanced Photon Source consists of two undulator beamlines providing circular polarized x-rays from 500 eV to 100 keV, thus allowing access to nearly all magnetically interesting absorption edges. We have used dichroism in absorption and reflectivity, combined with x-ray photoemission microscopy, to examine the interface structure and lateral coupling in a series of samples approximating real MRAM devices. We find evidence that the oxidation front proceeds through the Al layer preferentially through grain boundaries, and that barrier layers optimized for tunnel junction performance are nonstoichiometric. Over-oxidation results in coexisting metallic and oxidized regions in the underlying ferromagnetic layer. Field annealing to 200°C results in improved tunneling properties, reduction of ferromagnetic interface oxides, and improved magnetic ordering. We also find strong coupling between neighbors in rectangular patterned arrays of Co elements. At an interelement gap distance of 100 nm, coupling can persist out to the 5th nearest neighbor.

This work and use of the Advanced Photon Source was supported by the U.S. Department of Energy, Office of Science, under Contract No. W-31-109-ENG-38.

Nanoscale Fabrication and Characterization of Chemically Modified Silicon Surfaces Using Atomic Force Microscopy in Liquids

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The atomic force microscope has emerged as a powerful tool for patterning organic nanostructures on surfaces through such techniques as Dip Pen Nanolithography [1] and Nanografting [2]. These nanolithography techniques have been used to pattern organic molecules on gold [1,2] and oxidized silicon surfaces [3]. Here, we present a new Liquid Phase Nanolithography technique for patterning organic nanostructures bound covalently to hydrogen passivated silicon surfaces.

AFM tip-induced oxidation of hydrogen passivated silicon has been utilized for the fabrication of oxide nanostructures with ~10 nm resolution [4]. However, when hydrogen is desorbed from H-passivated Si(111) surfaces submerged in organic solvents using ultra-violet light, oxidation is avoided and 1-alkene molecules suspended in the solvent react directly with the depassivated regions [5]. In Liquid Phase Nanolithography, hydrogen desorption is induced by applying a bias across an AFM tip-sample junction submerged in an organic solvent. Appropriately chosen molecules suspended in the solvent directly chemisorb on the depassivated lines. We will present preliminary results for patterning nanostructures of 0.45 M *exo*-5-norbornene-2-ol in distilled dimethyl sulfoxide and neat undecylenic acid methyl ester on H:Si(111) using this technique and suggest approaches for utilizing this scheme to fabricate biomedical nanosensors.

This work has been supported in part by the Northwestern University Institute for Bioengineering and Nanoscience in Advanced Medicine.

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An AFM Study on Living PC12 Cells

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Atomic force microscope (AFM) is a powerful tool of imaging biological structures at high resolution in real-time fashion under physiological conditions. It also provides the opportunity of quantifying biomolecular interactions that are essential of protein functions in living cells. Here we report on the application of AFM to three-dimensional imaging of PC12 (neural) living cells, as well as the study of the specific interaction between nerve growth factor (NGF) and its receptor TrkA on cell membrane. PC12 cells are a secondary cell line that was originally derived from a pheochromocytoma (a tumor of the adrenal gland) that developed in an irradiated rat. We have first captured the images of PC12 cells from micrometer scale to nanometer scale in both fluid tapping mode and fluid contact mode in RPMI medium. The images showed rugged surface of PC12 cell corresponding to the cell membrane with various proteins embedded on it. Since NGF promotes neuronal survival and differentiation by activating TrkA receptors in PC12 cells, it is essential of understanding the distribution of TrkA receptors on the cell membrane. Using the NGF-TrkA specific interaction as a probe, we acquired TrkA distribution on PC12 cell membrane via force volume imaging. This was accomplished by modifying NGF molecules onto an AFM tip. As the NGF-coated tip scanned on the cell membrane, strong attractive forces (nano-Newton level) were detectable at local regions, indicating local concentration of TrkA. The NGF-TrkA specific interaction was derived from the statistical analysis of numerical force curves.

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Atomic level characterization and control of free radical surface chemistry using scanning tunneling microscopy

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A unique organosilicon surface chemistry has been explored with the ultra-high vacuum (UHV) scanning tunneling microscope (STM). The chemisorption of an organic free radical (2,2,6,6-tetramethyl-1-piperidinyloxy (TEMPO)) to reactive dangling bonds on the Si(100) surface was studied. Specifically, a clean Si(100)-2×1 surface was exposed to a series of controlled doses of gas phase TEMPO molecules ranging from 0.03 L to 0.57 L. The surface was characterized with STM and scanning tunneling spectroscopy following each subsequent dose from sub-monolayer coverage, in which individually isolated molecules are observed, to full monolayer coverage. Imaging of individually isolated molecules revealed a bias dependence, both in topography and two dimensional conductance maps.

To further control this surface chemistry, electron stimulated desorption of the hydrogen passivated Si(100) surface was implemented using the STM. This technique allows for the specific removal of hydrogen from the surface, yielding reactive dangling bonds on an otherwise inert substrate. Successful utilization of this STM based nanolithography has enabled selective adsorption of TEMPO to the pre-patterned areas.

Controlling the Nanoscale Morphology and Chemistry of Organic Films Deposited by Polyatomic Ions

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www.chem.uic.edu/hanley

The control of chemistry and morphology on the nanometer scale is critical to a range of new technological applications. Polyatomic ion beams with hyperthermal kinetic energies ranging from 1 to 500 eV are advantageous for practical surface modification and nanofabrication due to their ability to fabricate thin film nanostructures with controlled morphology, unique collision dynamics, and ability to transfer intact chemical functionality to the surface. Hyperthermal polyatomic ions also play a critical role in plasma processing, laser ablation, and several other energetic deposition processes. Several experiments are described in which mass-selected and non-mass-selected polyatomic ion beams are used to create nanometer organic thick films with controlled surface and buried interface morphologies. X-ray photoelectron spectroscopy, atomic force microscopy, x-ray reflectivity, and scanning electron microscopy are utilized to analyze the morphology and chemistry of these films. Polyatomic ions are found to control film morphology on the nanoscale through variation of the incident ion energy, ion structure, and/or substrate.

Abstracts for Posters

Direct Nanoscale Impedance Scanning Microscopy

L. S. Cavanaugh, E. F. Fabbroni, K. R. Shull, and M. C. Hersam

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Many atomic force microscopy (AFM) methods exist for examining electrical properties with nanoscale spatial resolution. Non-contact mode AFM techniques such as Kelvin Probe Force Microscopy, Scanning Impedance Microscopy, and some forms of AFM potentiometry rely upon relatively long-range electrostatic forces [1]. While these methods minimize surface perturbation by the tip, the measured data can be corrupted by uncontrolled surface variables [2]. Similarly, methods such as Scanning Capacitance Microscopy [3] and Scanning Capacitance Spectroscopy [4] rely upon electrostatic forces across a surface oxide, which can be affected by local non-uniformities in oxide thickness and dopant profile [1]. Other contact mode AFM methods, such as Spreading Resistance Profiling, rely on conduction paths close to the surface and across the sample [5]. By combining aspects of the aforementioned techniques, we have developed a nanoscale impedance spectroscopic measurement using conductive contact mode AFM in which an AC bias is applied across the tip-sample junction. Using a lock-in amplifier, the magnitude and phase of the resulting current through the tip is monitored as a function of space and driving frequency, thus yielding quantitative information about the local surface impedance. This presentation describes the development and initial proof of principle measurements for this new characterization scheme, which will be referred to as Direct Nanoscale Impedance Scanning Microscopy (DNISM).

Initial control experiments were performed on a set of 6 gold nanowires on SiO₂. The nanowires were electrically connected to known impedances with resistance of 1M Ω and capacitance ranging from 50 pF to 470 pF. The DNISM technique demonstrated excellent agreement with theoretical expectations for the magnitude and phase of the current for driving frequencies between DC and 10 kHz. Similar to DC mode AFM potentiometry [6], DNISM has demonstrated spatial resolution on the order of 10 nm, limited only by the radius of curvature of the conductive tip. Since this technique is especially appropriate for mapping conductive paths perpendicular to the sample surface, DNISM has also been applied to polyethylene matrices impregnated with carbon black nanoparticles above the percolation limit. Nanoscale variations in the AC conductivity through these samples extend previous DC mode AFM potentiometry measurements on this system [7].

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Change of Optoelectronic Properties in Vacuum Evaporated Tungsten Oxide during thermal Annealing

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Tungsten Oxide (WO_3) has been investigated for electronic device, photonics, sensor, and tribology applications. Study of evaporated WO_3 for gas sensors indicated that this material has capability to detect few PPM-NO and NO_2 and other chemically active gases. Thin films of WO_3 have been fabricated using vacuum evaporation, metal organic chemical vapor deposition (MOCVD), sputtering, and sol-gel methods. Among these techniques, vacuum evaporation became one of the most promising ways of producing device quality films because its simplicity, low contaminants, low cost, and scalability. In this study we have systematically investigated the optoelectronic properties of vacuum evaporated WO_3 films as a function of annealing temperature. The project aimed at enhancement of electronic properties of WO_3 films.

WO_3 films were fabricated on glass and silicon substrates by vacuum evaporation of WO_3 powder on a cold substrate. The coated films were annealed at a substrate temperature between 100-600 °C in an oxygen atmosphere. Films were investigated with Raman, X-ray Diffraction (XRD), Atomic Force Microscopy (AFM), optical transparency and electrical conductivity measurements. The results were analyzed to understand annealing effect on crystal structure, and the relationship between crystallinity and optoelectronic properties.

It was found that the crystalline structure of evaporated WO_3 gradually varied when annealing temperature is increased. Annealing temperature above 500 °C, the change of crystallinity is saturated. Moreover, we have measured the surface morphology with AFM. The change in surface morphology of as-deposited, annealed at 300 °C and 500 °C samples observed. When the annealing temperature was increased, the surface morphology changed from a rough surface to a smooth surface, and the grain morphology was also varied. These phenomena were supported by the Raman spectroscopy. The optical transparency is another important property of WO_3 films because their applications in photonic devices. We have investigated the optical transparency of these films in the range of 200-900 nm. The results indicate that the films annealed over 300 °C have drastic change of optical transparency. An attempt was made to investigate the electronic properties with the annealing temperature. These results revealed that the optoelectronic properties of WO_3 films were attributed to the change of crystallinity during annealing process. These changes are interpreted as the formation of nanocrystalline WO_3 by annealing. Detailed experimental results of this investigation will be presented in this conference.

Studies on the Surface of Resin-Matrix Dental Composites

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The surface chemical characterization of resin-matrix dental composites is examined by secondary ion mass spectrometry (SIMS), x-ray wavelength dispersion spectroscopy (WDS) and atomic force spectroscopy (AFM). Several polymethylmethacrylate resins are mixed with different weight percent glass fillers and thermally cured. SIMS measurements allow a relative quantitative analysis for dental composites by using carbon (C^+ , $m/z12$) or CH_3CO^+ ($m/z43$) as an internal reference present at large homogeneous and constant concentration in samples. These peaks are used to standardize the signal of SIMS data for the quantification of BaO and SrO on the surface of dental composites before and after the aging process. In WDS experiments, a thin layer of carbon is evaporated onto the surface of dental composites to avoid charging. The WDS results show that the BaO and SrO concentrations are much lower after the samples are aged in different media for four months, as confirmed by SIMS. In addition, AFM is used to compare the surface roughness of a number of dental composites prior to and after analysis.

Ion Assisted Deposition of MgB_2 Thin Films

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After the discovery of superconductivity in MgB_2 , research groups all over the world have focused on synthesizing this compound in many forms. Methods such as pulsed laser deposition, molecular beam epitaxy, dc magnetron sputtering and co-evaporation have been applied in the deposition of MgB_2 thin films. However, producing these films under UHV conditions has been hindered due to the high volatility of Mg at high temperatures. Here, we report a novel method for UHV fabrication of MgB_2 thin films using ion assisted deposition. Prior to deposition, the substrate was prepared by deposition of Mg on Hf(0001) with a Mg flux created by a heated Ta wire around which a Mg ribbon has been wrapped. Lattice mismatch of Hf(0001) to MgB_2 is 1.7%, and therefore favors epitaxial growth. Diborane (B_2H_6) and Decaborane ($B_{10}H_{14}$) have been used as B sources to generate positively charged ions. With the chamber backfilled with borane, a sputtering ion gun was employed to ionize the borane and then to direct it towards the substrate. X-ray photoelectron spectroscopy (XPS) and Temperature Programmed Desorption (TPD) were used to monitor the ion assisted deposition. The Mg 2s to B 1s peak area ratio is 1 to 2 for the films produced from diborane. TPD spectra of Mg ($m/e=24$) show two distinct peaks at 560 K and 780 K for the desorption of Mg from Hf(0001). The peak at 560 K is characteristic of multilayer desorption of Mg while the latter is seen only after the ion assisted deposition. Although these peaks are independent of the choice of B source, decaborane is clearly more efficient for ion assisted deposition and worthy of further investigation.

Quasi-Equilibrium During Epitaxial Growth: A Direct Verification of the Walton Relation with Kinetic Monte Carlo Simulations,

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Nucleation theory [1] is a well known theoretical tool for modeling epitaxial growth with rate equations. Fundamental to this rate equation approach is the idea of the critical nucleus size, i , which is defined as one less than the smallest-sized stable cluster of atoms on the surface. At low coverage and assuming quasi-equilibrium (detailed balance between attachment and detachment rates of atoms to and from the unstable islands), the somewhat complicated, coupled differential equations of the theory simplify to yield a closed-form scaling relation, $N \sim (D/F)^{-i/(i+2)}$, where N is the number density of stable islands, D is the monomer diffusion coefficient, and F is the deposition flux. This scaling relation has been applied to experimental studies [2] of epitaxial growth to extract important surface diffusion parameters for different epitaxial systems. Because this simple closed-form power law relation between N and the ratio D/F , which allows relatively transparent experimental determination of the parameters characterizing surface diffusion, depends strongly on the *assumption* of detailed balance, it is interesting to note that the realm of applicability of this quasi-equilibrium condition has not been determined directly (i.e. via simulations).

We have produced a square geometry solid-on-solid (SOS) kinetic Monte Carlo model to investigate the presence of a low coverage quasi-equilibrium regime during epitaxial growth. The SOS model is a restricted pair-bond model wherein atoms on the surface with one in-plane nearest neighbor are allowed to detach from island edge positions with a rate, r_1 . Thus, the simulation is applicable to homoepitaxial (100) metallic surfaces with $i = 3$. In the quasi-equilibrium regime the number density of islands of size j ($2 \leq j \leq i$) is predicted to scale with the number density of monomers, n_1 , according to the so-called Walton relation, $n_j \sim n_1^j$ [3]. We have studied the scaling of the number of unstable dimers and trimers with the number of monomers during growth to low coverages to determine the presence of detailed balance as evidenced by the verification of the Walton relation. We show that this relation does not always hold during epitaxial growth and that its presence depends strongly on the ratios, D/F and r_1/D . We report on the ranges of these ratios over which equilibrium is observed.

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Preparation and Properties of Titanium Oxide Films by Reactive Vapor Deposition

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The high refractive index, high hardness, photocatalytic nature and many other outstanding properties of titanium dioxides have made them useful for many applications. Ion-assisted, high-rate, reactive dc magnetron sputtering and e-beam evaporation techniques are used to deposit the oxides. Various characterization methods such as ellipsometry, Raman spectroscopy, XRD, SEM, hardness and stress measurement techniques were used to measure crystallinity, morphology, optical and mechanical properties of the films. Titanium oxides come in various compositions and crystal structures. The stoichiometric oxide-compounds of titanium include TiO, TiO₂, Ti₂O₃, Ti₃O₅ with varying colors. Depending on the growth parameters, these stoichiometric oxides were detected in the preparation of thin films. Under suitable conditions, the sputtered or evaporated atoms will recombine reactively with the partial pressure of supplied oxygen to form stoichiometric films of colorless TiO₂. The transparent films are of the rutile, anatase or mixed crystal forms depending on growth conditions. The rutile phase has a higher refractive index (up to 2.7) and a higher hardness (15-20 GPa) than the anatase phase, but it is the anatase that show the stronger photocatalytic effect. Increasing substrate bias, increases the hardness and the stress in the film and reduces the value of the refractive index. Thus, the deposition conditions must be carefully controlled to obtain the desired properties for a particular application, and certain properties may have to be compromised to obtain the desired product.

Templated growth of Styrene molecular wires on Si(100) using feedback controlled lithography

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This study combines the spontaneous growth of one-dimensional molecular wires on a semiconducting surface with the creation of atomically precise templates. Specifically, styrene molecules, which are known to experience self-directed growth on the Si(100) surface along dimer rows, have been induced to grow from individual dangling bonds that have been created on a hydrogen-passivated Si(100)-2x1 surface through feedback controlled lithography (FCL) using an ultra-high vacuum (UHV) scanning tunneling microscope (STM). The site-specific creation of individual dangling bonds allows control over the position and length of the styrene wires whose growth is confined along a dimer row.

In addition, the robustness and stability of the styrene chains to ambient exposure have been studied and confirmed. The thermodynamic stability of the chains in the ambient environment seems to be favored by certain growth orientations and the presence of proximal defect sites that raise the energy barrier for the reverse reaction (unzipping of the chains). The controlled growth of molecular arrays in UHV and their stability in ambient indicate the future possibility of *ex-situ* attachment of non UHV-compatible molecules by wet chemical methods on the technologically significant Si(100) surface.

Electron Beam Effects on Diethylsilane Covered Si (100) Surfaces Investigated by Temperature Programmed Desorption

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Ethylated silicon or germanium containing molecules are promising candidates to fabricate hetero-junction atomic layer epitaxy SiGe devices. However, thermal processes to dissociate unwanted ligands from parent molecules after dosing are not suitable for the device fabrication. Preliminary results of the electron induced dissociation of diethylsilane (DES) on Si(100) surface are reported. DES molecules were dosed onto Si (100) surface at 120 K and the thermally desorbed species with and without 600 eV electron beam radiation were investigated by temperature programmed desorption (TPD). Electron beam dissociation effects as well as electron induced state changes reflected in TPD spectra will be discussed for several different initial gas exposures at 120 K.

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Polyatomic Ion Deposition of Thiophenic Thin Films

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Oligo- and polythiophenes are utilized as conducting polymers in many applications. Polyatomic ion deposition at ion impact energies below 200 eV is an effective method for the growth of thin organic films on polymer, metal, and semiconductor surfaces.* We demonstrate here the growth of thiophenic thin films on aluminum and silicon substrates by mass-selected <200 eV C₄H₄S⁺ ion beams. Thiophenic films are also grown by non-mass selected ion beams containing <200 eV C₄H₄S⁺ and fragment ions. Our non-mass selected ion deposition method permits rapid film growth over wide substrate areas and it is described here for the first time. X-ray photoelectron spectroscopy and atomic force microscopy are used to compare the film chemistry and morphology for the two methods. Oxidation of the films during aging in air is observed.

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Silylation of a hydroxyl-terminated self-assembled monolayer surface through reactive collisions of mass-selected ions

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Chemical modification of surfaces in a spatially selective fashion is an objective with potential importance in materials science including the development of chemical sensors and other MEMS devices¹.

In this study, a well-known solution reaction, silylation of hydroxyl surfaces, was performed in the gas phase using a reactive, hyperthermal energy beam of ions as the chemical reagent. A hydroxyl-terminated self-assembled monolayer (HO-SAM) surface was modified using a tandem mass spectrometer with BEEQ configuration. Various tertiary silylium ions, with the general structure SiR_3^+ , where R represents CH_3 , OCH_3 , F, Cl, Br, and NCO, were used as the reagent ions. These reagent ions were mass-selected and made to impact at normal incidence at the HO-SAM surface at a kinetic energy of 12 ~ 15 eV and a current density of 1.4 nA/cm². Under these conditions, the $\text{Si}(\text{CH}_3)_3^+$ resulted in ca. 30 % conversion of the HO-terminated monolayer after 1 hour of treatment².

Various methods were employed to verify the character of the bond between the projectile ion and the surface. In situ chemical sputtering using CF_3^+ ion showed evidence for covalent modification. XPS and TOF-SIMS further supported the formation of the silyl-etherification. Surface patterning was also successfully demonstrated using $\text{Si}(\text{CH}_3)_3^+$ ion and the modified surface was imaged using the TOF-SIMS technique.

Not all the silylium ions tested reacted with the surface, and calculations were performed to seek correlations between ion structure and surface modification. At the 6-31G(d,p) level of theory, the results revealed that the amount of local positive charge is more or less related to the tendency of modification³. It is concluded that electrophilic attack is responsible for this covalent modification of HO-SAM surface.

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Reactivity Towards Oxidation of the TaB₂(0001) Surface

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Many early transition metal diborides adopt the AlB₂ structure, which has a simple hexagonal lattice with the c-axis normal to planes of close-packed metal atoms that alternate with planes of boron atoms arranged in a graphite-like structure. For metal diborides of this structure, a key question is whether the (0001) surfaces are metal or boron terminated. Previous studies have shown that the HfB₂(0001) surface is metal-terminated [1,2] whereas the TaB₂(0001) surface is terminated by a boron layer [3]. The bulk properties of HfB₂ and TaB₂ are generally quite similar in that they are both extremely hard, have melting points above 3000 EC, and have high metallic electrical conductivities. Growth of single crystals of the two diborides differs in that the c-axis is the preferred growth direction for HfB₂ whereas there is no preferred growth direction for TaB₂ [4]. The different terminations of HfB₂(0001) and TaB₂(0001) might be expected to impart rather different reactivity to the two surfaces. We have studied the reaction of a clean TaB₂(0001) surface with O₂ under ultrahigh vacuum conditions with X-ray photoelectron spectroscopy. We find that the surface is remarkably unreactive with a dissociative sticking probability for O₂ that is several orders of magnitude lower than that observed for the HfB₂(0001) surface. The reactivity is so low that it may be attributed entirely to defect sites implying that the ideal boron terminated surface has essentially zero reactivity towards oxidation at room temperature. In order to gain a better understanding of the structure of the clean surface and the nature of the defect sites present, we have obtained atomically resolved images of the surface with scanning tunneling microscopy.

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Thanks for coming to our meeting - your participation made it possible!