

Thursday Afternoon Poster Sessions

Surface Science

Room: Hall D - Session SS-ThP

Poster Session

SS-ThP1 Adsorption, Photo-Fragmentation, and Ion-Desorption Pathways of Organic Molecules at Semiconductor Surfaces using Synchrotron Radiation Techniques, T. Sekiguchi, Japan Atomic Energy Agency (JAEA), **H. Ikeura-Sekiguchi,** National Institute of Advanced Industrial Science and Technology (AIST), Japan, **Y. Baba,** Japan Atomic Energy Agency (JAEA)

The chemistry of organic molecules on semiconductor surfaces has attracted much attention due to the perspective of the molecular wires, self-assembled monomolecular layer (SAM), and semiconductor-organic hybrid formation such as SiC. We have investigated the adsorption interaction, photo-dissociation, and ion-desorption of multifunctional organic molecules such as acetone $[(CH_3)_2C=O]$ adsorbed on Si substrates. We used synchrotron radiation techniques including polarization-angular dependences of near-edge x-ray absorption fine structure (NEXAFS) and photon-stimulated ion-desorption (PSID). We measured photon-energy dependences of ion yields for a variety of fragments in the carbon 1s excitation region, along with the NEXAFS. We compare results for the following three systems: (1) dissociatively adsorbed monolayered molecules prepared at a room temperature (RT), (2) molecularly adsorbed monolayered molecules prepared by heating condensed molecules very slowly from liquid-N₂ low temperatures (LT) to RT, and (3) multilayered molecules prepared at LT. The results showed that mass-patterns and excitation spectra of PSID depend dramatically on the chemical states of adsorbed systems. We conclude that PSID and NEXAFS techniques are useful tools to investigate chemical states such as configuration, orientation, and charge-transfer interaction of adsorbed molecules at surfaces.

SS-ThP2 AFM Studies of poly-L-lysine Mediated Adsorption of Alginate to Hydrophilic and Hydrophobic Surfaces, C. Franqui, H. Applebaum, K.T. Queeney, Smith College

The poly-L-lysine (PLL)-mediated adsorption of alginate to hydrophobic and hydrophilic substrates is a useful model system for understanding the initial stages of biofilm formation. Work in our lab using a variety of techniques has shown that film continuity and morphology are strongly influenced by the underlying substrate. The current work uses atomic force microscopy (AFM) to examine differences in film morphology as a function both of substrate surface chemistry and of adsorption conditions. On a hydrophobic, electrically neutral alkylsilane monolayer, PLL films adsorbed from pH 11 buffer and air dried exhibit morphologies that are suggestive of polymer shrinking as water is removed from the film, with networks of PLL surrounding regularly-spaced patches of bare surface. The proportion of surface covered by PLL decreases with increasing PLL molecular weight, which suggests stronger PLL-surface interactions for the lower MW polymers. Since adsorption under these conditions is thought to be driven by a transition from alpha helix in solution to random coil for adsorbed PLL, these results may indicated a lesser amount of uncoiling for the larger MW PLL. The role of drying in determining film morphologies is explored by comparing subsequently-adsorbed alginate films on both pre-dried and undried PLL overlayers. On hydrophilic silica PLL adsorbed at neutral pH forms much more uniform films, consistent with strong electrostatic interactions between the positively charged PLL and the negatively charged surface. As ionic strength increases, PLL begins to aggregate on the surface to form a much more discontinuous film, consistent with competition for binding sites between PLL and cations in solution. Alginate adsorption to these PLL overlayers results in more complex morphologies indicative more of isolated molecular adsorption than of true film formation.

SS-ThP3 Experimental Aspects of Measuring Dissociative Sticking Coefficients of Hydrocarbons on Solid Surfaces with Independently Variable Gas and Surface Temperatures, V. Johánek, L. Valadez, G.W. Cushing, I. Harrison, University of Virginia

The thermal activation of alkanes on transition metals can be studied by a technique of effusive dosing of gases onto the metal surfaces where both gas and surface temperatures are independently variable. Dissociative sticking coefficients, $S(T_g, T_s)$, are measured by monitoring the deposited amount of surface carbon. This relatively simple method allows measurement of dissociative reaction rates of alkanes or other hydrocarbons with about 9 orders of magnitude dynamic range, however, a careful implementation is required to assure good accuracy and relevance. In particular, effects not related to the direct well-defined gas beam or to the surface under study have to be either eliminated or separated which brings

several experimental challenges. Ultimately, such $S(T_g, T_s)$ experiments can be used to define reaction rates and transition states for activated dissociative chemisorption reactions that are otherwise difficult to study under ultrahigh vacuum, surface science conditions.

SS-ThP4 Low Energy Electron Microscopy Study of Adsorbed C on Pt(111), G.W. Cushing, V. Johánek, I. Harrison, University of Virginia

Methane reforming rates on supported transition metal nanocatalysts at temperatures near 1000 K are apparently limited, in part, by the build-up and dynamics of adsorbed C.¹ We report on the use of a SPECS low energy electron microscope (LEEM) to examine the dynamics and reactivity of adsorbed C on Pt(111) at reforming temperatures. The adsorbed C coverage can be controlled by dosing hydrocarbons and/or oxygen at pressures as high as $\sim 5 \times 10^{-8}$ Torr whilst imaging with LEEM.

¹H. L. Abbott and I. Harrison, "Methane dissociative chemisorption on Ru(0001) and comparison to metal nanocatalysts", J. Catal. 254, 27-38 (2008).

SS-ThP5 Interaction of Water with BaF₂(111) at Ambient Conditions, S. Kaya, S. Yamamoto, Stanford Synchrotron Radiation Laboratory, **J.T. Newberg, H. Bluhm,** Lawrence Berkeley National Laboratory, **A.R. Nilsson,** Stanford Synchrotron Radiation Laboratory

Aggregation of water and ice nucleation on ionic surfaces have been a topic of interest for many years due to their importance in atmospheric and environmental chemistry. However, the fundamental questions such as the structure and chemical composition of thin film water on surfaces in equilibrium with ambient pressure water vapor are still largely unanswered. BaF₂(111) is one of the promising model substrates at which two dimensional hexagonal ice growth can be expected due to their matching lattice parameters. By using ambient pressure photoemission spectroscopy (APPEs) and O K-edge near-edge x-ray absorption fine structure (NEXAFS) spectroscopy, we have studied the interaction of water with the BaF₂(111) surface at water partial pressures up to 1.5 Torr. Water uptake curves indicate that monolayer coverage is achieved at relative humidities lower than 10 %. O K-edge NEXAFS findings reveal that the structure of submonolayer water on the BaF₂(111) surface is similar to the topmost surface of hexagonal ice which is lacking two dimensional long range order. Additional water layers obtained at higher relative humidities have slightly different hydrogen bonding structures. In addition, lateral hydrogen bonding network becomes more apparent with increasing water coverage.

SS-ThP6 LER Reduction by Means of a Grazing Incidence Ion Beam, C. Struck, D.N. Ruzic, University of Illinois, **R.L. Bristol,** Intel Corp.

As lithographic feature sizes continue to increase, the phenomena of line edge roughness (LER) becomes more pronounced. While many efforts are underway to decrease LER from the photoresist, post-develop smoothing techniques may be required to achieve acceptable results. We report on one such technique employing the use of an ion beam at grazing incidence unidirectional with the features. One key potential advantage of this approach over many other smoothing techniques is the ability to smooth LER at relatively long spatial length scales over large sections of, or whole wafers. LER reduction numbers are reported at both short and long spatial wavelengths using Ne, He, and Ar beams. The angle of incidence is varied, as well as ion energy, and process time. LER measurements are taken from top-down analytical SEM measurements and Hitachi image analysis software. Line profile data are taken with the SEM in cross-section mode. Tests have achieved a reduction in LER from 9.8 ± 0.67 nm to 5.5 ± 0.86 nm for 45nm CDs using an Ar beam at 500eV for 6s at an 85° angle of incidence. A reduction from 10.1 ± 1.07 nm to 6 ± 1.02 nm was shown using an Ar beam at 1000eV for 4s at a 60° angle of incidence.

SS-ThP7 Modification of PMMA Thin Films with Atomic Oxygen and Ultra-violet Light, H. Yuan, D.R. Killelea, S. Tepavcevic, S.J. Sibener, University of Chicago

The degradation and modification of polymeric surfaces by irradiation, oxygen plasmas and other reactive species have dramatic effect on their physical and chemical behavior. A molecular-level understanding of reactions at the polymer surface is necessary to guide further development of polymers in a wide range of fields, from microelectronics to aerospace. Here, we present the results of a study of photodegradation and oxidation of a model polymeric film. We exposed a poly(methyl methacrylate) (PMMA) film to vacuum ultraviolet (VUV) radiation and a collimated supersonic beam of O(³P) oxygen atoms. In separate experiments, we directly measured the mass loss of the film with a quartz-crystal microbalance (QCM) and identify the chemical changes in the PMMA film using in situ infrared spectroscopy. Previous work was limited by the necessity of removing the sample from vacuum for IR analysis; our new in situ IR system lifts this limitation and permits much greater time-resolution in our

studies of the polymer modification process. Our analysis has determined the kinetics of the reactions of PMMA with VUV and atomic oxygen, and we have investigated how exposing PMMA films to both atomic oxygen and VUV light alters the polymer properties. We have also found that exposure of the polymer to these two reagents simultaneously results in kinetics that differ from the two individual effects.

SS-ThP8 State-Resolved Measurements of CH_4 Activation on Ni(111) Without Laser Excitation. *N. Chen*, Tufts University, *R.R. Smith*, Independent Consultant, *D.R. Killelea*, University of Chicago, *V.L. Campbell*, *D.F. Del Sesto*, *A.L. Utz*, Tufts University

We describe experimental work that yields vibrational-state-resolved reaction probabilities for a polyatomic molecule without the need for selective laser excitation of the target state. The method relies on a detailed knowledge of the vibrational structure of the molecule under study, its vibrational cooling dynamics in a supersonic expansion, and an understanding of how individual vibrational states contribute to the state-averaged reactivity measured in the experiment. The reagents in beam-surface scattering measurements of surface reactivity typically have a well-defined translational energy and a narrow distribution of rotational states, but the vibrational state distribution of the reagents remains nearly thermalized at the nozzle source temperature. As nozzle temperatures are raised to access higher incident kinetic energies, the thermal population of excited vibrational states grows. The high vibrational state density of polyatomic molecules can result in hundreds, or even thousands of vibrational states contributing to the measured reactivity. In addition to yielding reaction probabilities averaged over many internal states, the state or group of states that dominate reactivity may vary as a function of incident kinetic energy, even at a fixed nozzle source temperature. Recent results from state-resolved measurements of methane activation on Ni(111) allow us to model vibrational-state-averaged beam-surface data to gain insight into how reactivity scales with increasing vibrational excitation. We use this approach to extract a state-resolved reaction probability for the $v=0$ vibrational ground state of methane dissociating on a Ni(111) surface. At intermediate nozzle temperatures, only the $v=0$, v_2 , and v_4 vibrations have sufficient population to impact reactivity. Non-equilibrium vibrational cooling in the expansion relaxes v_2 to v_4 . Knowledge of S_0 for the $v=0$ state allows us to extract S_0 for the v_4 vibrational fundamental of the "umbrella" bending vibration.

SS-ThP9 Interfacial Dynamics of Amorphous and Crystalline Thin Polymer Films. *J.S. Becker*, University of Chicago, *M.A. Freedman*, University of Colorado, Boulder, *S.J. Sibener*, University of Chicago

The surfaces of thin polymer films are a complex and dynamic macromolecular interface that have attracted significant attention. Presently, there is poor understanding regarding the modification of dynamics and crystallization at the free polymer surface by dimensional confinement of the polymer into a supported thin film. Helium atom scattering is a uniquely surface sensitive and non-destructive probe of vibrational motion and structure at complex interfaces. Elastic helium scattering reveals surface stiffening of amorphous poly(methyl methacrylate) (PMMA) in molecularly thin films as a function of diminishing film thickness. Furthermore, collisional energy transfer characteristics measured from amorphous PMMA, polystyrene, and polybutadiene films show remarkably similar lineshapes and temperature induced intensity decays, owing largely to the common methylene groups presented at the surface. Additionally, helium scattering provides exquisite sensitivity to surface order and crystallinity. Surface crystallization is presently being measured in thin films comprised of poly(ethylene terephthalate) and compared with related data obtained from glancing-angle Fourier-Transform Infrared Spectroscopy measurements acquired in an ultra high vacuum environment.

SS-ThP10 Interaction of Water with Pure and Mixed Monolayers of Hydrophobic and Hydrophilic Terminated Alkanethiols on Au(111). *N.M. Barrentine*, *R.L. Grimm*, *J.C. Hemminger*, University of California, Irvine

The interaction of water adsorbed on self-assembled monolayers (SAMs) with moieties that are either hydrophobic, hydrophilic, or mixtures of both were characterized by temperature programmed desorption (TPD). The SAMs were fabricated on Au(111) from dilute ethanolic solutions of alkanethiols terminated with either a methyl group (hydrophobic) or a polar group (hydrophilic). The goal of our experiments is to understand the interaction of water with localized regions of hydrophilic character on an organic surface as a function of the spatial extent of the hydrophilic region (in the 10's of nanometer size regime). TPD experiments of water desorption from pure hydrophobic surfaces show first order desorption kinetics at low coverage with an activation of energy of $\sim 34 \text{ kJ mol}^{-1}$. The peak temperatures seen in the pure hydrophilic TPD spectra are 10-60 K higher than that of the pure hydrophobic case, indicative of a stronger interaction with water. Surfaces functionalized with a mixture of the

hydrophobic and hydrophilic terminated alkanethiols display different properties from either of the pure cases and are not well described by simple weighted addition of the two limiting cases. The aim of this work is to develop a well characterized model system that mimics the surfaces of organic-coated aerosols found in the troposphere. These aerosol surfaces are typically hydrophobic when the aerosol is first formed and are thought to become more hydrophilic as the aerosol undergoes varying degrees of oxidation due to reactions with atmospheric oxidizing species such as O_3 and OH radicals. We will discuss how our results can be useful in understanding water interactions with atmospheric aerosols.

SS-ThP11 Optimization of Hardness of Ultra Water Repellent Silica-Based Film by Tuning Surface Structure and Film Matrix. *H. Sakurai*, *N. Saito*, *O. Takai*, Nagoya University, Japan

Ultra-water repellent film (UWR) has a water contact angle of more than 150° . The UWR property is governed by the hydrophobic groups and the geometrical structure of the surface. We have successfully fabricated UWR film by microwave plasma enhanced CVD (MPECVD) with trimethylmethoxysilane (TMMOS) as a raw material. However, the UWR film showed a poor mechanical property, because the film was composed of not a continuous film but aggregation of clusters. In order to improve the mechanical property of the UWR film, it is crucial to control the ratio of continuous film and aggregation of clusters in the film. The ratio is strongly related to the surface geometry accentuating the wettability. The large roughness makes the water repellency increase while the hardness of the structure decreases. In this study, we aimed to obtain UWR film with high hardness by tuning the surface structures and film matrix. The UWR film was deposited by MPECVD. A microwave generator (2.45GHz) was used at 250 W. Si wafer was used as substrate. TMMOS was used as a raw material, and Ar was introduced as excitation gas. The partial pressures of TMMOS and Ar were kept constant at 70Pa and 30Pa. And also, the distance between plasma and substrate was constant. The deposition time was changed 3 minutes to 30 minutes to change the surface roughness. Water contact angles on the resulting films were evaluated with a contact angle meter. Hardness of the films was measured by a nanoindenter as Vickers hardness. Surface structures of UWR films were observed by atomic force microscope (AFM). The surface roughness was evaluated by root mean square (RMS). The UWR films with smaller roughness were obtained. Even in the case, the relationship between water repellency and hardness depended on roughness. Smaller roughness would indicate the increase of continuous films. However, the Vickers hardness was not improved drastically. The film matrix was changed by the increase of oxygen and the addition of nitride and so on. The changes of film matrix have a great effect on the improvement of hardness.

SS-ThP12 Synchrotron Radiation-Induced Reactions of Astrochemical Interest*. *M.J. Abu Haija*, *R.A. Rosenberg*, Argonne National Laboratory, *P.J. Ryan*, Ames Laboratory

In molecular cloud regions of the interstellar medium (ISM), astronomical observations have revealed a rich chemistry with the detection of over 130 different chemical species ranging from simple diatomic molecules to complex organic molecules such as polycyclic aromatic hydrocarbons (PAHs). These molecules may have been involved in the prebiotic chemistry that led to life's origin. Our approach for simulating such chemistry is to in-situ monitor the x-ray induced chemical reactions of model compounds adsorbed on well-characterized substrates. We are currently pursuing two areas of research in this field. The first one is to understand the source of chirality in prebiotic molecules, which is a subject of great interest to a wide group of researchers. We have recently demonstrated that low-energy spin-polarized secondary electrons, produced by irradiation of a magnetized permalloy substrate can induce chiral selective chemistry of adsorbed (R)- or (S)-2-butanol on permalloy.¹ Using x-ray photoelectron spectroscopy (XPS) to monitor the intensity of the C-O peak, the results showed an enhancement of $\sim 10\%$ in the rate of C-O bond cleavage that depends on the chirality of the molecule and the spin polarization of the substrate secondary electrons. In addition to the C1s XPS measurements used to determine the rate constants, O1s XPS and O1s near edge x-ray absorption fine structure (NEXAFS) as well as x-ray magnetic circular dichroism (XMCD) measurements were performed. The second area of research is the investigation of x-ray induced chemical reactions of PAHs which are flat molecules based on rings of six carbon atoms. PAHs are of particular interest because they are often used as biomarkers that indicate life. A large variety of these molecules has been detected in meteorites after being delivered to Earth. We will present some preliminary results on the x-ray induced reactions of coronene ($\text{C}_{24}\text{H}_{12}$). The focus of this work will be to understand the kinetics and mechanisms of this system, as well as other PAHs. Experiments were performed under UHV conditions utilizing both XPS and x-ray excited optical luminescence (XEOL) to monitor the reactions.

SS-ThP13 CCD for Ion Detection, O. Hadjar, G. Kibelka, O.I. Analytical CMS Field Products

Photon imaging based on charged coupled devices (CCD) is a mature technology. Such detectors are used, for instance, in astrophysics instruments as well as in every day consumer products. As a consequence, the CCD underlying functionality is well understood and devices can easily be mass-produced. The common CCD is a fine-pitched, two-dimensional array detector, which can be operated in a vacuum as well as under high pressure. Replacement of the photosensitive layer of the CCD with a metal-oxide semiconductor (MOS) has proven to be a very successful and promising technique for ion imaging. Various instruments based on charge detection can benefit from such a device, particularly mass spectrometers (MS). Fusing the CCD with a miniaturized Matauch-Herzog type MS¹ results in a compact sector-field mass spectrometer with sufficient mass resolution and unmatched duty cycle. Using an electron-impact ion source, formed ions are m/z separated and detected by our CCD located at the focal plane of our instrument. The CCD response can be studied as a function of ion energies and incidence angles. Quantum efficiencies of singly and doubly charged rare gas ions are being investigated and results are compared with electron-impact ionization cross section found in literature.² These fundamental studies will increase the accuracy of quantifying abundances of ionic species and can be the base for future improvements.

¹ M. P. Sinha, M. Wadsworth. Rev. Sci. Ins. 76, 025103 (2005).

² A. Kobayashi, G. Fujiki, A. Okaji, T. Masuko. J. Phys. B: At. Mol. Phys. 35 2087 (2002).

SS-ThP14 Atomistic Approaches to Fischer-Tropsch Model Catalysts, B. Wang, A. Purdie, M. Caffio, R. Schaub, University of St Andrews, UK

Fischer-Tropsch synthesis, discovered in the 1920s, is one of the most researched topics within heterogeneous catalysis. Fe and Rh are two widely studied Fischer-Tropsch catalysts. The former strongly dissociates CO and catalyzes the preferential formation of methane and higher hydrocarbons, while the latter exhibits a unique catalytic activity on syngas reactions to form carbon-two oxygenates.¹ It has been demonstrated that additive Fe species to silica-supported Rh catalysts exert a significant promotion in CO hydrogenation by enhancing the yields and unexpectedly increasing the selectivities toward oxygen-containing products such as alcohols.² In this work, we investigated the FeRh catalyst system within a surface science approach, aiming to get atomic level information on the structure, composition and chemical state of different bimetallic catalysts, and hence an understanding of the Fe promotional role. The nucleation and growth of Fe deposited at room temperature on single-crystalline Rh(111) surfaces (flat and stepped) was investigated as function of Fe coverage. Upon annealing at high temperatures (>600K), STM data confirm the formation of a near surface alloy. By a thorough and systematic comparison of STM images following CO exposure on Rh(111) and on Fe/Rh(111), we investigated the promotional role played by Fe (site specific versus local electronic structure alteration). In an attempt to address more realistic systems, we also performed STM measurements on Rh and Fe physically vapour deposited onto SiO₂ thin films. The morphology of the resulting nano-particles, their dispersion and sintering, were studied as function of the Fe:Rh molar ratio. We observed that the addition of Fe dramatically enhances the dispersion of the active Rh loading, concomitant with a significant decrease in average particles size. The implications of our findings are discussed in light of the selective catalysis reported for FeRh systems.

¹ M. Ichikawa, Polyhedron, 7 (1988) 2351.

² M. M. Bhasin, et al., Journal of Catalysis, 54 (1978) 120.

SS-ThP15 Wettability of Self-Assembled Monolayer Surfaces of Alkane Thiols on Au, N. Yoshida, T. Watanabe, The University of Tokyo, Japan

Wettability of solid surface has attracted much attention in many fields, from basic surface science to practical uses. Up to now, numerous studies have sought to interpret the static hydrophobicity (contact angle of a droplet and surface energy/surface tension of solid surface) in terms of the interaction between liquid and solid surface. The static hydrophobicity has been well-clarified (controlled by surface energy and morphology), however, the dynamic hydrophobicity (sliding angle and velocity of a droplet), a measure of dynamic adhesive property against water, is still in controversy. Practically, dynamic hydrophobicity does not simply depend on static hydrophobicity. Thus far, no one could completely explain a fact that hydrophobic surfaces of similar water contact angles often show quite different adhesive property against water. In this study, we successfully prepared various hydrophobic surfaces on Au using alkane and fluoroalkane thiols with various adhesive properties against water in terms of solid-liquid interface engineering. We will demonstrate that the dynamic

hydrophobicity, a measure of the adhesive property against water, depended on the surface morphology (even of the order of a few nanometers) and surface composition (small amount of polar groups on the surface) and that we could control it independent of static hydrophobicity.

SS-ThP16 Surface Characterization of Hydrophobic Thin Films Deposited by Various Plasma Polymerization Methods, Y.S. Kim, K.-J. Kim, Korea University, Y.H. Lee, Korea Institute of Science and Technology

Plasma polymerization is a thin film deposition process and may be uniformly coated onto any substrate. Plasma polymers generally have different properties from those of conventional polymers due to their unique properties. Plasma polymer films have been used in a variety of applications including barrier coating, protective coating, anti-scratching coating, and dielectric layer in microelectronics. In this study, plasma-polymerized films fabricated by three different type plasma such as inductively coupled plasma (ICP), capacitively coupled plasma (CCP), and pulsed-plasma (PP). Different kinds of hydrocarbon gases and fluorine-containing gases were mixed to investigate their effect on the films. Also, process parameters for plasma polymerization such as gas ratio, gas pressure, plasma power, pulse width, and processing time were investigated. The physical properties of plasma-polymerized thin films made by three different methods were characterized using water contact angle measurement and mechanical test. The adhesion strength between plasma-polymerized thin film and substrate was measured by 90° peel test, and the mechanical properties of plasma-polymerized thin film surface were investigated by indentation. Surface analytical instruments such as Auger electron spectroscopy (AES), x-ray photoelectron spectroscopy (XPS), near-edge x-ray absorption fine structure (NEXAFS), and time-of-flight secondary ion mass spectrometry (TOF-SIMS) were also used to provide useful information about the chemical properties such as surface composition and functional groups.

SS-ThP18 Fabrication and Characterization of Well-Ordered Model Nanocatalysts using Anodic Aluminum Oxide (AAO) Template, Y.C. Chu, C.M. Kim, Kyungpook National University, South Korea

Heterogeneous catalysts are usually composed of 1 ~ 20 nm metal clusters. It is generally observed that the catalytic activity is greatly affected by the size of metal clusters. It is crucial to control the size of metal clusters in the fundamental studies of catalytic reactions. We fabricated ordered arrays of nanostructures for the study of size-selective model catalysts using porous anodized aluminum oxide (AAO) templates. The AAO templates whose pore sizes were 5 ~ 50 nm were prepared. A silver electrode was sputter-deposited on one side of the templates and Ni, Au and Pt were electrodeposited to produce nanocatalysts with a uniform size. The model catalyst surfaces were characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), atomic force microscopy (AFM), X-ray photoelectron spectroscopy and temperature-programmed desorption (TPD). Catalytic reaction of CO oxidation and propene epoxidation on these model catalyst surfaces will be presented.

SS-ThP19 Synthesis of Nanostructured CoSb2O6 by a Co-Precipitation Method and its Potential Application as a Gas Sensor Material, C.R. Michel, A.H. Martinez-Preciado, H. Guillen-Bonilla, J. Rivera-Dominguez, Universidad de Guadalajara, Mexico

Nanostructured powders of CoSb2O6 possessing the trirutile-type structure, were synthesized by a co-precipitation method, using antimony chloride and cobalt nitrate. During this process a precipitate was obtained when the reagents were mixed in ethanol, which was stirred for 24 h. Microwave radiation at low power was applied for the evaporation which produced a solid precursor. The thermal decomposition of the precursor, from room temperature to 700°C in air, was made in order to investigate the crystal structure evolution while increasing the calcination temperature. To perform this characterization X-ray powder diffraction was used, resulting that the tetragonal CoSb2O6, with cell parameters a = 4.6544 Å and c = 9.2823 Å, and space group P42/mnm, can be obtained from 600°C. The observation of the calcined materials by SEM shows that the main microstructure produced corresponds to a filamentary shape, with a length between 100 to 600 nm. The observation by TEM of these filaments revealed that are composed by an arrangement of nanoparticles with an average size of 20 nm. To test CoSb2O6 as a gas sensor material, the powder calcined at 700 °C was deposited on alumina substrates using the screen-printing method. DC electrical characterization was performed in air, O2 and CO2, from room temperature to 600°C. The dynamic response of resistance was studied by supplying alternatively the gases while recording the electrical resistance; which increased in approximately 1000 ohms when detecting CO2, whereas for O2 the change was in the order of 100 ohms.

SS-ThP20 Ion Implantation and Microstructure - How Each Affects the Other in Tool Steel, L.A. Autry, D.G. Goberman, H.M. Marcus, R.R. Ramprasad, The University of Connecticut

Ion implantation has been a useful technique for advanced materials processing for many decades. The range of materials that have been ion beam modified covers most classes of materials and many of these classes in great detail. However, with advances in analytical techniques and new manufacturing techniques and objectives, interesting and new observations of ion beam effects are often just waiting to be found. This research has focused on the affect of various ion implanted species on the chemistry and microstructure of tool steel. The inherently heterogeneous microstructure of tool steels affects both the implantation depth and concentration of implanted ions within the steel. This leads to a near surface region where the ultimate affect of ion implantation is, itself, affected by the local microstructure. Small spot surface spectroscopic analysis will be presented which highlights the magnitude of the phenomenon and the implications of this will be discussed. In addition to the affect of heterogeneous microstructures on ion implanted tool steel, the intertwined affect of surface preparation will be discussed. Often surface oxides are removed prior to ion implantation either as a by-product of normal materials preparation or intentionally in order to simplify characterization. However, oxides can be quite adherent and are found on many tool steels in use today. An analysis of ion implanted oxidized steel will be presented and tied into the discussion of how local microstructure can affect ion implantation profiles within tool steel.

SS-ThP21 Temperature-Dependent Surface Structure and Fermi Level of InGaAs, J. Shen, W. Melitz, A.C. Kummel, University of California, San Diego

The Si based MOS field effect transistors (MOSFETs) technology is rapidly approaching its theoretical physical limits. III-V compound semiconductors are known as a potential additional technology platform to silicon. The key to fabricating a practical III-V MOSFET is forming an unpinned oxide-semiconductor interface with low fixed charge. The correlation between the atomic bonding structure and the electronic structure at oxide-semiconductor interfaces is critical to understanding how atomic scale changes in electronic structure can cause localization of electrons or holes at these interfaces. We have used atomically resolved scanning tunneling microscopy (STM) images and scanning tunneling spectra (STS) to determine the atomic and electronic structure of clean InGaAs surface structure and gate-oxide/InGaAs semiconductor interface. Using a low temperature preparation we can get an InGaAs(001)-(2×4) surface reconstruction that is mostly β2(2×4) with some α2(2×4) regions. However these surfaces are very oxygen sensitive and reconstruction is not pure. Then increasing preparation temperature, we can get mixed surface reconstruction structure of InGaAs(001)-(2×4) and (4×2). For even high temperature, we can get pure InGaAs(001)-(4×2) surface reconstruction. Then oxides are deposited on InGaAs surface and STS measurements are being performed to determine the electronic properties of the interface and whether Fermi level is pinning or unpinning.

SS-ThP22 XPS and Ellipsometry Analysis of Process Variations for Direct Current Plasma Enhanced Chemical Vapor Deposition of Trimethylsilane, P.R. Scott, D.M. Wieliczka, University of Missouri-Kansas City

Thin films were deposited onto Aluminum and Silicon substrates utilizing DC PECVD of Trimethylsilane. The process parameters of gas pressure, discharge voltage, discharge current and deposition time were varied. The films were analyzed using X-ray photoelectron spectroscopy in conjunction with argon ion etching to determine the chemical properties as a function of film thickness and to examine the film-substrate interaction. Spectroscopic ellipsometry was used to obtain the optical properties and film thickness. Results from the comparison and correlation of these film properties to the process parameters will be presented.

SS-ThP23 Cycloaddition and Cyclocondensation Processes on Silicon: Nitrosobenzene on Si(100)-2x1 and Nitrobenzene on Hydrogen-Terminated Si(100), K.A. Perrine, T.R. Leftwich, C.R. Weiland, R.L. Opila, A.V. Teplyakov, University of Delaware

Reactions of nitrogen-containing bifunctional molecules with silicon substrates can play an important role in such areas of science and engineering as molecular electronics, surface passivation, and building organic/inorganic interfaces. These nitrogen-containing bifunctional molecules can be attached to the silicon surface via the nitro or nitroso group. The other end of the bifunctional molecule, a phenyl ring, remains intact after the reaction allowing for the model studies of electron transfer processes or for further surface modification. Nitrosoadducts are obtained from two different bifunctional molecules and two different surfaces. Nitrosobenzene reacts initially through a [2+2] cycloaddition on a clean Si(100)-2x1 surface through the N=O group leaving the phenyl ring intact.

The oxygen migrates subsurface leaving the phenyl nitrene adduct the dominant product from the reaction leaving the minor presence of the nitrosoadduct on the surface. However, nitrosoadducts are the dominant products from the condensation reaction of nitrobenzene with hydrogen-terminated Si(100). All these products and their distribution on surfaces are verified using X-ray photoelectron spectroscopy (XPS), infrared spectroscopic measurements (FTIR), and density functional theory (DFT) calculations. Analysis of the surface reaction pathways and spectroscopic investigations draw parallels between the nitrobenzene reaction on clean Si(100)-2x1 and hydrogen-terminated Si(100) and nitrosobenzene on clean Si(100)-2x1.

SS-ThP24 Formation and Collapse of Au/n-Si Schottky-Barrier Contact at the SiO₂/Si Interface and Oxidation Kinetics in Au-Contaminated and Thermally Oxidized n-Si (001) Surfaces, S. Shimizu, S. Shimada, N. Nagase, M. Muta, I. Ikeda, Nihon University, Japan

We have investigated an anomalous profile of Au in SiO₂/Si region as a function of oxidation temperature and then clarified an oxidation mechanism utilizing ellipsometer, X-ray photoelectron spectroscopy (XPS) and alternating current surface photovoltage (AC SPV) methods. When n-type Si wafers having hydrophobic surface were rinsed in Au aqueous solution (the Au surface concentration = ~2 10¹⁵ atoms/cm²) and then thermally oxidized at between 550 and 750°C, an Au cluster still resided both at the SiO₂/Si interface and the top area of SiO₂ film. Most of the Au at SiO₂/Si was identified to be detected as the Au cluster which did not make bonds with other elements such as O, H and Si. The Au at the SiO₂/Si interface formed Au/n-Si Schottky-barrier, causing depleted and/or inverted layer at the Si surface, thereby, giving rise to an occurrence of a frequency-dependent AC SPV. As the oxidation temperature and time increased, the frequency-dependent AC SPV decreased and disappeared, corresponding to the fact that the Au cluster at SiO₂/Si interface decreased and/or disappeared. At oxidation temperatures higher than at 750–800 °C, the frequency-dependent AC SPV was not detected. The Au was found to diffuse deeper in both SiO₂ bulk and Si substrate as the oxidation advanced. Regarding oxidation kinetics at between 550 and 900°C, Au caused a drastic SiO₂ growth enhancement for SiO₂ thickness less than ~10 nm. This result shows that Au acted as catalyst to promote the initial SiO₂ growth at the Si(001) surface. The behavior of the Au in SiO₂ layer explained the relationship between oxide thicknesses and oxidation time. Finally, the SiO₂ growth mechanism influenced by the addition of Au is proposed.

SS-ThP25 Oxidation of the PAH Coronene by Ozone and the Hydroxyl Radical, E.R. Mysak, J.T. Newberg, J.D. Smith, K.R. Wilson, H. Blumh, Lawrence Berkeley National Laboratory

Polycyclic aromatic hydrocarbons (PAHs) are a class of organic pollutants, consisting of two or more fused benzene rings, emitted directly into the atmosphere primarily through incomplete combustion processes and known to have allergenic, mutagenic, and carcinogenic effects. In the atmosphere, smaller PAHs are found primarily in gas-phase, whereas three or four-member ring compounds are partitioned between gas and particulate matter, and compounds with greater than five-member rings mostly reside in the particle phase. The atmospheric fate of these heavier PAHs is governed by heterogeneous reactions between the surface bound PAHs and gas-phase atmospheric oxidants such as ozone, the hydroxyl radical, and nitrates, however, these heterogeneous chemical reactions are relatively poorly understood and studied. In the current study, reactivity of the seven-member ring PAH coronene to oxidation sources ozone and hydroxyl radical is examined. To probe the extent of chemical reaction, product formation, and change in surface morphology as a function of reaction, we examine coronene adsorbed onto various substrates, from both a surface and bulk perspective, with ambient pressure photoemission spectroscopy (APPEs) and aerosol mass spectrometry (AMS), respectively. In bulk on-line analysis, a 20nm thick layer of coronene adsorbed onto NaCl seed particles and reacted with either oxidant in a flow tube showed very little reactant conversion to product in the AMS. However, surface analysis by the APPEs of the same reaction where coronene was adsorbed onto model substrates showed up to 90% conversion of the carbon species to volatilized or oxidized carbon. Data obtained with these two complementary bulk and surface techniques provide evidence for a surface selective reaction. Using APPEs, we are able observe the two oxidation reactions transforming on different timescales and through differing pathways, resulting in dissimilar final states.

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