

Tuesday Evening Poster Sessions, November 14, 2006

Surface Science

Room 3rd Floor Lobby - Session SS-TuP

Surface Science Poster Session

SS-TuP1 Design and Stability of Surface Alloys used for Catalytic Conversion of Fossil Fuel to Hydrogen, J. Knudsen¹, R.T. Vang, University of Aarhus, Denmark; *J. Schnadt*, Lund University, Sweden; *E.K. Vestergaard, T.M. Pedersen, B. Hammer, T. An, I. Stensgaard, E. Laegsgaard,* University of Aarhus, Denmark; *A.U. Nilekar, M. Mavrikakis,* University of Wisconsin-Madison; *F. Besenbacher,* University of Aarhus, Denmark

Clean, cheap and efficient production of high-purity hydrogen is an essential prerequisite for the emerging hydrogen economy. The vast majority of the present hydrogen production comes from catalytic conversion of fossil fuel, which relies heavily on the steam reforming (SR) reaction and the Water-Gas-Shift (WGS) reaction. Supported Ni particles are commercially used as catalysts for the SR reaction, whereas supported Cu particles are currently used for the low-temperature WGS reaction. In this study vacuum deposition of Cu onto Pt(111) at 800 K is used to synthesize stable near-surface alloys (NSA) of Cu/Pt(111). A combination of scanning tunneling microscopy (STM), Core-level photoemission (XPS), Thermal desorption spectroscopy (TDS) and Density functional theory (DFT) is used to characterize the NSAs, and it is found that Cu atoms are stabilized sub-surface, leaving a surface layer free of Cu atoms. Very interestingly, we find that the WGS activity of our new NSA is superior to that of Cu(111), and it is, therefore, very likely that real Cu/Pt near-surface particles could be used as new and improved catalysts for the WGS reaction. Finally, fast high-pressure STM experiments in a high CO pressure are used to examine the stability of this new Cu/Pt(111) near-surface alloy for the WGS reaction, and a previously found Au/Ni(111) surface alloy, which can be used for the SR reaction. From these experiments we conclude that the Cu/Pt(111) NSA remains stable in high pressure of CO in contrast to the Au/Ni(111) surface alloy, which is found to phase separate into small Au clusters on a Ni(111) substrate due to formation of Ni-carbonyls, which remove Ni from the surface.

SS-TuP2 Vibrational Energy Flow in a Gas-Surface Reaction, D.R. Killelea², A.L. Utz, Tufts University

Energy flow plays a central role in the activation of surface reactions. We measure how energy selectively deposited into the translational, rotational, and vibrational coordinates of methane influences S@sub 0@ on Ni(100) and Ni(111) to answer key questions about energy flow in this prototypical gas-surface reaction. Infrared laser excitation of CH@sub 4@ in a supersonic molecular beam prepares a microcanonical ensemble of reagents with well-defined internal and translational energies. We quantify reactivity for the state-selected reagents and observe non-statistical patterns of activation, including vibrational mode specificity. For example, the @nu@@sub 3@ C-H stretch is more reactive than the second overtone of the umbrella-bending mode, 3@nu@@sub 4@, even though 3@nu@@sub 4@ contains 30% more energy. On Ni(111) energy deposited in @nu@@sub 3@ activates dissociative chemisorption more than an equivalent amount of translational energy. To understand these results, we propose a framework for describing energy flow among the energetic degrees of freedom available to the molecule-surface reaction complex. Our model draws on and is consistent with descriptions of intramolecular vibrational energy flow in both the gas-phase and in liquids, but accounts for features unique to gas-surface reactivity. We focus on the characteristic timescales for energy flow and the molecule-surface interaction time. We conclude that for direct dissociative chemisorption of CH@sub 4@, there is insufficient time for full energy randomization among the energetic degrees of freedom in the molecule-surface reaction complex. Our model not only predicts vibrational mode-specific behavior - it also suggests a consistent explanation of surface temperature effects, explains the success of statistical theories to model ensemble-averaged reactivity even when energy flow is not statistical, and provides a framework for assessing the extent of energy flow in other gas-surface reactions.

SS-TuP3 Unexpected Growth Modes for Heteroepitaxial BaTiO@sub 3@ Films Due to Kinetic Limitation, J. Shin³, The University of Tennessee; *A.Y. Borisevich, S.V. Kalinin,* Oak Ridge National Laboratory; *E.W. Plummer,* The University of Tennessee; *A.P. Baddorf,* Oak Ridge National Laboratory

Fully strained BaTiO@sub 3@ (BTO) films have the strongest polarization because the c/a ratio is maximized. However, epitaxial growth of BTO films on SrTiO@sub 3@ (STO) is very difficult in oxygen pressures above 1 mTorr due to a large lattice mismatch (2.28%) and the Stranski-Krastanov (SK) growth mode with lattice relaxation is likely. To avoid the formation of 3D islands and prevent the system from reaching equilibrium, kinetic limitations can be used to reduce the surface diffusion length by changing the growth rate or the growth temperature. BTO films grown on (001)STO substrates by pulsed laser deposition have been investigated as a function of growth temperature and growth rate by atomic force microscopy, x-ray diffraction, reflection high energy electron diffraction, and transmission electron microscopy (TEM). The 125 nm thick BTO films deposited using the relatively high average growth rate (0.2 ML/s) with 10 mTorr oxygen pressure exhibit layer-by-layer or layer-then pseudo 2D island growth modes with increasing temperature, which is also related to thermal expansion differences between films and substrate. Compared with low growth rate (0.08 ML/s) condition, which shows conventional SK growth above 1 mTorr oxygen, this high growth rate condition provides 125 nm thick BTO films that are highly strained with visible terraces. In addition to the conventional layer-by-layer mode, an unusual pseudo 2D island growth mode is observed above 1050 K, where islands of several unit cell heights are observed between single height film steps. These islands are nearly steady-state; once formed, the film roughness does not increase with thickness as it does for 3D islands, and the island size and density remains fixed, with evidence of island-island repulsion. Pseudo 2D island growth appears related to the lattice of film dislocations observed with TEM. Research sponsored by Office of BES, U.S. DOE, under contract DE-AC05-00OR22725 with ORNL, managed by UT-Battelle, LLC.

SS-TuP4 Partially Dissociated Water Clusters on Ru(0001) Studied by Scanning Tunneling Microscopy, T.K. Shimizu, Lawrence Berkeley National Laboratory and University of California at Berkeley; *A. Mugarza,* Lawrence Berkeley National Laboratory and Institut de Ciencia de Materials de Barcelona, Spain, US; *J. Cerda,* Instituto de Ciencia de Materiales de Madrid, CSIC, Spain; *D.F. Ogletree, M. Salmeron,* Lawrence Berkeley National Laboratory

Individual molecules in partially dissociated water clusters have been imaged at 6K using a home-built low temperature scanning tunneling microscope (STM). After annealing the surface with pre-adsorbed oxygen and water above 140 K, elongated clusters with enhanced contrast at the perimeter were observed. By comparing the experimental data with STM simulations, we conclude that the clusters consist of mixed water and hydroxyl molecules lying flat. The presence of pre-adsorbed oxygen prevents the formation of a perfect hexagonal network inside the clusters and affects their overall shapes. Hydrogen atoms were observed both inside and outside the clusters, the latter reacting with the pre-adsorbed oxygen to form hydroxyl.

SS-TuP5 Gold Adatom-mediated Bonding in Self-assembly of Alkanethiols on the Au(111) Surface, P. Maksymovych⁴, University of Pittsburgh; *D.C. Sorescu,* U. S. Department of Energy; *J.T. Yates, Jr.,* University of Pittsburgh

The majority of self-assembled molecular monolayers (SAMs) are at present grown using the adsorption of alkanethiol molecules on the Au(111) surface. Despite decades of research in this field, the structural nature of the S-Au anchor bond of the thiolate to the Au(111) surface is still a matter of active debate. We addressed this issue by studying the decomposition of prototypical CH@sub 3@SH, CH@sub 3@SSCH@sub 3@ and C@sub 3@H@sub 7@SH molecules on the Au(111) surface using Scanning Tunneling Microscopy (STM) and Density Functional Theory. Initially, the CH@sub 3@S species were produced by STM-tip induced dissociation of CH@sub 3@SH or CH@sub 3@SSCH@sub 3@ molecules on the Au(111) surface at 5K. By comparing the experimental and calculated STM images of the CH@sub 3@S species produced in this way, we determined that the S-headgroup adsorbs on the two-fold coordinated bridge-site between two surface Au atoms, consistent with theoretical predictions for this system. In the next step, CH@sub 3@SSCH@sub 3@, CH@sub 3@SH and C@sub 3@H@sub 7@SH molecules were dissociated thermally in conditions typically used for SAM growth. Unexpectedly, we

¹ Morton S. Traum Award Finalist

² Morton S. Traum Award Finalist

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find that dissociation of the parent molecules in these conditions is mediated by gold adatoms, which populate the Au(111) surface at elevated temperatures. The product CH@sub 3@S (and C@sub 3@H@sub 7@S) species form self-assembled Au adatom-bound complexes, which have substantially higher calculated binding energy than CH@sub 3@S species bonded to the Au(111) surface. The involvement of Au adatoms in the self-assembly of alkanethiols resolves the current controversy around the headgroup-sulfur bonding, as we show for the case of the low-coverage stripe-phase SAM, and explains the morphological changes of the Au(111) surface that accompany self-assembly. We thank W. M. Keck Foundation and NEDO (Japan) for the financial support of this work.

SS-TuP6 Heterogeneous Oxidation of the Si(111) Surface Determined by Kelvin Probe Force Microscopy, B Poelsema, J.M. Sturm, G.O. Croes, University of Twente, The Netherlands; H. Wormeester, University of Twente, The Netherlands, Netherlands

A large change in work-function occurs during the initial oxidation of Si(111). The variation of the work-function after an initial exposure to O@sub 2@ allows the identification of a molecular precursor. An AFM with a conducting tip has been used as a Kelvin Probe Force Microscope (KPFM). It enables the in-situ, parallel recording of morphology and work-function with nanometer resolution. The clean Si(111) surface has been found to have a rms work-function variation of only 2 meV, indicative of an electrically very smooth surface. Exposure to molecular oxygen results in a very heterogeneous oxidation process in which morphology and work-function locally change in a non-correlated fashion. After an exposure of about 10 L(angmuir), the morphology remains similar, while over 100 L is required for the work-function to assume a stationary value. The change in work-function is only local as the average value is constant after 40 L and the rms of the work-function does not significantly change after 20 L. The heterogeneity of the oxidation process is also observed by a strong variation of the differential capacitance over the surface. This variation is strongly correlated to the local morphology indicating a large variation in local oxide thickness. The observations above can be rationalized via the presence of a molecular precursor. It actually has strong effects at sub-monolayer coverage.

SS-TuP7 Initial Oxidation Process of Si(100) Surface with O@sub 3@ Molecular Beam, I. Kinefuchi, The University of Tokyo, Japan; H. Yamaguchi, Nagoya University, Japan; Y. Sakiyama, S. Takagi, Y. Matsumoto, The University of Tokyo, Japan

The reaction of O@sub 3@ with Si(100) surface has been investigated by employing molecular beam techniques. The surfaces were oxidized at 673 K by exposure to 5.1%-O@sub 3@/O@sub 2@ beam and we examined the decomposition of the oxide adlayers using temperature programmed desorption (TPD). Compared with O@sub 2@, O@sub 3@ significantly enhances the oxidation rate in the low coverage regime. The coverage-exposure relationship up to 2.8 monolayers in thickness follows the modified Langmuirian kinetics, where the initial sticking probability of O@sub 3@ is almost unity. The desorption spectra exhibit higher peak temperatures and narrower distributions than those from the adlayers by pure O@sub 2@ beam. The surface adlayers formed with O@sub 3@ therefore have more stable and less heterogeneous structures than those formed with O@sub 2@. We also employed the molecular beam reactive scattering (MBRS) technique to investigate the reaction dynamics of the active oxidation process. The square-wave modulated beam of high concentrated O@sub 3@ gas (~60%-O@sub 3@/O@sub 2@ diluted with He) was directed to the surface at temperatures between 1033 and 1153 K. The surface transfer function shows that the reaction process is a sequential two-step first-order reaction as observed with O@sub 2@ beam. However, the reaction rate of the first step, which corresponds to the formation of the desorption precursor, is at least two times faster than that with O@sub 2@. This suggests that there is another reaction pathway involving atomic oxygen due to the decomposition of O@sub 3@ on the surface. @FootnoteText@ @Footnote 1@ One of the authors (I.K.) was supported through the 21st Century COE Program, "Mechanical Systems Innovation," by the Ministry of Education, Culture, Sports, Science and Technology.

SS-TuP8 Temperature Dependant Evolution of Co Islands on Ag/Si(111)-@sr@3x@sr@3and Ag/Ge(111)-@sr@3x@sr@3, S.L. Tsay, National Taiwan Normal University; C.L. Lin, Academia Sinica of China; T.Y. Fu, National Taiwan Normal University

Thermal evolution of Co islands on Ag/Ge(111) and Ag/Si(111) surfaces was studied by scanning tunneling microscopy and low energy electron diffraction. The Ag buffer layer with @sr@3x@sr@3 reconstruction can

avoid alloy formation of Co and Ge or Si during annealing below 800K. The morphology of 0.35ML Co on the Ag/Ge(111) surface transfers dispersion of clusters to nucleation of 2D islands. The 2D islands with @sr@13x@sr@13R14° reconstruction form after 573K annealing. Anneal to above 573K, the 2D islands grow up and the higher islands are reconstructed by 2x2. Submonolayer Co on Ag/Si(111) surfaces can not form 2D islands. The Co clusters just become larger as annealing temperature increases. However, 2x2 phase can be found on 1.8ML Co/Ag/Si(111) surfaces after 673K annealing. The different growth behaviors of Co atoms on Ag/Si(111) and Ge(111) surfaces are discussed from different structure factors.

SS-TuP9 Neutralization and Ionization during Impact of Low Energy Si@super +@ with Surfaces, X. Chen, Z. Sroubek, J.A. Yarmoff, University of California, Riverside

The interaction of low energy semiconductor ions with solid surfaces has been largely unexplored. In this work, 1-5 keV Si@super +@ ions are used to induce direct recoil (DR) from Al(100) and Si(111), and are scattered from electropositive and electronegative adatoms adsorbed on these surfaces. In the DR experiments, significant yields of fast, monoenergetic doubly and triply charged Al and Si ions are produced, which is in contrast to the secondaries formed during bombardment by noble gas ions. The Al@super 2+@ and Al@super 3+@ are attributed to an efficient promotion of Al 2p level during the electronically nearly-symmetric Si-Al collision, and subsequent shake-off processes. The yield of triply charged ions in DR from Si is reduced from that of Al, due to the more symmetric electronic structure. Si@super +@ ions were backscattered from submonolayers of Cs and I deposited onto Al(100) and Si(111). Because of the high ionization energy of Si, resonant charge transfer would be expected to completely neutralize the scattered projectiles. A considerable fraction of the Si backscatters from the adatoms as positive and negative ions, however. Mechanisms responsible for the ion formation will be discussed.

SS-TuP10 Running Current through a Single Non Resonant Quantum State in Silicon, M. Berthe, A. Urbiet, R. Stiefuic, B. Grandidier, D. Deresmes, C. Delerue, D. Stievenard, Institut d'Electronique, de Microelectronique et de Nanotechnologie, France; R. Rurali, N. Lorente, LCAR (UMR 5589), France; L. Magaud, Laboratoire d'Etude des Proprietes Electronique des Solides (LEPES-CNRS), France; P. Ordejon, Institut de Ciencia de Materials de Barcelona, Spain

Due to its ability to resolve geometric structures on the atomic scale, scanning tunnelling microscopy (STM) is a technique well suited to identify individual point defects on a surface. In principle, its versatility should allow to spectroscopically characterize the coupling of tunnelling electrons to the electronic states and the nuclear motions of a defect. Such a measurement, which has recently been achieved on isolated molecules adsorbed on a thin insulating layer still needs to be demonstrated for other systems, particularly semiconductor systems. We have studied the transfer of electrons through the localized dangling bond state of an isolated Si adatom lying in a passivated silicon surface at 5 Kelvin. While the state is electronically decoupled from the silicon bulk states, a strong electron-vibration coupling is evidenced by measurement of the inelastic current and supported by density functional calculations.

SS-TuP11 Valence-Band and Core-Level X-Ray Photoelectron Spectroscopy of Lead Sulfide Nanocrystal/Polymer Composites, D.J. Asunskis, L. Hanley, University of Illinois at Chicago

Lead salt nanocrystals have been the subject of intense recent interest due to their potential applications in photovoltaics, near infrared sensors, and other optoelectronic devices. However, relatively few studies have used photoemission to probe the electronic structure of these novel nanomaterials. Valence-band and core-level X-ray photoelectron spectroscopy (XPS) are therefore used to probe different lead sulfide (PbS) nanocrystal-polymer nanocomposites. Composite materials are prepared by trapping monodisperse 3 and 10 nm lead sulfide nanocrystals in two polymers, the non-conducting polymer, polystyrene, and the conjugated polymer, poly (2-methoxy-5-(2'-ethyl-hexyloxy)-p-phenylene vinylene or MEH-PPV. Additional composites with polydisperse lead sulfide nanocrystals were synthesized by growing the particles in the presence of MEH-PPV and poly (vinyl alcohol). These materials are initially characterized by UV/Vis optical absorption and transmission electron microscopy to monitor the particle size in the composites. Monochromatic XPS with charge neutralization is then used to collect both core-level and valence-band spectra. The composites with monodisperse particle sizes exhibit a shift to lower energy of the highest occupied molecular orbital as the lead sulfide particle size increases from 3 to 10 nm. Oxidation of the

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sulfur content in the particles by air during fabrication and transport was minimal as evident by the small contribution of oxidized sulfur in the XPS spectra. The core level XPS results also show additional states in the lead core XPS regions that change as the particle size changes. The monodisperse composites are compared to the other composites synthesized having varied particle size, showing the effects of size variance and polymer/particle bonding in the core level and valence band XPS spectra. ¹ ² ³ ⁴ ⁵ ⁶ ⁷ ⁸ ⁹ ¹⁰ ¹¹ ¹² ¹³ ¹⁴ ¹⁵ ¹⁶ ¹⁷ ¹⁸ ¹⁹ ²⁰ ²¹ ²² ²³ ²⁴ ²⁵ ²⁶ ²⁷ ²⁸ ²⁹ ³⁰ ³¹ ³² ³³ ³⁴ ³⁵ ³⁶ ³⁷ ³⁸ ³⁹ ⁴⁰ ⁴¹ ⁴² ⁴³ ⁴⁴ ⁴⁵ ⁴⁶ ⁴⁷ ⁴⁸ ⁴⁹ ⁵⁰ ⁵¹ ⁵² ⁵³ ⁵⁴ ⁵⁵ ⁵⁶ ⁵⁷ ⁵⁸ ⁵⁹ ⁶⁰ ⁶¹ ⁶² ⁶³ ⁶⁴ ⁶⁵ ⁶⁶ ⁶⁷ ⁶⁸ ⁶⁹ ⁷⁰ ⁷¹ ⁷² ⁷³ ⁷⁴ ⁷⁵ ⁷⁶ ⁷⁷ ⁷⁸ ⁷⁹ ⁸⁰ ⁸¹ ⁸² ⁸³ ⁸⁴ ⁸⁵ ⁸⁶ ⁸⁷ ⁸⁸ ⁸⁹ ⁹⁰ ⁹¹ ⁹² ⁹³ ⁹⁴ ⁹⁵ ⁹⁶ ⁹⁷ ⁹⁸ ⁹⁹ ¹⁰⁰ ¹⁰¹ ¹⁰² ¹⁰³ ¹⁰⁴ ¹⁰⁵ ¹⁰⁶ ¹⁰⁷ ¹⁰⁸ ¹⁰⁹ ¹¹⁰ ¹¹¹ ¹¹² ¹¹³ ¹¹⁴ ¹¹⁵ ¹¹⁶ ¹¹⁷ ¹¹⁸ ¹¹⁹ ¹²⁰ ¹²¹ ¹²² ¹²³ ¹²⁴ ¹²⁵ ¹²⁶ ¹²⁷ ¹²⁸ ¹²⁹ ¹³⁰ ¹³¹ ¹³² ¹³³ ¹³⁴ ¹³⁵ ¹³⁶ ¹³⁷ ¹³⁸ ¹³⁹ ¹⁴⁰ ¹⁴¹ ¹⁴² ¹⁴³ ¹⁴⁴ ¹⁴⁵ ¹⁴⁶ ¹⁴⁷ ¹⁴⁸ ¹⁴⁹ ¹⁵⁰ ¹⁵¹ ¹⁵² ¹⁵³ ¹⁵⁴ ¹⁵⁵ ¹⁵⁶ ¹⁵⁷ ¹⁵⁸ ¹⁵⁹ ¹⁶⁰ ¹⁶¹ ¹⁶² ¹⁶³ ¹⁶⁴ ¹⁶⁵ ¹⁶⁶ ¹⁶⁷ ¹⁶⁸ ¹⁶⁹ ¹⁷⁰ ¹⁷¹ ¹⁷² ¹⁷³ ¹⁷⁴ ¹⁷⁵ ¹⁷⁶ ¹⁷⁷ ¹⁷⁸ ¹⁷⁹ ¹⁸⁰ ¹⁸¹ ¹⁸² ¹⁸³ ¹⁸⁴ ¹⁸⁵ ¹⁸⁶ ¹⁸⁷ ¹⁸⁸ ¹⁸⁹ ¹⁹⁰ ¹⁹¹ ¹⁹² ¹⁹³ ¹⁹⁴ ¹⁹⁵ ¹⁹⁶ ¹⁹⁷ ¹⁹⁸ ¹⁹⁹ ²⁰⁰ ²⁰¹ ²⁰² ²⁰³ ²⁰⁴ ²⁰⁵ ²⁰⁶ ²⁰⁷ ²⁰⁸ ²⁰⁹ ²¹⁰ ²¹¹ ²¹² ²¹³ ²¹⁴ ²¹⁵ ²¹⁶ ²¹⁷ ²¹⁸ ²¹⁹ ²²⁰ ²²¹ ²²² 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prepared smooth surfaces were almost constant, regardless of chain length and whether alkyl or fluoroalkyl.

SS-TuP19 The Effect of Chemical Bonding on Energy Dissipation in Functionalized Silicon Resonators, A.M. Richter, D. Sengupta, M.A. Hines, Cornell University

Low cost chemical or biological sensors could potentially be fabricated from micromechanical resonators, such as simple cantilevers; however, the realization of this goal has been impeded by the low performance and stability of current micromechanical devices. The sensitivity of a resonant detector is determined, in part, by its rate of mechanical energy dissipation. High mechanical energy dissipation (i.e. low quality factor, Q) leads to poor sensitivity. In previous research, we have shown that the rate of mechanical energy dissipation in MHz-range silicon resonators is profoundly affected by the chemical state of the surface. By changing a single monolayer of molecules on the surface of a 5- μm -wide, 250-nm-thick silicon resonator - less than 0.07% of the total mass - the quality factor of the resonator can be improved at least 70%. In this study, we probe the chemical origins of this effect by comparing the performance of two different types of alkyl-terminated resonators. In the first type, the alkyl chain is directly bonded to the silicon surface through a Si-C bond, whereas in the second type, the alkyl chain is bonded through a Si-O-C linkage. These monolayers were formed by the direct reaction of primary alkenes (Si-C linkage) or primary alcohols or aldehydes (Si-O-C linkage) with H-terminated silicon surfaces. The monolayers were characterized using surface infrared spectroscopy, then their affect on resonator performance was characterized using interferometric detection. Both the chemical linkage (Si-C vs. Si-O-C) and the monolayer precursor (alcohol vs. aldehyde) significantly affected performance. The chemical basis of these differences will be discussed.

SS-TuP20 Selective Modification of Silicon-based Substrates: Reactions of Nitro-, Nitroso-, and Azido-aryls on Clean and H-terminated Si(100) and on a Surface of Silicon-filled Nanopits, T.R. Leftwich, S.P. Sullivan, T. Beebe, A.V. Tepyakov, University of Delaware

The modification of silicon-based substrates has been investigated with the purpose of selective delivery of organic functional groups over a wide range of conditions. Nitro-, nitroso-, and azido-derivatives of aromatic hydrocarbons have been investigated on clean Si(100)-2x1 surface under ultra-high vacuum conditions and on H-terminated Si(100) surface under ambient conditions. These reactions were compared to analogous processes on patterned silicon-filled nanopits of 50-100 nm diameters created on a surface of highly oriented pyrolytic graphite (HOPG). The pits were created from defects formed by controlled Cs or Ga ion bombardment that were then oxidized at 923 K. These reactions were investigated using a combination of temperature-programmed desorption (TPD), infrared spectroscopy, Auger electron spectroscopy (AES), X-ray photoelectron spectroscopy (XPS), and density functional theory (DFT). While 1,3-dipolar cycloaddition dominates the attachment chemistry on a clean Si(100)-2x1 surface, reactions of H-terminated silicon with nitro- or nitroso-compounds proceed through condensation reactions, releasing a water molecule. For reactions of azido-compounds with a clean Si(100)-2x1 surface, a novel intermediate is suggested computationally and identified spectroscopically. This intermediate can be described as a nitrogen molecule stabilized on a silicon surface dimer by a neighboring aryl group. Selected surface intermediates and reaction pathways have been investigated computationally. These findings were applied to modify silicon nanostructures formed on a surface of HOPG.

SS-TuP21 Initial Stages of the Diffusion Barrier Formation on Semiconductors: Mechanism of Decomposition of Tetrakis(dimethylamino)-titanium on Clean and Ammonia-modified Si(100) Surfaces, J.C.F. Rodriguez-Reyes, A.V. Tepyakov, University of Delaware

Tetrakis-(dimethylamino)-titanium (TDMAT) is a deposition precursor for titanium nitride and titanium carbonitride diffusion barriers. In spite of its crucial impact for the interface formation, the reaction of TDMAT with the practically important Si(100) surface has not been understood. In this work, the mechanism of decomposition of TDMAT on clean and ammonia-pretreated Si(100) surface is investigated by a combination of X-ray photoelectron spectroscopy (XPS), thermal desorption, infrared spectroscopy, and density functional theory (DFT). Adsorption of TDMAT on a clean Si(100) substrate proceeds through weak dative bonding of its ligands. Decomposition of TDMAT on a clean Si(100) surface leads to the evolution of a complex mixture of products including methane, dimethylamine and hydrogen cyanide. A chemometric approach is used to identify and quantify these compounds. The decomposition processes are

analyzed on a clean Si(100) surface and compared to the ammonia-modified surface. Specific surface reactive sites produced by ammonia adsorption and thermal decomposition on Si(100) substrate have been investigated computationally and identified spectroscopically. Several previously predicted structures existing on this surface at high temperature were confirmed experimentally and a novel surface structure relevant for nitrogen diffusion was proposed. Decomposition of TDMAT on ammonia-modified surfaces is experimentally observed to be more effective than on clean Si, which provides a way to change the surface energetics by pre-treating the surface. This approach is also applied to investigating the decomposition of TDMAT on a carbon-modified Si(100) surface.

SS-TuP22 Characterization of Orientation-Selective-Epitaxially Grown CeO@sub 2@ Layers on Si(100) Substrates by X-Ray Diffraction and Cross-Sectional Transmission Electron Microscopy, T. Inoue, S. Shida, Iwaki Meisei University, Japan; K. Kato, Fukushima Technology Centre, Japan

Orientation-selective-epitaxial (OSE) growth of CeO@sub 2@(100) and CeO@sub 2@(110) layers on Si(100) substrates is found to be capable by controlling substrate bias and plasma power in reactive dc magnetron sputtering. Although we have obtained a rough growth condition map to select growth orientation,@footnote 1@ at present, the detailed mechanism of OSE is not yet fully understood. In order to get insight into the origin of OSE, we characterized OSE grown CeO@sub 2@ layers using XRD and XTEM. The OSE growth procedure utilizing a two step growth method has been reported.@footnote 2@ Firstly, we carried out XRD measurements to study the orientation components of the epitaxial layers as a function of substrate bias. Analyses of (200) and (220) peak intensity variations with substrate bias proved that (100)-oriented growth regions exist at around ± 15 V bias with a half width of 5 V. In the other regions, (110)-oriented CeO@sub 2@ layers grow. In the vicinity of the border of the two orientation regions, XRD data contained both peaks and their intensity ratio reversed across the border. Secondly, we made XTEM observations. Lattice images of CeO@sub 2@(100)/Si(100) structure indicated following two facts. One is that lattice rows of CeO@sub 2@(100) inclined compared with those of Si(100), wherein defects such as dislocations were scarcely seen. The other is that no interfacial amorphous layers are seen when the Ce-silicide layer thickness is adequate, which indicates the advantage of the two step growth method. This is very exciting, since amorphous interfacial suboxide layers have been thought to be inevitable. A part of this work was conducted in AIST Nano-Processing Facility, supported by "Nanotechnology Support Project" of the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan. @FootnoteText@ @footnote 1@ T. Inoue et al., J. Cryst. Growth, 271, 176 (2004).@footnote 2@ T. Inoue et al., J. Vac. Sci. Tehcnol. A 22(1), 46 (2004).

SS-TuP23 Quantitative Analysis of SAM-Layers on Copper, C. Van der Marel, Y. Furukawa, N. Kahya, J.H.M. Snijders, Philips Research, The Netherlands

Recently, a method has been developed for the quantitative analysis of XPS-measurements on homogeneous layer systems.@footnote 1@ Starting from the apparent concentrations, measured at only one take-off angle, the method provides values for the composition and the thickness of all layers present in the system in a self-consistent way. The method works well for homogeneous layer systems (e.g. samples consisting of a Self Assembling Monolayer (SAM) on a substrate), provided that for each element or chemical state is known to which layer it belongs. Measurements at two or more different angles provide in general information about the depth-distribution of an element or a chemical state in a sample. The present calculation method has been extended to include measurements at two or three measuring angles; by doing so also the depth-distribution of the elements is obtained in a quantitative way. The method will be illustrated by experiments with various SAM-layers on copper. The Cu2p- and the Cu LMM lines were used to obtain information about the chemical state of copper. The copper surfaces were pre-cleaned by means of ion etching in the XPS instrument and incubated with the appropriate SAM-layer without contact with the ambient air. @FootnoteText@ @footnote 1@ C. van der Marel, M. Yildirim and H. Stapert, J. Vac. Sci. Technol. A23 (2005) 1456 - 1470.

SS-TuP24 Alkali Ion Scattering from Metal Nanoclusters, G.F. Liu, P. Karmakar, University of California, Riverside; Z. Sroubek, Czech Academy of Sciences, Czech Republic; J.A. Yarmoff, University of California, Riverside
Neutralization during the scattering of low energy (0.5-5 keV) alkali ions provides a sensitive measure of the confined quantum states of nanomaterials. The neutral fraction (NF) for Na@super +@ scattering from

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small Au clusters was previously shown to be surprisingly high (up to 50%), and to decrease with increasing cluster size.¹ This indicated that scattered alkali ions couple to atomic-like states specific to the nanoclusters, and the energy of the states is a function of the cluster size. In this work, Na⁺, Li⁺ and K⁺ ions are employed to probe the presence and position of the confined states of metal nanoclusters, and their dependence on cluster size is compared. Nanoclusters are formed by deposition of Au onto TiO₂ and self-organized clusters are produced from Au and Ag thin films by Ar⁺ ion sputtering. The ion scattering NFs have different dependences with respect to cluster size for each alkali projectile. The microscopic mechanisms involved in charge exchange between the alkali ions and the nanoclusters will be discussed. ¹G. F. Liu, Z. Sroubek, and J. A. Yarmoff, Phys. Rev. Lett. 92, 216801 (2004).

SS-TuP25 First Principles Studies of the Reactivity of Pt Islets on Ru(0001)*, M. Alcantara Ortigoza, S. Stolbov, T. Rahman, Kansas State University

A key element of direct methanol fuel cells is a catalyst for electro-catalytic oxidation of methanol. However, during this reaction, intermediate CO adsorbed on the surface blocks the active sites and poisons the reactivity of commercial catalysts. It was recently reported that nanoclusters of Ru with sub-monolayer of Pt are much more tolerable to CO than commercial alloy catalysts.¹ The mechanism of the reaction on this nanocatalyst is not clear. It apparently depends on the size of Pt islands whose optimum size is small (about 10 atoms). As a step towards understanding of the nature of this phenomenon, we have performed first principles studies, based on density functional theory, of the stability and reactivity of small Pt islands on Ru(0001), whose geometry represents that of the dominant facets of the Ru nanoparticles in the experiments of Brankovic et al. We have calculated energetics and geometric structures for 1- to 9-atom islands and one monolayer of Pt adsorbed on Ru(0001) using the pseudopotential method with the plane wave expansion for the wave function. We find the formation energy per atom of the islands to decrease monotonically from -5.1 eV to -6.1 eV, as the number of Pt atoms in the 2D island increases from one atom to one monolayer. The propensity of the systems to form as many interatomic bonds as possible thus overpowers the effect of stress caused by some misfit of Ru and Pd interatomic bonds. CO molecules are found to adsorb preferentially at the Pt island edges with a bond tilted towards the Ru atoms. The energetics of diffusion of CO and OH and their reaction pathways, as an intermediate step in methanol decomposition, are examined. ¹S. R. Brankovic, J. X. Wang, and R. R. Adzic, Electrochem. Sol.-St. Lett. 4 (12) A217 (2001). *Work supported in part by DOE under grant DE-FG02-03ER15465 and DE-FG02-03ER46058.

SS-TuP27 Adsorbate-Induced Faceting of Atomically Rough Re Surfaces, H. Wang, W.H. Chen, A.S.Y. Chan, T.E. Madey, Rutgers University

We report faceting of atomically rough Re(12-31) and (11-21) surfaces induced by oxygen or ammonia using AES, LEED, STM and synchrotron-based high resolution X-ray photoemission spectroscopy (HRXPS). Faceting is driven by thermodynamics (anisotropy of surface free energy) but is controlled by kinetics of surface diffusion. The Re(12-31) surface undergoes faceting once the oxygen coverage exceeds 0.5 monolayer (ML) and the surface is annealed at $T \geq 700\text{K}$. The morphology of the surface depends on oxygen coverage and adsorption temperature, ranging from long sawtooth ridges to complex structures exposing some of the following five different facets: (11-21), (01-10), (10-10), (01-11) and (10-11). For Re(11-21), adsorption of oxygen at room temperature followed by annealing causes the surface to become partially faceted with (01-10) and (10-10) facets forming zigzag chains. Under oxidation conditions, i.e. dosing a large amount of oxygen at high temperatures (900-1000K), the (11-21) surface is completely covered by four facets identified as (01-10), (10-10), (01-11) and (10-11). In contrast, after exposure to ammonia at 700K, the Re(11-21) surface only shows a (1x2) reconstruction and remains planar (ammonia dissociates on Re, and only N remains on the surface at $T > 700\text{K}$). By exposure to ammonia at 900K, the Re(11-21) surface becomes completely faceted, forming 2-sided ridge-like structures; the orientations of the ridge sides are different from any of those found in oxygen-induced faceting of Re(12-31) and Re(11-21). Our work demonstrates that it is possible to tailor the surface morphology by choosing appropriate adsorbate and annealing conditions, which in turn provides different but related model systems to study structural sensitivity in catalytic reactions as well as potential templates to grow nanostructures.

SS-TuP28 Methane Activation on Nickel Surfaces: Mechanistic Insights from State-Resolved Reactivity Measurements, A.L. Utz, D.R. Killelea, V. Campbell, D.F. Del Sesto, Tufts University

The molecular-level mechanism for methane activation on metal surfaces remains a subject of inquiry and debate. This has occurred in part because many experiments quantify the average reactivity of ensembles of reagents. The ensembles contain a distribution of molecules whose internal (vibrational and rotational) energies may vary significantly. The many energetic degrees of freedom available in this system severely hamper attempts to deconvolute ensemble averaging. This presentation describes experiments in which laser excitation prepares the methane reagents in specific vibrational and rotational states with well-defined total energy. We then quantify the reactivity of these state-selected molecules. Our ability to systematically vary the total energy of the reagents and its distribution among translational, rotational, and the stretching and bending vibrations of methane allows us to identify how energy deposited into specific reagent motions promotes reactivity. The presentation will highlight how these state-resolved results shed light on the mechanism for activation of methane and other hydrocarbons.

SS-TuP29 Rebound Transitions in Surface Diffusion, G. Antczak, University of Illinois

We have examined in detail the mechanism of surface diffusion on an atomic scale for the W(211) plane. Types of movement as well as their kinetics have been identified. The investigations are based on the distribution of displacements of single atoms on planes around 15 spaces in diameter. The distribution for any one temperature consists of at least 1200 observations. Special attention was paid to transient temperature effects during cooling and warming of the sample. At a temperature 1/10 the melting point we identified, in addition to standard single jumps in the direction, double jumps as well as rebound jumps which occur when an atom starts in the direction but turns back and lands at the starting point. In the investigated temperature range we have not observed any triple jumps. The kinetics of all kinds of jumps were derived, and the correlation between different types of jumps was investigated. We found that double as well as rebound jumps originate from single jumps. The increasing significance of non-nearest-neighbor transitions gradually diminishes the rate of single transitions, which almost reaches zero at 320 K. Rebound jumps start to be noticeable at 300K and seem to be quite frequent in diffusion over the W(211) plane. Surprisingly, their energy is lower than the activation energy for double transitions, 1.03 eV compared with 1.44 eV for double jumps. The reason for that is not completely clear, but possible factors involved will be presented. Research supported by the Department of Energy under Grant No. DEFG02-91ER45439 to the Materials Research Lab.

SS-TuP30 Adsorption and Displacement of Cetyltrimethylammonium Bromide (CTAB) on Model Gold Surfaces, S. Lee, V.H. Perez-Luna, Illinois Institute of Technology

The adsorption and displacement of the cationic surfactant, cetyltrimethylammonium bromide (CTAB) on model crystalline gold surfaces was studied. Adsorption of CTAB from aqueous media onto gold surfaces of different crystal orientations was studied by water contact angle measurements, spectroscopic ellipsometry, and FT-IR spectroscopy. Displacement of adsorbed CTAB molecules with 16-mercaptohexadecanoic acid (MHDA) from planar gold surfaces was performed using various MHDA concentrations and incubation times. The displacement reaction was also studied by water contact angle measurements, ellipsometry and FT-IR spectroscopy. The displacement of CTAB on gold is evident in the decreased water contact angle upon formation of carboxyl terminated surfaces. FT-IR spectra also show differences indicative of the displacement reactions. Differences in adsorption and displacement behavior at various crystalline surfaces are especially relevant to adsorption and displacement reactions of surfactants and alkanethiols on anisotropic gold nanoparticles such as nanorods. These studies will yield new insights on strategies for surface modification of nanoparticles presenting different crystalline surfaces.

SS-TuP31 Scanning Tunneling Microscopic Observation of Phospholipid Adlayer on Gold as a Model Cell Membrane, T. Yamada, RIKEN, Japan; S. Matsunaga, R. Yokomori, The University of Tokyo, Japan; D. Ino, RIKEN, Japan; M. Kawai, The University of Tokyo, Japan

Microscopic view of cell membranes in the molecular scale has been desired concerning the domain structures, or "rafts", formed by various phospholipids, which are related to important biochemical functions caused by inclusion of proteins. Physical-chemistry-based model study is

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needed to estimate the interaction between lipid molecules and to obtain information about domains formed with different kinds of phospholipids. We attempted to obtain STM images of phospholipid adlayer spread on modified gold substrates. First a Au(111) substrate modified by octanethiol was immersed in a neutral ammonium perchlorate buffer solution (50 mM, pH7.0), and the thiol adlayer was examined by STM within the solution. The thiol-covered surface was characterized by pores with diameters less than 10 nm, of which bottoms were also covered with thiol. Individual molecules within the adlattice were also discerned. Then the buffer solution was added with 1,2-dihexanoyl-sn-glycero-3-phosphocholine below the critical micellar concentration at 0.0 V vs. RHE of the Au electrode potential. Sequential STM images of a fluidic lipid adlayer spreading along the surface were obtained. The thickness of adlayer was observed to be a few angstroms. The motion of lipid monolayer was detected as deformation of holes on the monolayer. By changing the electrode potential to -0.2 V vs. RHE, the adlayer was gradually altered into solidified patches of striped patterns with a periodicity of 4 nm. By returning the potential to 0.0 V vs. RHE, the fluidic monolayer was restored. This change is considered related to polymerization of phospholipids. More times of potential cycling induced fragmentation of the solid striped patches. It was recognized that the functions of phospholipids are addressable on the viewpoint of nanometer-scale chemistry. The applicability of STM to lipid adlayer is promising. Some cross-checking spectroscopic evidences will be also presented.

SS-TuP33 Enhanced Initial Hydrophilicity and Biological Response of Microstructured Titanium Implants by Chemical Modification, M. De Wild, Institut Straumann AG Switzerland, Switzerland; F. Rupp, L. Scheideler, Poliklinik für Zahnärztliche Prothetik Tuebingen Germany; M. Wieland, Institut Straumann AG Switzerland; J. Geis-Gerstorfer, Poliklinik für Zahnärztliche Prothetik Tuebingen Germany; G. Zhao, Z. Schwartz, Georgia Institute of Technology; D. Cochran, University of Texas Health Science Center at San Antonio; B.D. Boyan, Georgia Institute of Technology
Surface topography and chemistry both influence initial wettability and peri-implant bone apposition of implants. Until now, sandblasted and acid etched (SLA) titanium surfaces are initially hydrophobic due to microstructuring and contamination with hydrocarbons and carbonates. The purpose of this study was to investigate initial hydrophilicity and protein adsorption and examine its role in the response of osteoblasts on a new developed chemically modified implant surface called SLActive. By chemical modification it is now possible to overcome the initial hydrophobic behavior of standard implant surfaces. The innovative clean-room production method influences protein/surface and cell/surface interactions in vitro. This study shows that surface energy controls osteoblast differentiation and local factor production. Histological and biomechanical observations of osseointegration approve the enhanced interactions between the SLActive implant surface and the tissue in the initial healing phase.

SS-TuP36 Chemicurrent Caused by Adsorption of -C=C -Contained Molecules on Pt Surfaces at Low Temperature, M. Sushchikh, M.N. Lapushkin, UC Santa Barbara; H. Nienhaus, University of Duisburg-Essen, Germany; D. Auerbach, Hitachi Global Storage Technologies; E.W. McFarland, UC Santa Barbara

A chemicurrent caused by directing beams of C=C -contained molecules (ethylene, propylene) at 100K on evaporated Pt films was measured using Schottky-type metal-semiconductor (MS) devices. Largest chemicurrent was observed for ethylene with overall yield 2×10^5 e/molecule. In the case of propylene the yield was 5×10^6 e/molecule. Increase in the kinetic energies of the impinging molecules (up to 0.5eV for ethylene and up to 0.45eV for propylene) using seeded beam techniques did not affect the chemicurrent overall yield. Beams of large molecules (benzene, propylene oxide, allylbenzene, styrene) did not cause observable chemicurrent.

SS-TuP37 Adsorption Reaction of C₂H₅SH on Rh(100) Surface Studied by XPS and Sulfur K-edge NEXAFS, S. Yagi, T. Nomoto, A. Koizumi, Nagoya University, Japan; G. Kutluk, Hiroshima University, Japan; K. Soda, Nagoya University, Japan; E. Hashimoto, M. Taniguchi, Hiroshima University, Japan
There are various environmental problems. One of the causes is automobile exhaust gas. Therefore an efficient automobile catalyst is needed for the exhaust gas (SO_x, NO_x, C_xH_y) purification. Since the purification catalyst loses its activity in a sulfur-containing molecular atmosphere, which is named "Sulfur Poisoning", the adsorbed sulfur has a great influence on the catalyst performance. It is important to investigate the reaction of sulfur containing molecules on the catalyst surface. In comparison with other platinum group metals, rhodium especially has

much resistance to the sulfur poisoning. In this investigation, we have studied the adsorption structure of C₂H₅SH on Rh(100) surface by X-ray Photoelectron Spectroscopy (XPS) and S K-edge Near Edge X-ray Absorption Fine Structure (NEXAFS) methods. The Rh(100) surface was cleaned by the repeated operation (Ar⁺ sputtering and annealing) and then exposed by C₂H₅SH at 85 K. Both XPS and NEXAFS measurements were carried out at the soft X-ray double crystal monochromator beamline BL-3 on Hiroshima Synchrotron Radiation Center (HSRC). C₂H₅SH coverage is submonolayer phase and estimated to be 0.15 ML. The S_{2p} XPS results show that the C₂H₅SH molecules dissociate to ethanethiolate C₂H₅S⁻ and atomic sulfur. The C_{1s} XPS results indicate that some hydrocarbons (C_xH_y) adsorb on Rh(100) surface. It is clear that the adsorbed C₂H₅SH, C₂H₅S⁻ and hydrocarbons behaviors depend on substrate temperature. @FootnoteText@@@footnote 1@ J.S. Hepburn et al., Energy & Fuels 2 (1988) 289.

SS-TuP38 Measurement of Residual Water on Aluminum Surface by PMIRRAS, H.P. Hsueh, NSRRC, Taiwan; C.W. Yeh, NTHU, Taiwan; G.Y. Hsiung, NSRRC, Taiwan; J.R. Chen, NSRRC and NTHU, Taiwan

Water always plays a vital role in the cleaning process of aluminum material used in UHV or XHV devices like the vacuum chambers used in large accelerators. Yet it is the residual water inside or on the thin alumina layer on top of the bulk aluminum material that was hated most in UHV or XHV regime since it is one of the major obstacles to achieve XHV. Phase modulated infrared reflection absorption spectroscopy (PMIRRAS) system has been setup and used in this study to explore how the residual water interacts with alumina surface layer of bulk aluminum as different cleaning method is applied. Both residual water quantity and their binding mechanism will be measured and analyzed. Cleaning methods include ozone water cleaning and traditional acid (HNO₃+HF) and alkali (NaOH) cleaning etc. With this study, it will be determined which cleaning method has the most effective way to clean aluminum surface (contaminations less than a certain level) and yet generate either less residual water or easier repelled residual water by baking at lower temperature or shorter period. Some spectra have been measured and water spectrum at 3450 1/cm has been identified. Further analysis of obtained data will be carried out. More samples will be measured and the results will be discussed.

SS-TuP39 The Interaction of Aluminum with 1,3,5-trinitro-1,3,5 Triazine, V.J. Bellitto, Naval Surface Warfare Center, US

Vibrational and photoelectron spectroscopies have become useful tools for identifying adsorbed aromatics and their orientation on surfaces. The adsorption geometry of aromatics, such as benzene, pyridine, and triazine on Al has been deduced. On sp-metal surfaces such as on Al, benzene has been shown to adsorb in a flat-lying geometry. Although the bonding orientation is similar to that of transition metals, the bonding interaction is different with only a weak benzene-Al interaction. For the adsorption of pyridine at low temperatures and low coverages, the molecular plane is parallel to the surface plane. At higher coverages, the molecular plane tilts toward the surface normal and is bonded through the nitrogen lone pair. We have previously reported on the chemisorption of triazine on an Al (111) surface using X-ray photoelectron spectroscopy (XPS) and infrared reflection absorption spectroscopy. The data showed that some s-triazine molecules dissociatively chemisorb on the Al surface, while others adsorb intact and bond to the surface through a nitrogen lone pair. The data revealed the molecular plane of the intactly adsorbed triazine is tilted with respect to the substrate surface plane. In this work, X-ray photoelectron spectroscopy (XPS) is used to characterize the interaction of 1,3,5-trinitro-1,3,5 triazine (RDX) with Al. XPS is used to determine the chemical species at the RDX/Al interface. Besides its usefulness as a tool for chemical analysis, XPS is useful in examining changes to chemical states of materials. For RDX, the spectrum of the N 1s region has two easily discernable peaks assigned to the nitro group and ring structure nitrogen. Upon the initial interaction of aluminum with RDX, the N 1s spectrum reveals that the nitrogen peak associated with the nitro group is diminished compared to that of the ring structure. This is an indication of the preferential reaction of the nitro group with the aluminum, leaving the ring structure intact.

SS-TuP40 Methanol Adsorption on Clean and O-Predosed V(100) Surfaces, M. Shen, F. Zaera, University of California, Riverside

The reaction of methanol has been studied on the clean and O-covered V(100) surfaces. On the clean surfaces, adsorbed methanol follows various reaction pathways leading to the production of methane, carbon monoxide, formaldehyde, and ethylene the main carbon-containing desorbing compounds. Methane desorption takes place mainly in two temperature regimes centered at around 350 and 500 K. Predosing of

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oxygen appears to significantly enhance the high-temperature methane production at the expense of the one at low temperatures. In addition, an upward shift is seen in the desorption temperatures of methane, ethylene and hydrogen in the presence of coadsorbed oxygen. Finally, the coupling mechanism for the formation of ethylene was investigated by using isotope labeling and also comparing the TPD spectra of several probing molecules. Our results indicated that $-\text{CH}_2\text{O}-$ and $-\text{CH}_2-$ are the most likely intermediates.

SS-TuP41 Metallization of Self-Assembling Monolayers of Conjugated Molecules by Electroless Deposition of Cu, C.T. Nottbohm, A. Turchanin, A. Götzhäuser, University of Bielefeld, Germany

Metallization of self-assembling monolayers (SAMs) is of great interest for various areas of fundamental and applied research: fabrication of microelectronic and molecular electronic devices, establishing of electrical contacts to single molecules, metal patterning of supramolecular assemblies. Here we present an investigation of the Pd catalysed electroless deposition (ELD) of Cu on top of the amino-terminated cross-linked biphenylthiol SAMs. The lateral cross-linking and formation of amino groups have been achieved by irradiation of nitrobiphenylthiol SAMs with low energy electrons. The x-ray photoelectron spectroscopy (XPS) and atomic force microscopy (AFM) data show that the cross-linked SAM acts as a barrier suppressing the catalyst-free ELD of Cu on the Au substrate. In order to deposit Cu on the cross-linked SAMs a Pd(0) catalyst was immobilized to their surface. This was realized by the chemical reduction of Pd(II) ions coordinated to the terminal amino groups. Angle resolved X-ray spectroscopy (ARXPS) verified every step of the Pd immobilization and unambiguously show that it forms an outermost layer of the cross-linked SAM. The AFM/XPS data show that Cu is then deposited in cross-linked areas at the catalytic site and hence on the surface of the SAM. A. Götzhäuser, W. Eck, W. Geyer, V. Stadler, Th. Weimann, P. Hinze, M. Grunze, Adv. Mater. 13, 806 (2001).

SS-TuP42 Adsorption Behavior and Reaction Properties of NO and CO on the Ir Surfaces, I. Nakamura, A. Takahashi, M. Haneda, H. Hamada, T. Fujitani, National Institute of Advanced Industrial Science and Technology (AIST), Japan

Selective catalytic reduction of NO in oxidizing atmospheres has recently received extensive attention, since it has potential as a practical measure to remove NO_x emitted from diesel engines, lean-burn engines and combustors. A few studies of selective catalytic reduction of NO have been made with such reductants as H₂ and CO over the Ir-based catalysts. However, no evidence for explaining this reaction mechanism and the active site has been obtained. To clarify the role of CO for NO reduction, we studied the surface structure dependence for the reaction of NO and CO on the Ir single-crystal surfaces using surface science techniques such as XPS and IRAS. We examined the adsorption state of NO and CO on the Ir(111) and Ir(211) surfaces using IRAS. The peaks due to the adsorbed NO on hollow and atop sites were observed at 1400-1444 cm⁻¹ and 1799-1820 cm⁻¹ on Ir(111). On the other hand, the peaks due to the adsorbed NO on bridge and atop sites were observed at 1580-1590 cm⁻¹ and 1790-1810 cm⁻¹ on Ir(211), indicating that the NO adsorption was depended on the surface structure. Concerning the CO adsorption state, we observed the peak of CO adsorbed on atop site at 2060 cm⁻¹ over Ir(111) and at 2080 cm⁻¹ over Ir(211), indicating that the CO adsorption was not depended on the surface structure. We also investigated the thermal reactivity of the NO and CO adsorbed on the Ir(111) and Ir(211) surfaces. It was clearly demonstrated that the Ir step was active site for the NO dissociation. Furthermore, it was found that the NO reduction with CO on Ir surface proceeded via the direct decomposition of NO.

SS-TuP43 Reactions of SO₂ and Between Atomic S and O₂ on the Ir(111) and Rh(111) Surfaces, T. Fujitani, I. Nakamura, M. Haneda, H. Hamada, National Institute of Advanced Industrial Science and Technology (AIST), Japan

It has been reported that Ir/SiO₂ shows marked catalytic activity for NO reduction with CO in the presence of O₂ and SO₂. However, no evidence was obtained for the role of SO₂. We examined the role of SO₂ for NO reduction with CO in the presence O₂. The reactions of SO₂ on Ir(111) and Rh(111) were investigated using XPS. On Ir(111), the peaks due to molecularly adsorbed SO₂ were observed after SO₂ exposure at 200 K. With the rise of temperature at 300 K, two S 2p peaks were observed at 165.9 and 162.4 eV. The peak at 162.4 eV was assigned to atomic S. The ratio of coverage of S 2p (165.9 eV) and O 1s (530.7 eV) was almost 3,

indicating that these peaks corresponded to the SO₂. After annealing to 400 K, the adsorbed SO₂ significantly decreased and the atomic oxygen was observed. The SO₂ and atomic oxygen were completely desorbed and the only atomic S was presented on the surface above 500 K. On Rh(111), SO₂ was molecularly adsorbed on the surface at 200 K. The adsorbed SO₂ dissociated to atomic S and oxygen above 300 K. The only atomic S was presented on both surfaces above 500 K, but the formation process of atomic S on Ir(111) was different from that on Rh(111). The reaction between atomic S and O₂ was examined on Ir(111) and Rh(111). On Ir(111), S coverage decreased with increasing O₂ exposure at 500 K, and then no atomic S was observed at 1000 s, indicating that atomic S reacted with surface oxygen and was removed from the surface in the presence of oxygen. In contrast, S coverage was almost constant on Rh(111). Thus, the reactivity of atomic S with oxygen on Ir(111) was significantly higher than that on Rh(111).

SS-TuP44 Study of Dye Molecule Orientation and Configuration in Dye Molecule Doped Polythiophene Films, H. Kato, S. Takemura, Y. Watanabe, T. Nara, T. Hayashi, T. Sugiyama, T. Hiramatsu, N. Nanba, Kanto Gakuin University, Japan

Conducting polymer polythiophene (PT) films incorporated with dye molecule such as crystal violet (CV) and brilliant green (BG) were prepared by electrochemical doping and casting injection methods. Electrochemical doping was conducted in dye dissolved acetonitrile by applying negative voltage in a triangle wave to an as-grown PT film. Casting of dye molecules was conducted by dipping a PT film in dye dissolved acetonitrile so that the dye molecules diffused into the polymer film. Vibrational states of the doped dye molecule and the polymer backbone were investigated by FTIR RAS and transmission measurements in order to examine the dopant orientation and configuration in polymer chains in the hybrid films. In the case of brilliant green doping, CH in plane modes of the PT backbone which appeared around 800 cm⁻¹ was almost identical in both spectra of doped polymer and non-doped polymer. In the case of electrochemically doped sample, however, ring stretching modes which appeared around 1585 cm⁻¹ was observed only in the FTIR transmission spectrum, not observed in the FTIR RAS spectrum. However, in the case of casting sample, the ring stretching mode was observed by both of FTIR RAS and transmission measurements. The similar results was obtained in the case of CV doped PT films. This result shows that CV and BG molecule planes doped in polymer are inclined to be planar to the film plane in the case of electrochemical doping under a negative voltage in triangle wave. In the case of casting sample, the dopants were supposed to be randomly oriented. The results suggest that the manipulation of the molecular orientation and configuration would be possible by the electrochemical doping method.

SS-TuP45 XPS and FTIR Study of Electrochemical Doping of Fullerene and Copper Phthalocyanine Molecules in Conducting Polymers, H. Kato, S. Takemura, Y. Watanabe, A. Ishii, I. Tsuchida, Y. Akai, T. Sugiyama, T. Hiramatsu, N. Nanba, K. Iwasaki, Kanto Gakuin University, Japan; O. Nishikawa, M. Taniguchi, Kanazawa Institute of Technology, Japan

Conducting polymer polythiophene (PT) films incorporated with fullerene C₆₀ and copper phthalocyanine (PcCu), which were highly functional molecule, were prepared by electrochemical doping and casting methods. Electrochemical doping of C₆₀ was conducted by adopting different applying voltage polarity. C₆₀ doping proceeded in C₆₀ dissolved toluene by applying positive or negative voltage to a PT film. Electrochemical doping of PcCu was also conducted in PcCu dissolved toluene by applying negative voltage to a PT film. Charge transfer and interaction between the doped molecules and PT polymer chains, varied with the doping measures, were investigated by XPS analysis of the core-level energies and spectral profiles of the atomic components. Vibration states of the doped molecule and the polymer backbone were also investigated by FTIR RAS and FTIR transmission. In the case of C₆₀ doped PT, regarding electrochemical doping, applied voltage polarity made quite a different C 1s core level spectral profiles. A large split peak associated with shifted peaks due to C₆₀ and the charged states appeared in the case of positive polarity while serial ordered peaks with the same energy distance appeared due to C₆₀ charged states in the case of negative polarity. In FTIR measurements, frequency position of F_{1u} mode at 1400cm⁻¹, which was sensitive to charged states of C₆₀ varied with applied voltage polarity. In the case of PcCu doped PT, PcCu-origin peaks on the higher energy side appeared in the C 1s spectrum associated with the signal detection of N 1s and Cu 2p. In FTIR measurements, characteristic vibrational modes to PcCu, in-plane, out-of-plane, and ring stretching modes were observed. Central metal-origin peak was also observed. New peaks at 1545 cm⁻¹ and 1680 cm⁻¹ indicates the possibility of the polymer- PcCu linkage.

Tuesday Evening Poster Sessions, November 14, 2006

SS-TuP47 Nickel-rich Bimetallic Phosphide Hydrotreating Catalysts, A.W. Burns, M.E. Bussell, Western Washington University

Our research group is interested in the design of novel transition metal phosphide catalysts to be used for the removal of sulfur from petroleum feedstocks. Hydrodesulfurization (HDS) is a process in which sulfur is catalytically removed from fossil fuels. This project focuses on the development and properties of nickel-rich bimetallic phosphide catalysts. Nickel phosphide (Ni_2P) has been found to exhibit high HDS activity as well as excellent stability under reaction conditions. By incorporating another metal such as Co or Fe, we are investigating the properties of bimetallic phases in order to optimize the nickel phosphide-based catalysts. Therefore, we have prepared a series of oxide-supported $\text{Co}_x\text{Ni}_{2-x}\text{P}$ catalysts, where x varies between 0 and 1. Our results show an increase in HDS activity with increasing Ni (decreasing Co) compositions. Interestingly, for $\text{Co}_x\text{Ni}_{2-x}\text{P}$ compositions where x is small but not zero, the HDS activity is higher than that of pure Ni_2P . As will be described, different results are observed for a series of $\text{Fe}_x\text{Ni}_{2-x}\text{P}$ catalysts. X-ray diffraction (XRD) is used to confirm the identity of the crystalline phosphide phase(s) present, to determine the average crystallite size, and to observe the transition from the Co_2P -like phase to the Ni_2P -like phase. BET surface area and O_2 chemisorption capacity measurements are used to determine the surface area and the number of active sites for the oxide-supported catalysts. Together with the results of elemental analysis and x-ray photoelectron spectroscopy (XPS) measurements, the surface area and chemisorption data are used to describe how the HDS activity is influenced by the surface properties of these catalysts. In this manner, we are determining the optimal composition for Ni-rich bimetallic phosphide catalysts for the HDS process.

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