## Surface Science Division
## Room 4C - Session SS-WeP
## Poster Session

**SS-WeP1 Strain and Strain Relief in Gadolinium(0001) Thin Films on Mo(112)*, T. Komesu,*** *H. Jeong, P.A. Dowben,* University of Nebraska, Lincoln

The electronic structure of strained and unstrained Gd(0001) has been studied with spin-polarized photoemission spectroscopy and spin-polarized inverse photoemission spectroscopy. In this work, we observed that relaxation of the expansively strained crystal in-plane lattice constant, of Gd(0001) on Mo(112), significantly diminishes the differences in the electronic structure from that observed for Gd(0001) grown on W(110). The defects incorporated in Gd films, with increasing film thickness, lead to both lattice relaxation and a loss of net polarization for Gd(0001) grown on Mo(112).

**SS-WeP2 Formation process of a Cu-Zn surface alloy on Cu(111) investigated by STM*, M. Sano,*** *S. Ishikura,* University of Tsukuba, Japan*; T. Fujitani,* National Institute for Resources and Environment, Japan*; J. Nakamura,* University of Tsukuba, Japan

We had previously shown that a Zn-deposited Cu(111) surface is a good model for methanol synthesis by the hydrogenation of CO@sub 2@, and a Cu-Zn surface alloy is active species for the reaction. Here, we investigated the formation process of the Cu-Zn surface alloy formed on a Zn-deposited Cu(111) surface by STM. The STM measurements were carried out using a UHV-STM apparatus equipped with LEED-AES. Zinc was deposited on Cu(111) by resistively heating a Zn wire. STM image of the surface after the Zn deposition at room temperature showed that the bright atoms were localized in the vicinity of step edges. These blight atoms were considered as Zn atoms substituted for the substrate Cu atoms. The density of Zn atoms decreased with increasing distance from step edges and no Zn atoms were observed on the terrace away from the steps. The migration of Zn atoms over the surface was observed by time resolved STM measurements. The migration rate was determined to be 6.67x10@super -3@ s@super -1@ and the mean residence time was 150 s. These results indicate that the alloying initially occurs around steps and then Zn atoms migrate over the terrace. On the other hand, after annealing the Zn-deposited Cu(111) at 523 K, STM images showed that Zn atoms were distributed homogeneously over the Cu(111) surface. The Zn coverage estimated by the STM images was in good agreement with that measured by AES. Pair-correlation analysis of the NN distribution for Zn atoms suggested that Zn atoms were randomly distributed on the terraces, indicating that Zn atoms were randomly substituted for Cu atoms leading to the Cu-Zn surface alloy.

**SS-WeP3 Microkinetics of Formate Synthesis on Cu Catalysts*, T. Fujitani,*** National Institute for Resources and Environment, Japan*; I. Nakamura, H. Nishimura, H. Nakano, J. Nakamura,* University of Tsukuba, Japan

The kinetics of formate synthesis by hydrogenation of CO@sub 2@ and formate decomposition has been studied on Cu(111) and Cu(110) surfaces using in-situ IRAS and STM apparatuses combined with a reactor (1 atm). It has been found that the formate synthesis does not depend on the surface structure of copper between Cu(111) and Cu(110). The activation energy of formate synthesis on Cu(111) and Cu(110) have been determined to be 68.3 and 69.7 kJ/mol, respectively. The microkinetics of the formate synthesis can be explained by that assuming an Eley-Rideal mechanism. On the other hand, the activation energy and the pre-exponential factor for formate decomposition on Cu(111) were different from those on Cu(110), indicating that the decomposition of formate species depend on the Cu surface structure. Furthermore, the decomposition rate of formate on Cu(111) is very different depending on the preparation method, the synthesis from CO@sub 2@ and H@sub 2@ at atmospheric pressure and the preparation by adsorption of HCOOH in UHV. However, the activation energy of the decomposition for both cases is close to each other, meaning that the frequency factor of the rate constant is different for the two cases. The difference can be explained by the different structures of formate observed by STM. In the presence of atomic hydrogen, the decomposition rate of the formate synthesized from CO@sub 2@ and H@sub 2@ increases and becomes equal to the decomposition rate of the formate prepared by the adsorption of HCOOH. The activation energies and the pre-exponential factors for both the formate synthesis and the formate decomposition on Cu/SiO@sub 2@ were in good agreement with those on Cu(111), suggesting that the surface structure of Cu for the Cu/SiO@sub 2@ catalyst is identical with the Cu(111) surface.

**SS-WeP4 The Adsorption-Desorption Properties of CO on W(111) Surface*, S.-B. Lee,*** *S.-Y. Lee, Y.-D. Kim, T.S. Yang, J.-H. Boo, C.Y. Park,* SungKyunKwan University, Korea*; H.-T. Kwak,* Kook Min University, Korea

The adsorption and desorption properties of CO have been studied on W(111) surface in the temperature range of 300 - 1100 K by LEED, XPS, UPS, and TDS. After CO saturation at 300 K, four adsorption states obtained from TDS experiment were observed at 400, 850, 1000, and 1100 K, called @alpha@, @beta@@sub 1@, @beta@@sub 2@, and @beta@@sub 3@ states, respectively. The desorption temperature of @beta@@sub 3@-CO state shifted to higher temperature with increasing CO exposure signifying an attractive lateral interaction between adsorbed species. Using Bragg-Williams approximation the lateral interaction energy (-5.7 kJ/mol) was calculated and the TD-spectra obtained experimentally were successfully simulated using by quasi-chemical approximation. The desorption kinetic order of the @beta@@sub 3@-CO state is followed by the first order indicating that the adsorbed state of @beta@@sub 3@-CO seems to be a molecular state rather than that of dissociated state. With UPS and XPS, the CO adsorption property (especially the @beta@@sub 3@-CO) on W(111) was clearly confirmed. The adsorption of CO on W(111) at 300 K exhibited only one emission peak at -6.3 eV below Fermi level due to 1@pi@+5@sigma@ molecular orbitals of CO. With heating the adsorbed CO to 1000 K, however, an additional emission peak was also observed at -7.1 eV due to an orbital energy splitting of 1@pi@+5@sigma@. This is strongly supported with a theoretical result calculated by ASED-MO method. Comparing the O state of @beta@@sub 3@-CO with that obtained from the dissociatively adsorbed oxygen species, we can identify that the @beta@@sub 3@-CO is different with that for dissociated CO suggesting a non-dissociated CO species with different geometry. From these results, a lying-down species of adsorbed CO is proposed.

**SS-WeP5 Ordered Structures of Oxo Overlayer on Cu(111) Electrode Surface in an Alkaline Electrolyte Revealed by Electrochemical STM*, O. Matsuoka,*** *S. Yamamoto, S. Sugiyama,* Mitsui Chemicals, Inc., Japan*; H. Nozoye,* National Institute of Materials and Chemical Research, Japan

Redox behavior of copper surface in aqueous solution is of great interest in many industrial fields, such as energy, catalytic, and microelectronic applications. Many characterization studies on copper electrode surface revealed that surface oxygen is not entirely removed even at the potential corresponding to the onset of hydrogen evolution. This oxo overlayer on surface is considered active for catalytic reactions.@footnote 1@ Information about the structure and behavior of oxo overlayer in aqueous solutions seems to provide a proper understanding of reacting mechanism of copper catalysts. We have investigated the structure of Cu(111) electrode surface that have an oxo overlayer in an 0.01M NaOH aqueous solution by using electrochemical scanning tunneling microscope (EC-STM). Two kinds of periodical structures of bright spots were observed.@footnote 2@ Dimensions of these periodical structures were similar to the unit cell for the (@sr@7 x @sr@7) and (2@sr@7 x 2@sr@7). The periodical structure similar to (@sr@7 x @sr@7) appeared at a cathodic wave at -0.9 V vs. Ag/AgCl on cyclic voltammogram, and this periodical structure was converted into (2@sr@7 x 2@sr@7) at more negative potential. Anodic wave related with the cathodic wave at -0.9 V appeared in anodic sweep. The potential of this anodic wave was different between these two periodical structures. We consider these periodical structures show an alignment of CuOH surface species which created by the reduction of sub-surface oxygen.@footnote 3@ @FootnoteText@ @footnote 1@L.D.Burk, et al., J.Electrochem.Soc., 137,553(1990) @footnote 2@O.Matsuoka, et al., Chem.Lett., 947(1998) @footnote 3@S.Haetinger, et al., J.Electroanal.Chem., 397,335(1995).

**SS-WeP6 Structure of MnO@sub x@/Rh(100) studied by STM*, H. Nishimura,*** *T. Tashiro,* University of Tsukuba, Japan*; T. Fujitani,* National Institute for Resources and Environment, Japan*; J. Nakamura,* University of Tsukuba, Japan

A modified Rh/SiO@sub 2@ catalyst with Fe or Mn shows excellent catalytic activity for the hydrogenation of CO into C@sub 2@ oxygenates such as acetic acid, ethanol and acetoaldehyde. The active sites may be located at the interface between Rh and MnO@sub x@ species. We have studied the structure of a MnO@sub x@ deposited Rh(100) surface using an ultra high vacuum scanning tunneling microscope (UHV-STM). The deposition of Mn over a Rh(100) surface was performed by resistively heating a Ta boat and then the Rh sample was annealed in an oxygen atmosphere to prepare the MnO@sub x@ species. The STM images showed a c(2x2) structure and a characteristic square unit (30 Å x 30 Å), which were tentatively assigned to Mn-Rh surface alloy and MnO@sub x@ species, respectively. A (111) like structure with six-fold symmetry was also assigned to MnO@sub x@ species.

**SS-WeP7 Electrochemical Scanning Tunneling Microscopy of Copper Adlayers on Iodine-Covered Au(111) in Sulfuric Acid Solution***, A. Martinez-Ruiz,* CICESE & Fac. de Ciencias, UABC, MEXICO*;* ***J. Valenzuela-Benavides****, L. Morales de la Garza,* CCMC-UNAM, Mexico*; N. Batina,* UAM-Iztapalapa, Mexico*; F. Castillon,* CCMC-UNAM, Mexico

We present structural and electrochemical studies of copper electrodeposition on the Au(111) surface precovered with iodine in a sulfuric acid solution. In situ electrochemical scanning tunneling microscopy (STM) studies reveal different adlayer structures depending on the potential of the gold working electrode. Before initiating the underpotential deposition (UPD) of copper, a (5x@sr@3) structure of the iodine adlayer is observed on wide terraces as reported in a similar study with perchloric acid solution. For more negative potentials, the (5x@sr@3) structure transforms to a (3x3) structure around 320mV (vs a Cu/Cu@super ++@ electrode). Cyclic voltammetry (CV) suggests that not enough copper is depositing at this potential to cause the observed (3x3) structure to form, since only a significant ammount of copper deposition begins at potentials below 250mV. This is in sharp contrast to the reported study performed in perchloric acid solution, where the (3x3) is attributed to the UPD of copper of approximately less than half of a monolayer. At the end of the UPD process a (@sr@3x@sr@3)R30@super o@ structure is observed. All these structures are also observed during the CV anodic cycle, returning to the initial (5x@sr@3) structure of the iodine adlayer, which can be removed at a more positive potential with the iodine atoms diffusing into the solution, leaving a bare Au(111) surface. The above results strongly indicate that the stable iodine layer exist on the top layers of Cu and Au during deposition and stripping of Cu. The presence of anions is discussed which may explain the difference between the CV data and the STM images.

**SS-WeP8 Lateral Compression of a Xe Film Physisorbed on the Surface of a Silver Single Crystal***,* ***S. Igarashi****, A. Tosaka, T. Hirayama, I. Arakawa,* Gakushuin University, Japan

The layering transition of a physisorption system on a metal single crystal has been investigated by means of an ellipsometry and an eXtremely-low-current LEED (XLEED). Our XLEED system is operated at the primary electron current of about 1 pA or less, which minimizes the effect of desorption, defect formation, and charging.@footnote 1@ We observed the surface structure of Xe/Ag(111) by XLEED while monitoring the layer growth by the ellipsometry from a submonolayer film to a thick one. An equilibrium between the Xe film and coexisting three-dimensional Xe gas has been maintained throughout the experiment. From a monolayer film to a sufficiently thick film, the Xe overlayer has clear hexagonal structure whose directions of the unit vectors are coincident with those of the substrate. The Xe-Xe spacing in the monolayer film on Ag(111) is known to be a few per cent larger than that of bulk. Our interest is how the Xe-Xe spacing varies in the process of layer growth. We have made a systematic observation of the change of the Xe-Xe spacing in one and two monolayer films at pressures between 10@super -7@ and 10@super -2@ Pa and at temperatures between 50 and 100 K. In the case of isothermal growth at 78.4 K, for example, the Xe-Xe spacing of the monolayer film is 4.53 Å at immediately after the first layer condensation at 1x10@super -5@ Pa and decreases gradually to 4.5 Å with increasing a surrounding pressure up to 1x10@super -3@ Pa. Then the spacing decreases rapidly and reaches almost that of bulk, 4.39 Å, just before the second layer condensation at the pressure of 4x10@super -2@ Pa. @FootnoteText@ @footnote 1@ S. Igarashi, Y. Abe, Y. Irie, T. Hirayama and I. Arakawa, J. Vac. Sci. Technol. A 16, 974 (1998).

**SS-WeP9 A Comparative Study for Small Molecule Adsorption onto Stoichiometric and Defective TiO@sub 2@ and SrTiO@sub 3@ Surfaces***,* ***K.F. Ferris****, L. Wang,* Pacific Northwest National Laboratories

Interactions of water and HCOOH with stoichiometric and defective TiO@sub 2@(100), TiO@sub 2@(110), and SrTiO@sub 3@(100) surfaces have been studied using electronic structure calculations. This paper presents a comparative study for the relationship between adsorbate interactions and reactivity focusing on the role of surface structure. Preliminary results for formate interaction with SrTiO@sub 3@(100) indicate strong adsorption consistent with experimental results, but in a distinctly different geometric arrangement due to absence of bridging oxygens present for the TiO@sub 2@ surfaces. This absence directly affects the water adsorption and dissociation behavior for SrTiO@sub 3@. Structural differences again modulate the reactivity of defect sites. Further results will be discussed in terms of potential reaction mechanisms and correlations with ongoing experimental studies.

**SS-WeP11 Structural and Chemical Investigations on Different Polar ZnO Surfaces***,* ***St. Hoevel****, Th. Beker, Ch. Boas, U. Burghaus, K. Weiss, M. Wuehn, C. Kolczewski, V. Staemmler, Ch. Woell,* Ruhr-Universität Bochum, Germany

We report on investigations of the structural and chemical properties of the two differently terminated Zn(0001) surfaces. The clean, oxygen terminated surface was studied with helium atom scattering (HAS) and LEED. The peak-shapes of the He-atom diffraction peaks and the variation of the He-atom reflectivity as a function of He-atom wavelength provide detailed information on the surface morphology (step height distribution, average terrace width, type of defects). As regards the chemical properties of the surface (e.g. presence of acidic sites), we studied the adsorption behaviour of pyridine on the two differently terminated ZnO(0001) surfaces with thermal desorption spectroscopy (TDS), x-ray photoelectron spectroscopy (XPS), and x-ray absorption spectroscopy (NEXAFS). The interpretation of the latter results is based on precise ab-initio electronic structure calculations for a model compound. The binding energy of pyridine on the O-terminated (000-1)-surface amounts to 57 kJ/mol and the spectroscopic data reveal only small modifications of the pyridine electronic structure, indicating the presence of a physisorbed species. On the Zn-terminated ZnO(0001)-surface the binding is substantially stronger, 112 kJ/mol, and the N1s NEXAFS-data for the pyridine @pi@*-resonance shows a shift of 0.6 eV towards higher binding energies. This observation indicates a substantial interaction between the nitrogen lone pair and the Zn d electrons, as confirmed by the ab-initio calculations.

**SS-WeP12 Formation of a Smooth and Pure Chromium Oxide Film on Stainless Steel Surface by Oxidation***,* ***B. Cho****, S. Chung,* Pohang University of Science and Technology, South Korea

Oxidation of stainless-steel for annealing temperature of 450 °C in oxygen partial pressures of 10@super -9@ to 10@super -4@ Torr was tested to form a smooth and pure chromium oxide film on the surface. Atomic force microscopy and scanning tunneling microscopy images show that oxidations in low oxygen pressures (10@super -9@ and 10@super -8@ Torr) favor the formation of not only macroscopically but also atomically smooth oxide films, which is almost total chromium oxide, as characterized by X-ray photoelectron spectroscopy. But oxidations in high oxygen pressures (10@super -6@ and 10@super -4@ Torr) prefer the development of very rough oxide films with distinct grains and significant proportion of iron. Considering that rough surfaces usually provide more adsorption sites for impinging molecules than smooth surfaces and pure chromium oxide films block hydrogen diffusion from bulk material more efficiently than inhomogeneous iron-rich oxide films, oxidation with low oxygen pressure may be a promising technique for the fabrication of a stainless steel vacuum chamber with enhanced outgassing characteristics.

**SS-WeP13 The Interaction of Water with the Basal Plane of @alpha@-Cr@sub 2@O@sub 3@: Dissociation and Multiply Coordinated Adsorption Sites***,* ***M.A. Henderson****, S.A. Chambers, C.L. Perkins,* Pacific Northwest National Laboratory

We have examined the interaction of water with an @alpha@-Cr@sub 2@O@sub 3@(001) thin film surface using TPD, HREELS and LEED. The @alpha@-Cr@sub 2@O@sub 3@(001) film is the terminus of an alternating @alpha@-Cr@sub 2@O@sub 3@/@alpha@-Fe@sub 2@O@sub 3@ heterostructure grown on an @alpha@-Al@sub 2@O@sub 3@(001) substrate using molecular beam epitaxy. The @alpha@-Cr@sub 2@O@sub 3@ lattice is 2@super o@ expanded inplane due to lattice matching to the @alpha@-Fe@sub 2@O@sub 3@. Water interacts strongly with the @alpha@-Cr@sub 2@O@sub 3@(001) surface, desorbing in two prominent TPD states at 345 and 297 K, both of which exhibit first-order desorption behavior. Weaker binding TPD states are observed at 210 and 185 K. Using a calibrated doser, TPD results indicate that the coverage of water in the 345 and 297 K TPD states is twice that of the surface Cr@super 3+@ coverage suggesting that each surface cation site binds two water molecules. Although no irreversible decomposition is detected by TPD, HREELS (acquired at room temperature to avoid sample charging) shows prominent losses at 3605, 2890 and 915 cm@super -1@. Using D2O, the latter two losses shift to 2645 and 2135 cm@super -1@ and the former is undetected (shifted under the lattice phonon modes). The 3605/2645 cm@super -1@ and 915/(?) cm@super -1@ losses are indicative of the hydroxyl stretching and bending modes, respectively, of a terminal hydroxyl group, whereas the 2890/2135 cm@super -1@ losses are suggestive of a very weak hydrogen-bonding interaction, probably between the deposited hydrogen/deuterium atom and the terminal OH/OD group. Although this hydrogen-bond is weak, as suggested by its low O-H stretching frequency, the dynamic dipole of its O-H stretch is as strong as that of the terminal OH group. Although HREELS analysis of the 297 K TPD state is in progress, our tentitive model is that each surface Cr@super 3+@ site binds both a molecular and dissociative form of water. The absence of strong coverage dependence in the TPD suggests that these water species are only weakly interacting. The role of lattice expansion will also be discussed, in comparison with studies on an unstrained @alpha@-Cr@sub 2@O@sub 3@(001) film (to be conducted).@footnote 1@ @FootnoteText@ @footnote 1@ This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences. Pacific Northwest National Laboratory is a multiprogram national laboratory operated for the U.S. Department of Energy by Battelle Memorial Institute under Contract DE-AC06-76RLO 1830. The research reported here was performed in the William R. Wiley Environmental Molecular Science Laboratory, a Department of Energy user facility funded by the Office of Biological and Environmental Research.

**SS-WeP14 In-situ Study on the Formation of SiC Thin Films on Si(111) Surface with 1,3-disilabutane: Adsorption Properties and Initial Deposition Characteristics***, H.G. Yoon, J.-H. Boo, S.-B. Lee,* ***W.L. Liu,*** SungKyunKwan University, Korea*; S.-C. Park, H. Kang,* Pohang University of Science and Technology, Korea*; Y. Kim,* Korea Research Institute of Chemical Technology, Korea

The adsorption properties of 1,3-disilabutane (DSB), SiH@sub 3@-CH@sub 2@-SiH@sub 2@-CH@sub 3@, and an initial deposition characteristics for the formation of SiC thin films on Si(111) surfaces have been studied in the temperature range of 150 - 1200 K in situ by XPS, UPS, TDS, and Cs@super +@ ion reactive scattering methods. After DSB dosing at 300 K, only one adsorbed state was obtained from XPS and UPS. The C 1s and Si 2p XP spectra appeared at ca. 283 and 99.5 eV showed no chemical (binding energy) shifts between RT and 600 K indicating a SiC cluster and/or islands formation. With increasing the surface temperature to 1200 K, however, a gradual binding energy shifts of both Si 2p and C 1s XP peaks to the higher values were observed due to a crystalline SiC thin film deposition. During deposition, moreover, we also identify the intermediate states of the thermal decomposition reaction of DSB on a Si(111) surface with Cs@super +@ ion reactive scattering. Several kinds of intermediates as CsCH@sub 4@Si@super +@, CsC@sub 2@H@sub 8@Si @sub 2@@super +@, CH@sub 4@Si@super +@, and CH@sub 3@Si@super +@ were detected at 150 K. In the case of DSB deposition between 800 K and 950 K, on the other hand, only one intermediate (i.e. CsCH@sub 4@Si@super +@) was observed indicating that most of C@sub 2@H@sub 8@Si@sub 2@ adsorbates have been reacted away at these temperatures, forming either CH@sub 4@Si or SiC thin films on the surface. Based on the experimental results of XPS, UPS, TDS, and Cs@super +@ ion reactive scattering, in this work, we proposed a possible chemisorption geometry and decomposition mechanism of DSB.

**SS-WeP15 Real-time VT-STM Studies of Dewetting Processes: Ag/Si(111)***,* ***K. Th@um u@rmer****, E.D. Williams, J.E. Reutt-Robey,* University of Maryland

Under typical MBE-conditions thin film morphology is often limited by kinetics. An excellent model system for film growth proceeding far from equilibrium is silver, deposited at room temperature on Si(111) (see review@footnote1@). At a mean film thickness of 1nm, the substrate is completely covered by worm-like structures. Using a variable temperature STM, we have studied the transformation of these metastable structures into equilibrium shaped hexagonal crystallites. By tracking the annealing process in real time, we encounter an astonishing variety of transition shapes. At ~200C the onset of de-wetting exposes substrate areas with a root3 x root3 reconstruction. The higher mobility on these denuded areas acts as a positive feedback, accelerating the decay of adjacent structures. At ~300 C the morphology is dominated by 500 nm wide and 100 nm high crystallites, exhibiting networks of partial dislocations on their (111)-top facets. This work has been supported by the NSF-MRSEC at University of Maryland under grant #DMR-96-32521. @FootnoteText@ @footnote 1@ H.Neddermeyer, Critical Rev. in Solid State and Material Science 16(5),309 (1990) 29, 30, 53-55, 57, 68.

**SS-WeP16 Dissociative Reaction of HBO@sub 2@ Molecules on Si(111)-7x7 Surface Studied by Scanning Tunneling Microscopy***,* ***K. Miyake****, T. Kaikoh, Y.J. Li, H. Shigekawa,* University of Tsukuba, Japan

Boron (B) has been attracting considerable attention as a promising c andidate for the formation of atomic-layer doped structure. Atomic-layer dop ing process on Si substrate consists of two parts; adsorption of a monolayer fraction of dopant atoms on Si surface and subsequent Si growth. Therefore, precise control of B atoms on Si surface is essentially important. Recently, HBO@sub 2@ molecules were found as a most appropriate boron source because o f its higher vapor pressure compared to the metal boron cases. However, how HBO@sub 2@ molecules react with the Si surface still remains as an open ques tion. In order to clarify this point, we characterized the chemical reaction process of HBO@sub 2@ molecules on Si(111)-7x7 surface in detail. We succeed ed in confirming two different states of HBO@sub 2@ molecules on the surface . When the substrate temperature during HBO@sub 2@ irradiation was kept at 3 00°C, the adsorbed HBO@sub 2@ molecules remained on the surface witho ut dissociation. On the other hand, when the substrate temperature was kept at 600°C, HBO@sub 2@ molecules were dissociated, and the oxygen- and boron-related adatoms were produced at corner and center adatom sites in 7x7 units, respectively. Taking the difference in the electronegativity between the oxygen and boron atoms into consideration, oxygen and boron atoms in HBO @sub 2@ molecules are expected to react with adatoms and rest atoms, respect ively. Then, as a result of the dissociation of HBO@sub 2@ molecules, oxygen and boron atoms may adsorb at the corner and center adatom sites, respective ly. In order to confirm this reaction process, the sample formed by HBO@sub 2@ irradiation at 300°C was annealed at 600°C for 1min. As exp ected, non-reacted HBO@sub 2@ molecules disappeared and the oxygen- and boro n-related adatoms were observed after annealing. These results indicate high controllability of chemical reaction process of HBO@sub 2@ molecules on Si(1 11)-7x7, and high potential exists in this system. @FootnoteText@ http://dora.ims.tsukuba.ac.jp

**SS-WeP17 Investigation of Sulfur-terminated GaAs(001) Surfaces by Selective Atoms Sublimed Method***,* ***S. Tsukamoto****, T. Ohno, N. Koguchi,* National Research Institute for Metals, Japan

Recently, a novel S-termination method has been developed by exposure to S vapor in molecular beam epitaxy system, observing not diffused (2x1), commonly reported, but clear (2x6) reconstruction by reflection high-energy electron diffraction and scanning tunneling microscopy(STM).@footnote 1@ Then, we found that the separations, 0.19 - 0.28 nm, between S atoms of S dimers by STM well agreed with the first-principles pseudopotential calculated result, 0.237nm, with the condition of one electron transferred from each S dimer.@footnote 2@ However, the (2x6) structure is still not clear. In this paper, we study the detail of this (2x6) by the investigation of the structural change by a selective atoms sublimed method which uses the thermal desorption of selective S-S dimer from the (2x6). The calculated maps of the charge-density contours of the S-S structures show that the center of the charge-density is as same as the poison of the S atom in the case with the transfer of one electron. On the other hand, in the case without the transfer, the center of the charge-density is about 0.05nm far from the position of the S atom. Therefore, if the charge-density balance is destroied by the thermal desorption, the observed S-S bond length by STM will be drastically changed. The (2x6) structure turns into the (2x3) structure at around 520°C releasing about 20% surface sulfur atoms, which amount consist with the central dimer pairs of the (2x6) structure, however, without interdiffussion and with keeping the same S-S bond length. In addition, the Ga small clusters appeared on this (2x3) surface. It seems that these Ga clusters kept the charge-density balance of the (2x3) structure, keeping the same S-S bond length. @FootnoteText@ @footnote 1@S.Tsukamoto and N.Koguchi, Jpn.J.Appl.Phys., 33 (1994) L1185; Appl.Phys.Lett., 65 (1994) 2199; J.Cryst.Growth., 150 (1995) 33. @footnote 2@S.Tsukamoto, T.Ohno, and N.Koguchi, J.Cryst.Growth., 175/176 (1997) 1303.

**SS-WeP18 Dynamical Behavior of Hydrogen Molecule on GaAs(001) Surface***,* ***M. Ohashi****, M. Ozeki, J. Cui,* JRCAT - ATP, Japan

Hydrogen plays important roles as an important reactant and a carrier gas in various surface processes of III-V compound semiconductors. However there are no sufficient data on dynamical behaviors of hydrogen on III-V compounds surface. Supersonic molecular-beam scattering enables us to bring valuable dynamical parameters such as reaction probability, reaction pathway, reaction kinetics, and activation energies of reaction steps. We have been studying in dynamical behaviors of hydrogen on GaAs(001) surface by supersonic molecular beam apparatus. We measured angular distributions of reflected beams, when hydrogen molecule was injected with 110 and -110 directions onto GaAs(001) 2x4 surface. The existence of trapping/desorption channel was clearly discovered and the depth of potential well of hydrogen molecule on GaAs(001) 2x4 surface was estimated 0.4 kcal/mol by the trajectory simulation of trapping probabilities. The angular distribution of reflected hydrogen molecule of trapping/desorption channels direct scattering was largely affected by the surface corrugation of GaAs(001) 2x4 surface. The experimental result was compared by classical trajectory simulation for this system. The experimental result agreed excellently with classical trajectory simulation. This indicated the important information of the energy exchange from translational to rotational modes was indicated. This work is supported by New Energy and Industrial Technology Development Organization (NEDO).

**SS-WeP19 Study on Properties of Defects and Boron at the Si/SiO@sub 2@ Interface using Empirical Interatomic Potential Energy Function***, **J.-W. Kang**, H.-J. Hwang,* Chung-Ang University, Korea

Properties of silicon/oxide interface were computed using novel interatomic potential-energy function that was recently developed@footnote 1@ for modeling the interactions between silicon and oxygen atoms. For boron-silicon interaction, we used the Stillinger-Weber (SW)-type interatomic potential with the repulsive part of the two-body term being splined to the Ziegler-Biersack-Littmart (ZBL) universal repulsive potential.@footnote 2@ For boron-oxygen, We used the Born-Mayer-Huggins potential.@footnote 3@ Effects of dangling bonds and oxygen clusters at SiO@sub 2@/Si interface and silicon vacancy and oxygen vacancy in the oxide film were calculated. We have investigated the SiO@sub 2@ evolution on the silicon surface with rich boron and various defects. The evolution of the structure at the Si/SiO@sub 2@ interface according to the presence of boron atom provided an overview of the behavior of boron dynamics at the Si/SiO@sub 2@. @FootnoteText@ @footnote 1@ T. Watanabe et al., Jpn. J. Appl. Phys. Vol.38 Part 2.No. 4A (1999) pp. L366-L369. @footnote 2@ J. W. Kang, E. S. Kang, H. J. Hwang, will be published in May, J. Kor. Phys. Soc. Vol. 34 (1999). @footnote 3@ J. M. Delaye, V. L-Achille, D. Ghaleb, J. Non-Cry. Solids, 210(1997) 234-242.

**SS-WeP20 Cesium-induced Structural Transformation from the Si(113)3x2 to the 3x1 Surface***, **C.C. Hwang**,* Sung Kyun Kwan University, Korea*; K.S. An,* High Energy Accelerator Organization, Japan*; S.H. Kim, C.Y. Park,* Sung Kyun Kwan University, Korea*; A. Kakizaki,* High Energy Accelerator Organization, Japan

Adsorbates such as H, Na, Cs, etc. on the Si(113)3x2 surface are known to induce a structural transformation to the 3x1 surface. The origin, however, seems to be still unclear due to the lack of informations about the adsorption behavior of several adsorbates as well as the structure of the 3x2 surface. To investigate the adsorption behavior of cesium on the Si(113)3x2 surface at room temperature, we measured the change of workfunction, core level (Si 2p, Cs 4d), and valence band spectra with increasing cesium deposition time by using low energy electron diffraction (LEED) and synchrotron radiation photoemission spectroscopy. As previously reported, the adsorption of cesium induced the structural transformation from the Si(113)3x2 to the 3x1 surface. When cesiums adsorbed on the Si(113)3x2 surface, the workfunction decreased to about 3.2 eV and surface states from dangling bonds disappeared gradually with increasing cesium deposition time. These results indicate that cesiums adsorb preferentially on dangling bond sites at the initial stage of adsorption. We also observed that two shoulders at higher and lower binding energy than the bulk peak in Si 2p core level spectrum from the 3x2 surface disappeared by the adsorption of cesium. Rehybridized surface atoms towards sp@super 2@- and s@super 2@p@super 3@-like configurations thus seem to be changed to sp@super 3@-like ones with the structural transformation. Based on these results, we will discuss the possible origin of the cesium-induced structural transformation at room temperature.

**SS-WeP21 Investigations of the Effects of P and Ge on the Desorption of D@sub 2@ from Si(100) and Si(111)***, **J.L. Stepnowski**, C. Dougherty, G.J. Batinica, M.L. Jacobson, M. Chiu, B.M.H. Ning, J.E. Crowell,* University of California, San Diego

The desorption of D@sub 2@ from Si(100) covered with various concentrations of both P and Ge has been investigated using temperature programmed desorption (TPD). Chemical vapor deposition was used to prepare the surfaces. Phosphorus at different concentrations was deposited at 873K using phosphine as the molecular source gas, and separately, various Ge coverages were prepared by exposing the surface to digermane at approximately 160K. After each exposure, the crystal was flashed to 873K to desorb hydrogen. The resulting P and Ge surface coverage was determined by Auger Electron Spectroscopy. The P,Ge modified Si surface was then exposed to D atoms produced by cracking D@sub 2@ gas with a hot tungsten filament and then a TPD spectrum was taken. Previous studies in our laboratory found that addition of phosphorus alone shifts the @beta@1 desorption state to higher temperatures relative to clean Si(100) while the presence of only submonolayer germanium on the Si surface decreases the @beta@1 peak temperature. This investigation will detail the combined effect of P and Ge on the Si(100) surface. Furthermore, the combined system of P and Ge on Si(111) has been previously examined in our laboratory and a comparison of the effect of these additives on the desorption behavior of Si(100) versus Si(111) will also be presented.

**SS-WeP22 Direct Absorption of Thermal H Atoms by Crystalline Silicon: A Narrow Substrate Temperature Window***, J.H. Kang,* Kyung Won University, S. Korea*; **S.K. Jo**,* Kyung Won University, S. Korea, South Korea*; J. Lee,* Seoul National University, S. Korea*; B. Gong, J.M. White, J.G. Ekerdt,* University of Texas at Austin

Si(100) surfaces exposed to gas-phase thermal-energy hydrogen atoms, H(g), were studied by temperature-programmed desorption (TPD) together with H/D isotope exchange experiments. We find that direct absorption of H(g) into crystalline bulk of Si(100) substrates occurs within a narrow substrate temperature window of 400 - 600 K. The bulk-absorbed hydrogen evolved out molecularly from Si(100) at a temperature 70 - 120 K higher than that of surface-adsorbed monohydride phase (@beta@@sub 1@) in TPD. This bul k-phase hydrogen (@alpha@) uptake increased with increasing H(g) exposure without saturation within our experimental limits. While pre-adsorbed hydrogen atoms on the surface, H(a), were readily abstracted and replaced by D(g), the amount of pre-absorbed H in the bulk remained unchanged by subsequent D(g) exposures. Our result of extensive H/D isotope mixing suggests that absorbed H atoms remain trapped atomically, rather than molecularly, at interstitial sites. We propose a model, in which the (2x1) surface dimer structure of Si(100) serves as a two-way barrier for both direct H(g) absorption and thermal evolution of molecular hydrogen.

**SS-WeP23 Low Energy Electron Damage to Condensed Phase Cyclic Ethers Studied by Electron Stimulated Desorption***, **L. Parenteau**, D. Antic, L. Sanche,* University of Sherbrooke, Canada

Low-energy electron (E@sub i@ < 20 eV) damage to condensed molecules prepared under ultra-high vacuum conditions has been the focus of intense study in recent years.@footnote1@ This research has particular relevance to the field of radiation science as it is well known that a large amount of low-energy secondary electrons are produced along the radiation tract following the interaction of ionizing radiation, the majority of which are created with initial kinetic energies well below 20 eV. At these low energies, fragmentation may occur following dissociative electron attachment (DEA) via the formation of negative ion resonances or by dipolar dissociation (DD). These processes are generally monitored in condensed-phase systems by electron stimulated desorption (ESD) which measures the negative ion yield desorbing from the surface. Below the DD threshold negative ion formation arises exclusively via DEA, whereas above this threshold the ESD yield is dominated by anions produced largely via DD. In recent years, there has been a shift in emphasis towards molecular systems of biological relevance, such as DNA bases,@footnote2@ radiosensitizing 5-halo-uracils and homo-oligonucleotides.@footnote3@ We are now studying the chemical consequences of the interaction of low energy electrons with the deoxyribose backbone of DNA and its constituents. Preliminary results on DEA damage to DNA sugar-like backbone analogues, tetrahydrofuran, 3-hydroxy-tetrahydrofuran and tetrahydrofurfuryl alcohol will be presented. In addition to a core excited resonance observed in the H@super -@ ESD yield near 10 eV incident electron energy, we find significant H@super -@ production via DEA to occur above the DD threshold for incident electron energies near 23 eV. @FootnoteText@ @footnote1@L. Sanche, Scanning Microscopy 9, 619 (1995). @footnote2@D.V. Klyachko, M.A. Huels, and L. Sanche, Radiat. Res. 151, 177 (1999). @footnote3@P.C. Dugal, M.A. Huels, and L. Sanche, Radiat. Res. 151, 325 (1999).

**SS-WeP24 Electron- and Photon-stimulated Desorption of Alkali Atoms from Silicon Dioxide Surfaces***, **B.V. Yakshinskiy**, T.E. Madey,* Rutgers University

As part of a program to probe the mechanisms by which Na and K atoms originate in the atmospheres of the planet Mercury and the Moon, we are studying the electron- and photon-stimulated desorption of Na deposited on model mineral surfaces: amorphous SiO@sub2@ thin films, grown on a Re(0001) substrate. The measurement scheme for electron- stimulated desorption (ESD) of Na atoms includes an efficient pulsed low energy electron source, a highly sensitive detector of Na based on surface ionization, and a time-of-flight technique. For photon-stimulated desorption (PSD), a 500 W Hg arc lamp photon source, a mechanical chopper, and appropriate filters are used. We find that bombardment of Na / SiO@sub2@ surface by ultraviolet photons or by low energy electrons (E > 4 eV) causes desorption of 'hot' Na atoms with the velocity distribution peak at 1000 m/s. The desorption cross section is ~ 10@super-20@ cm@super2@ at 5 eV excitation energy for both ESD and PSD. The ESD yield demonstrates a resonance-like feature at ~11 eV. We interpret the ESD / PSD of Na as occuring via a substrate mediated charge transfer process, in which ionic Na@super+@ is converted to neutral Na, which desorbs. These data provide evidence that DIET mechanisms (e. g., PSD) may contribute as source processes for Na in tenuous planetary atmospheres. Although there are insufficient electrons in the solar wind to produce the observed lunar sodium atmosphere, there appear to be sufficient UV solar photons to maintain the atmosphere by desorbing Na from the surface.

**SS-WeP25 Metastable Surface Structure of KTaO@sub 3@(001) by Helium Atom Scattering@footnote 1@***, J.A. Li,* ***T.W. Trelenberg****, E.A. Akhadov, J.G. Skofronick, S.A. Safron,* Florida State University*; L.A. Boatner,* Oak Ridge National Laboratory

Helium atom scattering is used for measurements of the surface structure of KTaO@sub 3@ immediately after cleaving in situ in a UHV scattering chamber. Angular distributions (ADs) of this simple perovskite insulator are measured under destructive interference conditions for steps of one-half the unit cell of KTaO@sub 3@(2Å). Initially the specular peak is very small and is flanked on each side by a satellite peak at ±0.043Å@super -1@. Over a period of one to three hours, depending upon the surface temperature, the specular peak grows in intensity while the satellite peaks decrease in intensity until they essentially disappear. The result is what appears to be a typical AD. A model consisting of uniform-width step-up and step-down terraces is presented which agrees with the initial observations. With increasing time, the terrace widths become more nonuniform and the step heights increase to the lattice spacing of the full unit cell(4Å) due to the mass transport. The first of these developments leads to a reduction of the satellite peak intensities and the second leads to an enhanced specular signal because of the constructive interference. @FootnoteText@ @footnote 1@Supported by U. S. Department of Energy grant number DE-FG02-97ER45635.

**SS-WeP26 A Calibrated Adsorption and Thermal Desorption System using Glass Capillary Arrays and a Capillary Valve Flow Source***,* ***R.H. Jackson****, B.G. Frederick, D.J. Dwyer,* University of Maine

We demonstrate a calibrated thermal desorption system utilizing a glass capillary array doser as a calibrated beam source. Absolute calibration of the mass spectrometer signal in molecules per second is achieved using both calculated and measured flux distributions from the doser to calibrate the doser flux to the inlet appeture of a differentially pumped thermal desorption mass spectrometer. By a re-parameterization of the formalism of Winkler and Yates,@footnote 1@ we have reduced the order of the necessary integrations from 3 to 2, which simplifies treatment of arbitrarily shaped planar targets. Fourier convolution methods are used to calculate of the flux to a target at any position in a plane parallel to the doser face. These calculations are compared to direct measurements of the doser flux in 3 dimensions. The pressure versus time, measured by a spinning rotor gauge in a gas cell of known volume, determines the flow rate to the doser. The flow closely obeys the simple effusion model after accounting for finite base pressure. A transient molecular flow model is applied to the establishment of the flow from the capillary valve, providing good estimates of the time to steady state for the flow. This Calibrated Thermal Desorption Spectrometer is applied to a study of oxygen on Pd(110) and the coverage results are compared to values from nuclear reaction analysis. @FootnoteText@ @footnote 1@A. Winkler and J. T. Yates Jr. "Capillary array dosing and angular desorption distribution measurements: A general formalism", J. Vac. Sci. Technol. A 6(5), Sep/Oct 1988.

**SS-WeP27 Corrosion Inhibition of Aluminum by Self-Assembling Monolayers***,* ***S.M. Wetterer****, P. Dharia, S. Xie, J.J. Donofrio,* Oakite Products, Inc.

Self-assembling monolayers have been evaluated as an alternative to traditional chromium-based treatments for corrosion protection of aluminum surfaces. With good water solubility and long-term solution stability, alkyl phosphonic acids were found to be suitable candidates for the formation of a well-ordered, passivating layer on a series of aluminum alloys. Application process parameters such as immersion time, bath temperature, and anneal time significantly affected the development of the monolayer with implications for the resultant protective benefit of the layer as assessed by humidity and salt-spray corrosion testing. Additional characterization of monolayer-treated panels by SEM and EDAX has provided information regarding monolayer performance over surface defects and edge sites. Modeling of the mechanisms of corrosion protection and eventual breakdown of phosphonate monolayers will be presented.

**SS-WeP28 Structure of the (0001) Surface of Hafnium and Hafnium Diboride and of Epitaxial Thin Films of Hafnium Diboride Grown on Hafnium***,* ***R. Singh****, C.L. Perkins, M. Belyansky, M. Trenary,* University of Illinois, Chicago

Scanning tunneling microscopy (STM), x-ray photoelectron spectroscopy (XPS), and low energy electron diffraction (LEED) have been used to investigate the surface structure of single crystals of Hf, HfB@sub 2@, and epitaxial thin films of HfB@sub 2@ grown on a Hf substrate through the thermal decomposition of diborane. A comparison of the properties of HfB@sub 2@(0001) and Hf(0001) is of interest because the topmost atomic layer of both surfaces consists of a close-packed two-dimensional array of Hf atoms with lattice constants that differ by only 1.7%. In the bulk structure of HfB@sub 2@, the (0001) Hf atom planes are hexagonal close-packed and are separated by 0.348 nm. A graphite-like honeycomb lattice of boron atoms lies between the Hf planes. A clean well-annealed HfB@sub 2@(0001) surface is found to consist of Hf-terminated terraces separated by 0.35 nm with no boron layers exposed. When the HfB@sub 2@ sample is not well-annealed or when contamination is present, reconstructed surfaces are observed with both LEED and STM, including a (3x3) structure induced by carbon. The Hf(0001) surface consists of flat (0001) terraces separated by monoatomic steps 0.25 nm in height. The high reactivity of the group IV metals is reflected in the difficulty in obtaining contamination free images of the Hf surface. From the determination of the basic structural features of the HfB@sub 2@ and Hf surfaces by STM, patches of Hf and HfB@sub 2@ can be clearly distinguished in STM images acquired during different stages in the growth of epitaxial thin films of HfB@sub 2@ on a Hf substrate. The thin film growth mechanism can thereby be inferred from such images.

**SS-WeP29 Molecular-scale Origins of the Surface Memory Effect at a Liquid Crystal - Solid Interface***,* ***D.M. Scott****, A.J. Brackley, J.D. Mougous, K.M. Foland, D.L. Patrick,* Western Washington University

The surface memory effect (SME) describes the phenomenon in which an initially isotropic surface is rendered anisotropic through contact with anisotropic medium, such as a liquid crystal (LC) fluid. At a LC - solid interface, the SME leads to imprinting of the director orientation onto the surface, which can in turn induce uniform alignment in the bulk LC fluid. The SME is important in LC - based opto-electric devices such as liquid crystal displays. We studied the SME in LC droplets on a polycrystalline graphite substrate using polarized optical and scanning tunneling microscopy (STM). A single crystalline monolayer with macroscopically uniform orientation was prepared by depositing material from the LC droplet in an external magnetic field. The system was found to retain memory of the original bulk orientation, even when the field was removed and the LC was heated beyond its isotropic transition temperature. Loss of the SME coincided with monolayer melting. Comparison of STM images with optical micrographs establish a direct link between molecular alignment in the monolayer adsorbed to the graphite substrate and bulk LC director orientation.

**SS-WeP30 Investigation of the Dehalogenation of 1,1-Dichloroethene on Pd(111) Studied by Laser-Induced Thermal Desorption Fourier Transform Spectroscopy (LITD-FTMS)***,* ***D.E. Hunka****, D.P. Land, D.C. Herman,* University of California, Davis

The chemistry of chlorinated ethenes on transition metal surfaces is of great interest due to their prevalence as contaminants in groundwater. The decomposition of geminal dichloroethene (g-DCE) on a clean Pd(111) surface is investigated using thermal desorption spectroscopy (TDS) and laser-induced thermal desorption with FT mass spectrometry (LITD-FTMS). Preliminary results of g-DCE decomposition show that HCl is the major reaction product. The TDS studies have been performed as a function of coverage. At very low coverages, only one peak of HCl is seen to desorb in the range of ~600 K - 1000 K. As coverage increases, a significant portion of g-DCE desorbs intact, the HCl peak shifts to lower temperatures and a second HCl peak grows in with a Tp= 450 K, indicating a step-wise decomposition. At these higher coverages of g-DCE, separate TDS experiments monitoring hydrogen evolution from the surface show a sharp peak at 474 K (in between the two HCl traces). Interestingly, the LITD survey experiments reveal decomposition of g-DCE occurs by 150 K with the concomitant appearance of HCl. These results indicate that both C-H and C-Cl bond cleavage happens at low temperatures, although no chloroacetylene is produced as a second product, which would be indicative of an @alpha@-@beta@ elimination. Further decomposition of the surface intermediates occurs to yield a second formation of HCl which is subsequently liberated from the surface.

**SS-WeP31 CV, XPS, SIMS and ISS Examination of Zirconium Passive Film Breakdown in the Presence of Sulfate***, **R Schennach**,* Lamar University &Texas A&M University*; A. Mamun, N. Kunamneni, D.L. Cocke,* Lamar University

Passive films on zirconia have been prepared by potentiodynamic polarization in the presence of a range of anions and at various pH values. Sulfate has been found to produce unique transpassive peaks that appear to be associated with an amorphous to cyrat alline transitionand subsequent enhanced species transport along the resulting grain boundaries. The passive film breakdown can be qualitatively described by E@sub np@ = E@sub c@ + @eta@ + @PHI@ +E@sub inh@. Where E@sub np@ is the pitting potential, E@sub c@ the corrosion potential in acidified solution, @eta@ the polarization necessary to obtain a current density high enough to maintain acidity inside the pit, @PHI@ the potential drop inside of the pit and E@sub inh@ the contribution to pitting potent ial resulting from inhibitors present. XPS, SIMS and ISS have been used to characterize the films before and after the passive film breakdown. The results of these surface studies along with the variation in CV scans have been used to describe the process and to present a model that involves either IR drop and/or local acidification. The involvement of chemically bound water oxidation and local oxygen evolution are presented as well.

**SS-WeP33 Composition and Orientation at the Surface of a Room-Temperature Ionic Liquid Observed by Direct Recoiling Spectrometry***, **P.R. Watson**,* Oregon State University, U.S.*; T.J. Gannon, G. Law,* Oregon State University*; A.J. Carmichael, K.R. Seddon,* Queen's University, Ireland

Direct recoil spectrometry (DRS) has recently been applied to investigate the structure and orientation at the surface of low vapor-pressure liquids. Room temperature ionic liquids are generating considerable interest as low vapor-pressure clean technology solvents. We report the first measurements of the composition and molecular orientation at the surface of the room temperature ionic liquid - 1-butyl-3-methylimidazolium hexafluorophosphate, [bmim][PF@sub6@]. Recoil spectrometry using rare gas ions on continuously refreshed liquid surfaces in vacuo shows that neither ion is significantly enriched in the surface. The average orientation of the cation is with the plane of the ring vertical. The cation ring is rotated about an axis through its center such that the nitrogen atoms and side chains are deeper in the surface with the surface normal passing between the two nitrogen atoms (with an estimated error of ±30°).

**SS-WeP34 Surface Structures of @beta@-(BEDT-TTF)@sub 2@PF@sub 6@ Induced by Its Polar Surface Characteristics***, **M. Ishida**,* University of Tsukuba, Japan*; T. Mori,* Tokyo Institute of Technology, Japan*; H. Shigekawa,* University of Tsukuba, Japan

Bis(ethylenedithio)tetrathiafulvalene (BEDT-TTF or ET) based organic compounds, one of the low-dimensional conductors, are distinct from the others due to their polar surface characteristics. For @beta@-(BEDT-TTF)@sub 2@PF@sub 6@, an ordered-defect structure was observed on the anion (PF@sub 6@) surface similarly as the typical reconstructions of the inorganic polar surfaces. And characteristic properties such as superstructures and fluctuation of surface structures were observed on the cation (ET) surface. On the other hand, it is well known that @beta@-(BEDT-TTF)@sub 2@PF@sub 6@ undergoes a metal-insulator transition at 297 K, and formation of the 2x|c| superstructure due to 2k@sub F@ CDW is confirmed by X-ray diffraction. However, several superstructures with considerably longer modulations were observed by STM at 285 K instead of the 2x|c| superstructure. From the results of the STM, AFM, XPS studies, and molecular orbital calculations, the observed cation surface structures were concluded to be influenced by charge localization, relaxation of individual molecules, and symmetry breaking in the molecular relaxation. Concerning the modulated CDW phases, susceptibility @chi@(Q) for the surface layers was calculated in order to investigate the origin of the larger modulations, by taking into account the change in the molecular charge on the polar surface. As a result, the observed STM result were in good agreement with the CDW structure derived from the susceptibility calculation.

**SS-WeP35 Free Radical Based Amination of Polymeric Interfaces***, H. Fairbrother, **A. Wagner**, K. Han, A. Vaught,* Johns Hopkins University

The introduction of nitrogen containing functionality into organic surfaces is often used to modify interfacial characteristics, including permeability, wettability, adhesion, friction, wear and biocompatibilty. Compared to wet-chemical treatments for surface modification vacuum-based technologies are dry, fast and environmentally benign. Compared to the more traditional ion and plasma based modification treatments, the use of gas phase radicals is a relatively underdeveloped component with considerable promise. For example, nascent radical kinetic energies are typically in the range of 0-5eVs in contrast to the several hundred eVs of energy typically associated with ions. To address this issue a new NH radical source, based upon the thermal pyrolysis of hydrazoic acid (HN3) has been developed and characterized using mass spectrometry. Results from the interaction of NH radicals with thiol-based self-assembled monolayers using mass spectrometry, infrared spectroscopy and X-ray Photoelectron Spectroscopy will also be presented.

**SS-WeP36 An Ultra High Vacuum Compatible Matrix Assisted Laser Desorption/Ionization Time-of-Flight Mass Spectrometer***, **T.L. Porter**, S. Hermann,* Northern Arizona University

The emerging technique of matrix assisted laser desorption/ionization (MALDI) time-of-flight mass spectrometry allows for the mass determination of surface bound polymeric materials that suffer from fragmentation effects using conventional MS techniques. Using MALDI, the sample to be analyzed is combined with a strong UV absorbing "matrix", such as 3-hydroxypicolinic acid or 2,5-dihydroxybenzoic acid. Short UV laser pulses desorb the matrix plus sample material from the topmost sample surface, while simultaneously gently ionizing the sample material. The ionized species are then injected into a time-of-flight analyzer for mass determination. The gentle ionization process allows polymers and bio-materials on surfaces that would normally suffer from fragmentation effects to be detected intact. In this paper, we describe an ultra-high-vacuum MALDI instrument that has been constructed from primarily off-the-shelf components at minimal cost. This instrument may be used to detect the presence of pico-mole amounts of material with atomic weights from a few hundred to over one hundred thousand.

**SS-WeP37 Iodobenzene Reactions and cis-1,2-Dichloroethene Chemistry on Pd(111) Studied by Laser-Induced Thermal Desorption Coupled with Fourier Transform Mass Spectroscopy (LITD-FTMS)***, **D.M. Jaramillo**, D.P. Land, D.E. Hunka,* University of California, Davis

Halocarbons are important compounds for obtaining alkyl groups on metal surfaces. The thermal and photo dissociation of the carbon-halogen bond allows us to probe the chemistry of hydrocarbon fragments which have shown to be transient intermediates in catalytic processes. In addition, the reactions of halocarbons on metal surfaces relates to the remediation of chlorinated solvents from waste water. Elucidation of the mechanism of halocarbon decomposition will aid in determining better catalysts for remediation. The chemistry of iodobenzene and cis-1,2-dichloroethene have been investigated on Pd(111). Submonolayer iodobenzene adsorption at 90 K results in the formation of phenyl groups and iodine on the surface. The phenyl groups are hydrogenated by subsurface hydrogen to form benzene which desorbs around 500 K. Higher exposures of iodobenzene show iodobenzene desorbing at 200 K and benzene observed only at 140 K. The adsorbed iodine changes the reactivity of iodobenzene. Molecular desorption of cis-1,2-dichloroethene occurs at 160 K for low exposures and at around 200 K for higher exposures. Hydrogen is seen to desorb around 300 K for even the lowest exposure studied. No HCl was observed in TDS or LITD.

**SS-WeP38 Energy Transfer in Collisions of Nitric Oxide with Ordered Molecular Adlayers***, M.K. Ainsworth, V. Fiorin, **M.R.S. McCoustra**, M.A. Chesters,* University of Nottingham, UK

Detailed dynamical measurements have been made of the scattering of nitric oxide from well-characterised and well-ordered monolayers of carbon monoxide (CO) and ethylidyne (CCH@sub 3@) adsorbed on a Pt(111). The scattering dynamics have been probed using a combination of molecular beam and laser spectroscopic techniques for incident NO translational energies in the range 5 to 50 kJ mol@super -1@ at substrate surface temperatures from 100 to 300 K. Time-of-flight measurements were used to determine the translational energy of the scattered NO, while resonance-enhanced multiphoton ionisation was used to recover its rotational quantum state distributions. The results of both types of experiment will be reported. Significant loss of incident NO translational energy is observed and evidence from these measurements suggests that scattering occurs into both a direct inelastic scattering channel and a trapping-desorption channel. The scattering dynamics from both adlayers are found to be similar, with only slight differences that may be interpreted in terms of different interaction potential strengths.

**SS-WeP39 Surface Diffusion of Photogenerated Hydroxyl Radicals as Probed by FTIR*, Y. Paz*,** *H. Haick,* Technion-IIT, Israel

Titanium Dioxide is a well-known photocatalyst for water and air treatment as well as for catalytic production of gases. For many organic materials, destruction of contaminants occurs through an oxidation mechanism, where hydroxyl radicals formed on the surface of the catalyst attack adsorbed compounds. Structures comprised of photoactive titanium dioxide and inert adsorbents may promote the overall performance of the photocatalyst by concentrating molecules, that usually do not adsorb on TiO@sub 2@, at the vicinity of the photocatalyst. Furthermore, one may consider the modification of the inert domains to achieve selective physisorption of contaminants of interest. This selectivity can be achieved by coating the inert areas with chemisorbed organic molecules, tailored for specific physisorption of the contaminants. The growing interest in such combined structures is strongly coupled with the debate over possible surface diffusion of the oxidizing species (namely OH radicals), which might migrate to the inert domains where they might mineralize the organic templates. The destruction of templates of alkyl-trichlorosilane organized organic monolayers, chemisorbed in the vicinity of TiO@sub 2@ domains, is studied. Based on in-situ FTIR measurements, it is shown that OH radicals, formed on the titanium dioxide micro-domains, are capable of inducing the mineralization of the fixed chemisorbed aliphatic chains, within minutes, even when these chains are located as much as 20 microns away from the titanium dioxide domains. These results, measured as a function of domain size and surface temperature, are now being evaluated in order to deduce surface diffusion parameters.

**SS-WeP40 The Interactions of Azomethane and Methyl Radical with Cu(111)*, P. Chuang,*** National Taiwan University, Taiwan*; Y.L. Chan,* Academia Sinica, Taiwan*; C.H. Chuang,* National Central University, Taiwan*; S.-H. Chien, T.J. Chuang,* National Taiwan University, Taiwan

We have employed TPD, XPS, LEED and HREELS to investigate the interactions of CH@sub 3@ radicals and CH@sub 3@N@sub 2@CH@sub 3@ molecules with Cu(111). The subject is of interest@footnote@ due to the importance of the radical in many heterogeneous reactions involving hydrocarbons. It is found that distinctive adsorption states exist for azomethane on Cu at 90K depending on surface coverage. Molecular desorption is detected at 205K, 145K and 120K corresponding to the first chemisorbed layer, the second layer and the bulk-like multilayer, respectively. Both first-order and zero-order desorption kinetics are observed. Methyl radicals can be chemisorbed on Cu(111) at 300K showing partial decomposition to CH@sub 2@(ads) and H(ads), mediated possibly by defect sites. CH@sub 3@ thermal desorption signals exhibit two channels at about 360K and 440K, corresponding to the second-order and the first-order desorption kinetics. The behavior is closely related to H and CH@sub 3@ coadsorption and reaction during the desorption process. The results of TPD, XPS and HREELS are correlated with each other and compared with previous work. @FootnoteText@ @footnote 1@T.J. Chuang, Y.L. Chan, P. Chuang and R. Klauser, J. Electr. Spectr. Relat. Phenom. 98-99, 149 (1999).

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