Surface Science
Room Exhibit Hall B - Session SS-TuP
Poster Session

SS-TuP1 HREELS and TPD Investigation of Electron Irradiation Effects on Diethylsilane-Covered Si(100) Surfaces at 100K, ***J. Lozano,*** *D. Early, J.H. Craig, Jr., P. Wang, K.R. Kimberlin,* Bradley University

The effects of 600-eV electron irradiation of diethylsilane (DES) adsorbed on Si(100) was studied using high-resolution electron energy loss spectroscopy (HREELS) and temperature programmed desorption. The effects of electron irradiation at submonolayer and multilayer DES coverages will be discussed. Previous electron stimulated desorption and TPD studies suggested an electron-induced beta hydride elimination process as a pathway for ethyl group desorption at 100K. The results of HREELS experiments performed to probe such processes will be discussed.

SS-TuP2 FTIR and XPS Studies of Porphyrin Containing Monolayers on Si(100) Surfaces, ***D.A. Syomin***, *A.A. Yassery, F. Zaera, D.F. Bocian,* University of California Riverside

A number of mono-coordinated monolayers of redox-active Zn-containing porphyrins with a variety of organic linkers were prepared by thermal assembly onto hydrogen-terminated Si(100) surfaces. The porphyrin monolayers were characterized using attenuated total reflection (ATR) infrared and X-ray photoelectron spectroscopy (XPS) as well as standard electrochemical methods. The molecular orientation of the adsorbates within the monolayer films as a function of molecular coverage and type of organic linker used was investigated.

SS-TuP3 STM Study of Phosphine Adsorption on Si(111)-7x7 Surfaces, ***J.-Y. Ji,*** *T.-C. Shen,* Utah State University

PH@sub 3@ reaction with Si(111) surfaces has been studied by Yates et al. and Avouris et al. using a number of analytical techniques including UPS, AES, EELS and ESD in 1990. They concluded that PH@sub 3@ adsorbs dissociatively at 100 K and the surface is chemically inert. We are interested to revisit this system because the P-delta layer in the (111) direction may have interesting technological implications. In this report we present real space images of the PH@sub 3@ adsorption on Si(111)-7x7 at room temperature for various exposures between 0.3-60 L. Applying different sample biases we identify reacted and unreacted adatom sites. Similar to the ammonia adsorption, we find that center adatoms are more reactive than corner adatoms. However, careful analysis shows three different types of reacted sites which can be considered as PH@sub 3@, PH@sub 2@, and H adsorption sites. The coverage counting of the species suggests that most of PH@sub 3@ is dissociatively adsorbed on the surface at initial exposure generating H and PH@sub 2@ adsorption sites, followed by molecular adsorption of PH@sub 3@. Issues involving dissociation and desorption stimulated by electrons, saturation coverage at different substrate temperatures, and surface structures after annealing will be discussed. This work is supported by DARPA-QuIST program under ARO contract DAAD 19-01-1-0324.

SS-TuP5 Irradiation Effects of Undulator Synchrotron Radiation Beam on Hydrogen-Terminated Si (111) Surfaces Studied by STM, ***Y. Nonogaki***, *T. Urisu,* Institute for Molecular Science, Japan

Undulator synchrotron radiation (USR) is a powerful light source for observation of surface VUV-photochemical reactions, since it is quasi-monochromatic and has high photon flux. It is also very attractive for semiconductor device processes using photochemical reaction. We have designed and constructed a beamline for surface photochemistry and nanofabrication of semiconductor at the UVSOR facility. Using this beamline hydrogen desorption on hydrogen-terminated Si (111) surfaces (H-Si (111)) was investigated using the USR and STM observation. We successfully observed that H-Si (111) was drastically changed after the USR irradiation. H-Si (111) was prepared with atomic H exposure to Si (111) 7x7 at surface temperature of 350°C for 10 min. The H-Si (111) was exposed to the USR at room temperature for 5 to 60 sec, where 1st harmonic of the USR was centered at 100 eV. Correspondent irradiation dose is 1000 to 10000 mAsec (ring current x time). STM observation was performed with tungsten tips at room temperature. STM observation of H-Si (111) showed that there were adatom islands and small protrusions on rest-atom monohydride surface. The adatom islands have triangular shape and bilayer height typically, of which coverage was ~15%ML. On the rest-atom monohydride surface, extension of unfaulted regions were observed and faulted regions was ~20%ML. Surface morphology was changed after USR irradiation. Density of the small protrusions significantly increased with irradiation dose from 1.4%ML at 0 mAsec to 12.8%ML at 10000 mAsec. The distribution of small protrusions were random whether on unfaulted and faulted region. The rest-atom monohydride surface seems to be unchanged. The small protrusions are assigned to dangling bond formed by irradiation-stimulated H-desorption from the rest-atom monohydride on the surface.

SS-TuP6 Theoretical and Experimental Comparison Studies of the Electronic Structure of Molecular Carborane Films, ***S. Balaz,*** *L.G. Rosa, A.N. Caruso, J.I. Brand,* University of Nebraska-Lincoln*; Y.B. Losovyj,* Louisiana State University*; P.A. Dowben,* University of Nebraska-Lincoln

Semiconducting boron carbide represents a new class of semiconductoing materials with applications in neutron detection and radioactive decay calorimetry [1,2]. The key to making a good boron carbide semiconductor requires materials fabrication by chemical vapor deposition (usually with plasma, electron beam, or synchrotron radiation assisted decomposition of the molecular precursor). The properties of the semiconducting boron carbide appear to be intimately connected to the source compound used. There is no obvious reason why different isomers of the closo-carborane, dicarbadodecaborane C@sub 2@ B@sub 10@H@sub 12@, should result in such different semiconducting properties [2,3]. Utilizing the synchrotron photoemission, and exploiting photovoltaic charging as a test of the n-type and p-type semiconductor behavior [4], during the deposition process, is key to developing the necessary understanding. Theory suggests little difference in electronic structure but profound differences are observed in experiment. Theoretical calculations from semiempirical calculations of the isolated 1,2 closo-carborane (orthocarborane) and 1,7 closo-carborane (metacarborane) molecules indicate that these isoelectronic carboranes should be very similar in HOMO-LUMO gap (highest occupied - lowest unoccupied molecular orbital). These calculations predicted 10.97 eV for the orthocarborane and 10.87 eV for the metacarborane. Since the two carboranes differ only in the positions of the two included carbon atoms and theory predicted the electronic states to be so close, great similarity in chemical and physical behavior would be expected, but is not observed. @FootnoteText@ [1]Robertson et al.,JP APL 80(19): 3644-3646 (2002) [2]A. N. Caruso et al., Journal of Physics Condensed Matter 16, L139 (2004) [3]A. N. Caruso et al., APL 84, 1302 (2004) [4]J.E. Demuth et al., Phys. Rev. Lett. 56, 1408-1411 (1986)[5]A.P. Hitchcock et al. J. Phys. Chem. B 101, 3483 (1997) .

SS-TuP8 Scanning Tunneling Microscopy Study of GaCrN Grown by MBE, ***M.B. Haider,*** *H.A. Al-Brithen, R. Yang, C. Constantin, D. Ingram, A.R. Smith,* Ohio University

According to Sato et al., (Ga,Cr)N is expected to show ferromagnetism above room temperature if the bulk Cr@sub Ga@ concentration is above 2%.@footnote 1@ Although many (mainly bulk) techniques have been applied to study dilute magnetic nitride systems here we apply in situ STM to investigate issues of Cr incorporation, Cr diffusion/segregation, and the effects of growth parameters. Cr-doped GaN(000-1) has been grown using rf-plasma MBE on sapphire (0001) at Ts ~ 700°C. The Ga/N flux ratio has been varied from 65-100% with variable Cr/Ga flux ratio between 3-11% for GaCrN growth. Based on the Ga/N flux ratio, three growth regimes were found: N-rich, metal-rich, and Ga-rich. It was found that under all three conditions GaCrN surfaces are smoother even to atomistic level forming 3x3 reconstructions after the growth as revealed by RHEED and AFM. This is in contrast to Ga-polar GaMnN case, where N and metal-rich surfaces are not smooth and under Ga-rich conditions Mn droplets of micron size are formed due to the Ga bilayer which exists during Ga-rich GaN(0001) growth.@footnote 2@ Atomic scale STM images of Ga-rich GaN(000-1) covered with 0.05ML of Cr deposited at 700°C show 3x3 and 6x6 reconstructions indicating the presence of Cr atoms within the surface structure. STM images of GaN(000-1) with Cr deposition of 0.2ML and above show some linear features suggesting transition from Cr substitution to 2nd order phase nucleation at the surface. The 3x3 reconstructions have been observed upon exposure of GaN(000-1) 1x1 to Cr at room temperature by RHEED and STM. These STM images suggest that on GaCrN surface, at low Cr concentration, Cr occupies Ga position. Another interesting phenomenon of contrast reversal of 3x3 and 6x6 reconstructions has been observed by STM on 5% Cr doped GaN(000-1) surface, which depends on the tip condition. @FootnoteText@ @footnote 1@Sato et al. J. Superconduc, 16 (2003) 31@footnote 2@Haider et al. J. Appl. Phys., 93 (2003) 5274.

SS-TuP9 Spatial Persistence and Survival Probabilities for Fluctuating Interfaces, ***M. Constantin***, *S. Das Sarma,* University of Maryland; *C. Dasgupta,* Indian Institute of Science, India

We report the results of numerical investigations of the steady-state (SS) and finite-initial-conditions (FIC) spatial persistence and survival probabilities for (1+1)-dimensional interfaces with dynamics governed by the nonlinear Kardar-Parisi-Zhang (KPZ) equation and the linear Edwards-Wilkinson (EW) equation with both white (uncorrelated) and colored (spatially correlated) noise. We study the effects of a finite sampling distance on the measured spatial persistence probability and show that both SS and FIC persistence probabilities exhibit simple scaling behavior as a function of the system size and the sampling distance. Analytical expressions for the exponents associated with the power-law decay of SS and FIC spatial persistence probabilities of the EW equation with power-law correlated noise are established and numerically verified.

SS-TuP10 Sublimation Behavior of SiO@sub 2@ from Low and High-Index Si Surfaces Studied by Atomic Force Microscopy, ***J.C. Moore***, *A.A. Baski,* Virginia Commonwealth University

We have used atomic force microscopy (AFM) to investigate the sublimation behavior of 100-nm thick oxide layers on the low-index Si(001) and high-index Si(5 5 12) surfaces. During high vacuum anneals, we have observed the formation of holes that nucleate at defects and grow laterally with annealing time (1 to 4 min, 1150@degree@C to 1350@degree@C). The depth of these holes is ~200 nm, or approximately twice the thickness of the oxide film. This is consistent with the thermal decomposition of SiO@sub 2@, where Si is extracted from the bulk in equal ratio to SiO@sub 2@ in order to form volatile SiO. As expected, the lateral growth of these holes is linear with annealing time (2 @micron@/min for 1200@degree@C). Interestingly, it is possible to obtain hole diameter data vs. annealing time by performing sequential anneals in vacuum, and then observing by AFM the formation of rings correlated to each anneal cycle at the bottoms of the holes. With regard to shape, holes formed on Si(5 5 12) have smooth edges and are circular, while those on Si(001) typically are not as circular. For both surface orientations, the holes oftentimes incorporate pits (5 @micron@ dia, 500-700 nm depth) or vertical structures (1 @micron@ dia, 150 nm height) at their centers. The conditions resulting in such structures, as well as their formation mechanism, are now under investigation. @FootnoteText@ This work is supported by the National Science Foundation.

SS-TuP11 The Structure of the (111) Surface of Bismuth, ***J. Sun,*** University of New Hampshire; *H. Mönig, J. Wells, P. Hofmann,* University of Aarhus, Denmark; *K. Pohl,* University of New Hampshire

Bismuth is a group V semimetal with a very low density of states at the Fermi level. However, a small distortion of its rhombohedral (A7) bulk structure would give a cubic lattice, which should be a good metal. In view of this close relation between structure and electronic structure it is not surprising that the surfaces of Bi are very different from the bulk material. They are good, two-dimensional metals with an electronic structure governed by spin-orbit coupling@footnote 1-3@. The changes in the geometric structure which lead to these interesting properties are totally unknown. We have studied the surface structure of clean Bi(111) and the mean-square displacement of the surface atoms by low energy electron diffraction (LEED). Experimental and theoretical diffraction intensities are analyzed for sample temperatures of 140, 171, 218, 268 and 313K. The optimization of the structural and nonstructural parameters is carried out by minimizing a R-factor with the quadratic tensor model algorithm. This results in an excellent agreement between the experimental and calculated data and R-factors of less than 0.1 are obtained. Moreover, the short termination of the bulk on the surface is confirmed. The temperature-dependent relaxations of the first layer distances and the atomic vibrations in the surface region are discussed. @FootnoteText@ @footnote 1@S. Agergaard, C. S@phi@ndergaard, H. Li, M. B. Nielsen, S. V. Hoffmann, Z. Li and Ph. Hofmann, New Journal of Physics 3, 15.1 (2001)@footnote 2@Ch. R. Ast and H. Höchst, Phys. Rev. Lett. 87, 177602 (2001)@footnote 3@Yu. M. Koroteev, G. Bihlmayer, J. E. Gayone, E. V. Chulkov, S. Blügel, P. M. Echenique, and Ph. Hofmann, cond-mat/0404461 .

SS-TuP12 Tunable Lattice Parameter of Ultrathin Bismuth Film, ***J.T. Sadowski***, *Y. Fujikawa, T. Nagao, A. Al-Mahboob, T. Sakurai,* Tohoku University, Japan

The study of the structure and electronic properties of ultra-thin metal films on semiconductor surfaces has always attracted significant attention. To establish better control of the crystalline and electronic properties of the metallic layers, it is necessary to understand the factors governing their epitaxial growth, namely, surface free energies and stress relaxation effects. Semimetal bismuth (Bi) has distinctive electronic properties due to its covalent-like bonds and highly anisotropic Fermi surface. Moreover, results of our electron diffraction and scanning tunneling microscopy (STM) experiments show that Bi undergoes an allotropic transformation as a function of thickness on the scale of several layers, during the RT growth on Si(111)-7x7. After the initial formation of the Bi wetting layer, Bi grows with a new {012}-oriented phase, with a structure different from bulk Bi. With increasing the Bi coverage, above the critical thickness the film transforms into the bulk-like Bi(001) phase. Calculations suggest that the {012} phase with even-number layers is stabilized by forming a puckered-layer structure, which results in the formation of flat and well ordered film, reflecting the 2D structure of the {012} phase. Most interestingly, the lattice parameter of the Bi{012} phase can be tuned to a great extent by changing the nature and strength of the interactions between the Bi film and the substrate. Using the results of systematic diffraction and STM studies combined with the theoretical calculations, we will discuss the atomic structure of the Bi{012} film grown on the various surfaces (clean Si(111), H-Si(111), Bi and Au superstructures on Si(111)).

SS-TuP13 Stacking Fault Formation on Ir(111), ***C. Busse,*** RWTH Aachen, Germany, Denmark; *C. Polop, T. Michely,* RWTH Aachen, Germany

The formation of stacking faults during homoepitaxial growth was observed in the model system Ir/Ir(111) (crystal structure: face-centered cubic) under a wide range of deposition parameters (sample temperature and deposition rate) using scanning tunneling microscopy (STM). A quantitative model can explain the observations and proves that stacking faults form out of small clusters that can occupy faulted hexagonal close-packed adsorption sites with significant probability in thermal equilibrium. Metastable areas in the wrong stacking sequence then grow out of these clusters by sufficiently fast addition of adatoms. This model is expected to hold for other systems as well. Upon further growth, islands in the same stacking coalesce, but islands in different stacking sequences do not. In the latter case, atoms can, however, move to the energetically favourable, regular stacking via a kink-flip process (self-healing). In the ideal case this leads to a complete disappearance of the wrong stacking and a defect-free film evolves. This effect can be observed in situ by annealing experiments.

SS-TuP14 Observation of Standing Waves in Si(111)@sr@3x@sr@3-Ag Islands at Room Temperature, ***T. Ishizuka***, *H. Hirayama,* Tokyo Institute of Technology, Japan

It is widely accepted that Si(111)@sr@3x@sr@3-Ag surface has S1 surface state with a free electron like dispersion. The free-electron like surface dispersion has been confirmed by observing standing wave patterns at the @sr@3x@sr@3-Ag domain boundaries in STM at 5K [1]. In this study, we demonstrated that the free-electron like @sr@3x@sr@3-Ag surfaces can be utilized as the template for the nano-sized quantum structure construction. We obtained nano-scale @sr@3x@sr@3-Ag islands by depositing sub monolayer Ag on the Si(111)7x7 substrate surfaces at 770K. The standing wave patterns of electrons confined in the nano-islands were observed by a STM-based dI/dV mapping at 70K and room temperature. In the dI/dV images, the standing wave patterns were observed in the inside of the @sr@3x@sr@3-Ag islands of the size below 20nm. We found that the patterns persisted even at room temperature in the islands of 10nm scale. Then, we calculated the standing wave patterns numerically by solving Schrodinger equation for some islands with complex shapes using Finite Element Method(FEM). The numerical results reproduced characteristics of the observed standing wave patterns successfully, though the coincidence was not perfect. Furthermore, we fabricated point defects on @sr@3x@sr@3 Ag island artificially by using STM tip, and observed the resultant change of standing wave pattern. These results indicated that the 10nm scale islands still worked as Quantum Wells(QWs) even at room temperature. The shape of the islands could be modified by the STM tip induced atom manipulation. The confined electronic states are numerically predictable. These are preliminary demonstrations of the artificial design and fabrication of nano-sized QWs workable at room temperature on the template of the @sr@3x@sr@3-Ag surfaces.[1]N.Sato and S.Takeda PRB.59.3.2035(1999).

SS-TuP15 Electronic Structure of KDP and DKDP Nonlinear Optical Crystals Studied by Soft X-Ray Absorption and Emission Spectroscopies, ***S.O. Kucheyev***, *C.F. Bostedt, T. van Buuren, T.M. Willey, S.G. Demos, T.A. Land, A.V. Hamza, T.E. Felter, L.J. Terminello, A.J. Nelson,* Lawrence Livermore National Laboratory

The surface and bulk electronic structure of KD@sub 2x@H@sub 2(1-x)@PO@sub 4@ single crystals, so-called KDP (x = 0) and DKDP (x > 0), with a deuteration degree x of 0.0, 0.3, and 0.6, is studied by soft x-ray absorption near-edge structure (XANES) and x-ray emission (XES) spectroscopies. High-resolution O K-edge, P L@sub 2,3@-edge, and K L@sub 2,3@-edge XANES and XES spectra reveal that the element-specific partial density of states in the conduction and valence bands is essentially independent of deuteration x. Projected densities of states in the conduction band also appear to be essentially identical for tetragonal and orthorhombic phases, consistent with previous band structure calculations. A decrease in sample temperature from 300 to 77 K results in an ~0.4 eV shift in the valence band edge (probed by XES), with negligible changes to the conduction band edge (probed by XANES) as the material transforms from the tetragonal to orthorhombic phase. We assign XANES and XES peaks based on previous molecular orbital and band-structure calculations. Results also show that high-intensity x-ray irradiation results in material decomposition into water and KPO@sub 3@ cyclo- and polyphosphates.

SS-TuP16 Nanoparticle Diffusion on Desorbing Solids: The Role of Elementary Excitations in Buffer-Layer-Assisted Growth*, V.N. Antonov,* *J.S. Palmer, P.S. Waggoner, A.S. Bhatti, J.H. Weaver,* University of Illinois at Urbana-Champaign

Physical vapor deposition onto rare gas buffer layers leads to the spontaneous formation of clusters. During the thermal desorption of the buffer, these clusters diffuse and aggregate into larger structures, a process known as buffer-layer-assisted growth and desorption assisted coalescence. We studied the effect of buffer thickness and the rate of buffer desorption on the extent of this aggregation for Ag, Au, Cu, Pd, Co, and Ni particles on a solid Xe surface. On the basis of these experiments, results from Monte Carlo simulations and the existing theoretical models for cluster-cluster aggregation, we report the Arrhenius parameters for nanoparticle slip-diffusion. The effective activation energies range from 0.12 for small Ag clusters (few hundred atoms) to 0.60 eV for ramified Ni islands (millions of atoms), and the giant pre-exponential factors were found to differ by many orders of magnitude. Significantly, the pre-exponential factors follow a Meyer-Neldel type dependence on the corresponding effective activation energy, with a characteristic Meyer-Neldel energy of 6.9 meV. This energy is associated with the phononic excitations in solid Xe that are responsible for nanostructure mobility. This dependence should be a characteristic feature of nanoparticle diffusion.

SS-TuP17 Epitaxial Cu Nanowire Arrays Grown on H-Si(110) using Glancing Angle Deposition*, H. Alouach,* *G.J. Mankey,* The University of Alabama

We report the growth of epitaxial nanowire arrays using the technique of glancing angle deposition with substrate rotation. Epitaxial copper nanowire arrays were deposited on H-terminated Si(110) using electron beam evaporation. The nanowire arrays were characterized with x-ray diffraction, atomic force microscopy and scanning electron microscopy. Individual nanowires were confirmed to be single crystal by examination with transmission electron microscopy. The epitaxial growth involves twin formation with the epitaxial orientation relationships: Cu(111)//Si(110) with Cu[1-10]//Si[001] and Cu[-110]//Si[001]. As the angle of incidence is increased, the Cu grows as isolated columns with a spacing that increases as the angle of incidence is increased. However, the thickness limit for epitaxial growth is reduced as the angle of incidence is increased, and it is approximately 300 nm for a deposition angle of 75°. The X-ray rocking curves for samples deposited at increasing polar angles show steadily improving crystal orientation up to a deposition angle of about 35°. Beyond 65° deposition angle, the rocking curves show split diffraction peaks indicating that there are two distinct orientations. In addition, the split peaks have a much lower FWHM. The observed behavior will be explained based on arguments involving unidirectional diffusion arising from adatom parallel momentum. This work was supported by the NSF.

SS-TuP18 Modification of Surface Electronic Structure Due to Scattering from a Quasi-Periodic Potential in Ag/GaAs(110)*, D. Eom,* *C.-S. Jiang, H.-B. Yu, Q. Niu,* University of Texas at Austin*; P. Ebert,* Institut für Festkörperforschung, Germany*; C.-K. Shih,* University of Texas at Austin

An extensive study has been done on the metal films grown on the semiconductor substrates because of their practical and scientific issues. One interesting system is the silver film deposited on the GaAs(110) surface using the so-called two-step process: If Ag is deposited on GaAs (110) surface at low temperature (~77K) and subsequently annealed to room temperature, then it will form an atomically flat film. A detailed morphology, however, looks more like an array of two stripes, one is thick and one is thin, whose sequence is quasi-periodic. By using this model system, we explore the effect of quasi-periodic potential on the surface states of the silver film using a low-temperature scanning tunneling microscope (LT-STM) operated at 5.5 K. Spatially resolved tunneling spectra are analyzed in reciprocal space (i.e. Fourier space). We found that such a quasi-periodically modulated potential leads to a very complicated electronic structures. Unlike the periodic potential that leads to energy gaps in the well-defined Brillouin zone boundary, the quasi-periodic potential results in a hierarchical structure of gaps in the k-space. Detailed analysis combining theory and experiment will be presented.

SS-TuP19 Structure and Thermal Stability of Thin Fe Films on Al(001) Surfaces with Ti Interlayers@footnote 1@*, C.V. Ramana,* Montana State University-Bozeman*; B.-S. Choi,* Jeonju University, South Korea*; R.J. Smith,* Montana State University-Bozeman

Thermal effects and chemical reactions can induce complex changes in the electrical and magnetic properties of thin metal film device structures. Achieving stability of these structures at elevated temperatures is therefore important to operation, and becomes more difficult as the film thickness is reduced to the nanometer regime. In the present work we investigate the structure of Fe films grown on the Al(001) surface with extremely thin Ti interlayers at the interface. Using Rutherford backscattering and channeling (RBS/c), we identify the bcc structure of the Fe(001) film, with the [100] axis rotated 45° relative to the [100] axis of the Al(100) substrate, and an interplanar distance of 1.44Å. RBS/c and low-energy ion scattering (LEIS) were then used to evaluate the thermal stability of the interface. The resulting epitaxial structure is observed to be stable for temperatures up to ~200°C, at which point the diffusion of Al towards the surface begins. At ~400°C, the sample structure begins to disorder. @FootnoteText@ @footnote 1@Work Supported by NSF Grant DMR-0077534.

SS-TuP20 XPS and AFM Study of K Promoted Supported Au Nanoclusters*, Y. Yang,* University of Calfornia, Santa Barbara*; M.M. Sushchikh, **S.A. Sardar**, E.W. McFarland,* University of California, Santa Barbara

It has been observed in high pressure reactors that K can increase the activity for CO oxidization of Au nanoclusters formed in block copolymer micelles and deposited on titania supports. UHV in situ characterization shows that the surface species, K@sub 3@ N and carbonates are discomposed after heating the surface to 800 K in UHV. K remains on the surface, however, the XPS signal from Au disappears during the heating process. Surprisingly, repeat XPS following exposure of the surface to air shows an observable Au signal. The appearance/disappearance of the Au XPS signal is reproduced by cyclically exposing the sample to the air then re-heating to 800 K in UHV. Sputtering the surface heated in UHV recovers the Au XPS signal. A K-shell model is proposed to explain the data with the formation of a K@sub 2@ CO@sub 3@ overlayer on the Au cluster during heating in UHV. The concentration ratio between Au and K is approximately1:1.

SS-TuP22 Formation and Characterization of Au Coatings Deposited by Pulsed Laser Deposition on Alumina Particles for Low Temperature Oxidation of CO*, C.E. Allmond, M.C. Raphulu, **J.T. Calla**, R.J. Davis, J.M. Fitz-Gerald,* University of Virginia

Laser induced atomic flux processing affects a wide range of existing and emerging products used in aircraft, cutting tools, lithium-ion rechargeable batteries, superconductors, pharmaceutical drug formulations that employ micron to submicron sized particulate precursors in their manufacturing process. By attaching atomic to nano-sized clusters either in discrete or continuous form on the surface of the core particles, i.e. nano-functionalization of the particulate surface, materials and products with significantly enhanced properties can be obtained. In this paper we present an alternative use for these materials in the area of Au catalysis. Bulk gold is considered the least reactive metal in heterogeneous catalysis due to repulsion between the orbitals of the adsorbate and gold's filled d states. Gold's catalytic potential is not realized until it is present as supported nanoparticles. Supported gold nanoparticles are recognized as active catalysts for a variety of reactions, such as oxidation, epoxidation of propene, hydrogenation, water gas shift, and NO reduction. Despite intense effort, the underlying principles and the degree of their contribution to the activity of gold catalysts are currently debated. Although not conclusive, several factors have been proposed to explain the high activity of gold nanoparticles. These factors can be generalized into three classifications; metal particle size, metal oxidation state, and synergy between the metal particle and the support.

SS-TuP23 The Development of Pd and Ag Nanoparticles with Pulsed Laser Deposition*, **C.E. Allmond**, J.M. Howe, V.P. Oleshko, J.M. Fitz-Gerald,* University of Virginia

Small particles in the 1-100 nm range often exhibit significant properties that are promising for various practical applications, such as catalysis, electronics, imaging systems, etc. Therefore, it is important to develop preparation methods that are simple, effective and flexible in controlling particle size distributions. The development of novel materials has grown considerably with the introduction of nanoscale processing. A wide range of synthetic approaches regarding the preparation of metal nanoparticles in various matrices and at the surfaces, including reduction, sol-gel precipitation, solvent evaporation of hydrophobic colloids, cross-linking in colloidal aggregates, templates-directed methods, and biopolymer superstructures, has been reported. As an alternative, pulsed laser deposition is a novel preparation method. Palladium and silver nanoparticles, with sizes ranging from 1-10 nm, were deposited onto transmission electron microscope grids using pulsed laser deposition. Analysis of these nanoparticles incorporated high-resolution transmission electron microscopy, electron energy loss spectroscopy (EELS), and electron dispersion spectroscopy (EDS). The rationale behind this is two-fold: (1) is to obtain mean particle size and crystal structure as a function of fluence, gas pressure, and gas type and (2) is to establish parameters for site-specific catalysts.

SS-TuP24 Characterization of the Near-surface Structure, Composition and Surface Chemistry of Ultrathin Au Films on Pd{111}*, **T.G. Owens**, C.J. Baddeley, T.E. Jones,* University of St. Andrews, UK*; T.C.Q. Noakes, P. Bailey,* CCLRC Daresbury Laboratory, UK

There are many examples where bimetallic catalysts are known to outperform their monometallic counterparts. The synthesis of vinyl acetate monomer (VAM) from acetic acid and ethylene by Pd/Au catalysts is one such example exploited commercially by BP. In order to gain a fundamental understanding of the catalytic role of Au, we are interested in how the chemistry of Pd/Au bimetallic surfaces is influenced by surface structure and composition. Previous studies of the Pd{111}/Au system have reported that the first Au monolayer grows psuedomorphically on Pd{111} at 300 K while subsequent growth consists of films possessing a more Au-like structure, i.e. classic Stranski Krastanov growth. Medium Energy Ion Scattering (MEIS) has a unique ability to probe structure and composition of crystalline surfaces as a function of depth with monolayer resolution. In parallel with Scanning Tunnelling Microscopy (STM) measurements, we reveal that Au growth is more complex than previously assumed and identify an interfacial alloy structure with a quite different structure to either Au or Pd. In addition, we report the behaviour of ultrathin Au films as a function of pre-annealing treatment and we probe how the structure and composition of the near surface region is influenced by the adsorption of simple probe molecules.

SS-TuP25 Highly Stable Variable Temperature STM for Atomically and Time Resolved Imaging: The Dynamics of Self-Assembly at Surfaces*, **B. Diaconescu**, G. Nenchev, K. Pohl,* University of New Hampshire

Self-ordering growth of nanoarrays on strained interfaces is an attractive option for preparing highly ordered nano-templates of specific feature size densities. High-tech methods used for reducing of the feature sizes may thus be supplanted by this simple and elegant patterning technique. Reconstructed surfaces, e.g. Au(111) or Pt(111), and monolayer thick strained films, e.g. Ag or Cu on Ru(0001), exhibit well-ordered networks of misfit dislocations. These networks can serve as templates for the growth of mesoscopic-scale structures of large-scale order and size uniformity. The combination of interfacial stress and corrosion creates self-ordering arrays of unprecedented regularity. The great potential of this natural templating approach is that the feature sizes and densities are predicted to depend on the interfacial stress in these strained layers. We have the unique capability of being able to measure the resulting driving forces of self-assembly directly through time-resolved scanning tunneling microscopy. This enables us to determine the stability and elastic constants of 2D nano-templates@footnote 1@. For this purpose we designed and build a highly stable VT-STM@footnote 2@. It allows us to study the dynamics of self-assembly at strained metallic interfaces at the atomic scale in the temperature range 80-400K. An overview of the instrumental setup and it's performance will be given by variable temperature studies of self-organisation of nanostructures on Au(111) and Ag, and Cu films on Ru(0001) at different thicknesess. @FootnoteText@ @footnote 1@ K.Pohl et al. Nature 397,238 (1999)@footnote 2@ Supported by NSF-CAREER-DMR-0134933 and ACS-PRF-37999-G5.

SS-TuP26 Preparation and Chemical Oxidation Kinetics of Microcrystalline Tungsten Bronze Thin Films*, **E.B. Kadossov**, P. Rajasekar, N.F. Materer,* Oklahoma State University

Microcrystalline tungsten bronze (H@sub x@WO@sub 3@) thin films are prepared using wet chemical techniques or atomic hydrogen to reduce a tungsten oxide thin film. The oxide film is prepared by thermal oxidation of sputter deposited tungsten metal film on a quartz substrate. The crystallinity of these films is determined by X-ray diffraction. X-ray photoelectron and ultra-violet photoelectron spectroscopy show that these films are indistinguishable from conventionally prepared tungsten bronze powders. The quartz support allows the total amount of incorporated hydrogen in the film to be quantified by monitoring the absorbance at 900 nm. This technique is utilized to study the oxidation kinetics of these films by either oxygen gas or hydrogen peroxide aqueous solution. The resulting decay of the 900 nm absorbance intensity with time can be satisfactory fit to a kinetic model composed of two elementary steps. First, a proton must diffuse from the bulk to the surface. Next, a chemical reaction between the surface proton and the oxidant must occur. Conditions are such that the surface concentration of the oxidant adsorbed on the surface is effectively constant. In addition, this model implicitly assumes that the electron transfer step required for reduction of the oxidant is not rate limiting. From this kinetic model, both the proton diffusion coefficient and the surface activation energies can be estimated. The results are compared with previous nuclear magnetic resonances studies and electrochemical measurements.

SS-TuP27 Growth Studies of Thin Pt Films on the Cu(100) Surface by CAICISS, LEED and XPS*, **M. Walker**, C.R. Parkinson,* University of Warwick, UK*; C.F. McConville,* University of Warwick, UK, United Kingdom

The formation of a surface alloy upon room temperature deposition of Pt on the Cu(100) surface is observed by co-axial impact collission ion scattering spectrscopy (CAICISS), low energy electron diffraction (LEED) and X-ray photoelectron spectroscopy (XPS). Simulations of the CAICISS results are given to support the proposed alloy structures from Pt coverages of 0.25 ML upwards, with comparisons between layer-by-layer, alloy and Pt surface cluster models. With increasing Pt coverage the surface region becomes Pt rich, with a small Pt overlayer observed at a Pt coverage of 2.35 ML and above. This indicates the onset of layer-by-layer growth of a pure Pt film. LEED observations indicate that this film is disordered. The effects of annealing at temperatures up to 600 °C are also shown for samples with Pt coverages of 0.25 ML and 2.75 ML. CAICISS and XPS clearly demonstrate the penetration of Pt in to the Cu substrate upon annealing. For Pt coverages greater than 2.35 ML, annealing at 300 °C causes Pt to penetrate down to the fourth and fifth layers of the substrate, forming a CuPt surface layer and Cu@sub2@Pt sub-surface layers. For Pt coverages of ~ 0.25 ML, annealing at 200 °C resulted in a small amount of Pt migrating towards the bulk. After annealing at 300 °C the sample contained approximately 7% Pt in each of the top three layers of the sample and small Pt concentrations in the fourth and fifth layers. Annealing at 600 °C results in the onset of significant migration in to the substrate in both cases.

SS-TuP28 NO Decomposition over K-Deposited Pd(111)*, **I. Nakamura**, H. Hamada, T. Fujitani,* National Institute of Advanced Industrial Science and Technology (AIST), Japan

The adsorption and thermal reaction properties of NO on a K-deposited Pd(111) surface were investigated using infrared reflection absorption spectroscopy, X-ray photoelectron spectroscopy, and temperature-programmed desorption. For the K-deposited Pd(111) surface, two different NO adsorption sites were observed in addition to the Pd site. On the clean Pd(111) surface, the adsorption of NO was purely molecular and reversible, but on the K-deposited surface, the adsorbed NO decomposed to N@sub 2@ at two different temperatures, 530 and 610 K. The N@sub 2@ desorption at 530 K was due to the dissociation of NO, indicating that the NO dissociation sites were created on the Pd(111) surface by the deposition of K. On the other hand, the N@sub 2@ desorption at 610 K was due to the decomposition of NO@sub 2@, which was formed by the reaction of adsorbed NO with oxygen produced by NO dissociation. It was clearly shown that two active sites for the decomposition of NO to N@sub 2@ were newly created on the K-deposited Pd(111) surface.

SS-TuP31 Charge Exchange between Alkali Ions and Cerium Oxide Surfaces*, **G. Liu**, J. Yarmoff,* University of California, Riverside

CeO@sub 2@ has interesting catalytic properties, which are presumably the result of an electronic configuration that includes many valence electrons. Earlier, we showed that the probability for neutralization of low energy alkali ions scattered from metal surfaces is determined by resonant charge transfer (RCT) along the exit trajectory, and it depends on the local electrostatic potential (LEP) a few Å's above the scattering site.@footnote 1@ We also showed that RCT is effected by localized confined states in nanomaterials.@footnote 2@ The present work investigates the charge exchange between alkali ions and cerium oxide surfaces. The neutral fractions of 3 keV @super 23@Na@super +@ ions singly scattered from the Ce sites on CeO@sub 2@ single crystal surfaces were measured with time-of-flight spectroscopy. The angular dependence of the neutralization was found to be isotropic for CeO@sub 2@(111), while for CeO@sub 2@(100) the neutralization decreases for more grazing angles. The results from either surfaces cannot be explained by simple RCT theory, which predicts increased neutralization at grazing angles, and may therefore suggest that a new mechanism for charge transfer is operative with these materials. In order to ascertain the influence of the work function on ion neutralization, Cs and Br were deposited onto the CeO@sub 2@ surfaces to controllably decrease and increase the work function, respectively. Results for scattering from CeO@sub 2@(100) and CeO@sub 2@(111) will be compared and contrasted. @FootnoteText@ @footnote 1@C. B. Weare and J. A. Yarmoff, Surf. Sci. 348 (1996) 359.@footnote 2@G. F. Liu, Z. Sroubek and J. A. Yarmoff, Phys. Rev. Lett., in press. .

SS-TuP32 Inelastic Energy Losses and Ion Yields of Low Energy Ar@super +@ and Ne@super +@ from Transition Metals*, **A. Kutana**,* *K.P. Giapis,* California Institute of Technology

Inelastic losses and relative ion yields of 100-1300 eV Ar@super +@ and Ne@super +@ ions reflected off polycrystalline V, Nb, Ta, Zr, and Y surfaces were measured using a low energy scattering beamline apparatus. Use of a floating ICP source coupled to a small beam accelerator had overcome many problems pertinent to conventional sources in the sub-keV energy range and allowed measuring scattering energies with much greater precision. From the acquired energy spectra, peak positions of singly scattered ions were plotted versus the primary beam energy E@sub 0@ and compared with energies of totally elastic single collisions. For energies above 100 eV, the inelastic losses of singly scattered ions can be described by the power law E@sub 0@@super a@ with a<1. Scattering simulations based on the binary collision approximation with added local and nonlocal inelastic losses yielded the theoretical loss values that were related with the ones observed in experiment. For a given primary ion, the relative ion yields were generally found to vary insignificantly from one metal to another, except for the Ne@super +@-Y pair, where a much more efficient neutralization of Ne@super +@ was observed. Characteristic neutralization velocities were also estimated for the above projectile-target combinations.

SS-TuP33 Epitaxial Iron Oxide Growth on Vicinal Pt(111): Well-defined Defective Model Systems?*, **G. Ketteler**,* Lawrence Berkeley National Laboratory, University of California*; W. Ranke,* Fritz-Haber-Institute of the MPG, Germany

Heterogeneous catalysts consist often of metals in contact with oxides and the activity depends on the interaction between them. In addition, the defect structure of the surface is of high importance for the catalytic activity. The common electron-based surface science techniques allow the characterization of model catalyst surfaces with atomic precision. Studied model catalyst systems include single crystal surfaces, epitaxial compound films, or well-defined particles deposited on single-crystalline supports. However, real catalysts contain a defect structure which is difficult to model in a well-defined manner. In order to study the controlled introduction of defects into iron oxide model catalysts for the dehydrogenation of ethylbenzene to styrene, we have grown different iron oxide phases on a stepped Pt(9 11 11) single crystal surface and characterized the film structures by STM and high-resolution SPA-LEED measurements. The hope was that this may provide a way to introduce well-defined step defects into the epitaxially grown films. For coverages below 1 ML, FeO(111) films wet the vicinal Pt substrate. The step structure changes under formation of doubled and triplicated terrace widths and step heights. Further cycles of iron deposition and oxidation lead to a Stranski-Krastanov-type growth of Fe@sub 3@O@sub 4@(111) islands which initially are elongated along the edge direction. However, the morphology of a coalesced closed film is almost unaffected by the underlying substrate step morphology. High pressure oxidation of Fe@sub 3@O@sub 4@ films results in poorly defined Fe@sub 2@O@sub 3@(0001). Although FeO films grown on the vicinal Pt surface may serve as model systems for systematic studies of well-defined defective oxide surfaces, the catalytically more relevant Fe@sub 3@O@sub 4@ and Fe@sub 2@O@sub 3@ phases could not be obtained reproducibly with a well-defined defect structure.

SS-TuP34 Anomalous Diffusion Permeability of an Interphase Interface in Mo-Ni System Under High-Energy Electron Irradiation*, **G.G. Bondarenko**, M.M. Yakunkim, A.V. Artamonov,* Moscow Institute of Electronics and Mathematics (Technical University), Moscow, Russia*; S.P. Ostashkin,* Russian State University of Innovational Technologies and Management, Moscow, Russia

Some of the problems of the theory of transport in solids are anomalous atomic mobility and deviations from the equilibrium concentrations at an interphase interface caused by high-energy irradiation. The problem of anomalous mass transfer of components during long-term electron irradiation can be solved using information on phase diagrams. We study the Mo-Ni system during electron irradiation over the time it takes for stationary state to be achieved and compare the states obtained with equilibrium states. Samples in form of two-layer plates 0.05 (Mo) and 1.5 mm (Ni) in thickness were irradiated in a linear electron accelerator at energies of E = 2-8 MeV in steps of 2 MeV for the time it took for equilibrium structures to be formed. Irradiation was carried out in a special temperature-controlled chamber at 1000 K. The isothermal section of this system at E = 0 was preliminary obtained. Isothermal sections of the phase diagram at various values of E were constructed from the data of phase analysis. We found that the quasi-equilibrium irradiated diffusion zone at the interface is a nanoregion ~20 nm in size. The concentrations of components at the interphase interface significantly change during irradiation. As a result of electron irradiation, the maximum nickel content in the @delta@-phase increases by 12%, the nickel concentration in the molybdenum-based solid solution at the interface increases by a factor of almost four and is equal to ~10% at E = 8 MeV. Changes in the component concentrations at interphase interfaces can be described without applying thermodynamics by introducing the concept of the diffusion permeability of an interphase interface. Given the appearance of a phase diagram at various values of E, it is possible to calculate the diffusion permeability of the interface for all cases. This approach was used to account for the concentration deviations detected at the interphase interface during high-energy electron irradiation.

SS-TuP35 Structure Transformation of Palladium and Iridium Clusters on the W (110) Surfaces at Initial Stage*, **T.-Y. Fu**,* National Taiwan Normal University, Taiwan, ROC*; Y.-H. Wang,* National Taiwan Normal University, Taiwan, Taiwan R.O.C.*; T.T. Tsong,* Institute of Physics, Taiwan

The initial stages of cluster nucleation of Pd or Ir adatoms on W (110) surfaces and in the vicinity of surface steps are observed directly by a field ion microscope (FIM). At the beginning, the most stable structures of Pd and Ir clusters are both linear chains, which are parallel to the nearest-neighbor stacking directions of the substrate. Different to the Pd clusters which the preferred structure is a 2-D compact island when the chain length is beyond 8 atoms, the linear Ir chains are apparently more stable and the greater coverage and higher temperature are necessary conditions for 1-D to 2-D transition. Both of Pd and Ir 2-D islands are pseudomorphic structure. As the number of Pd adatoms increasing to approximate monolayer coverage, the structures of clusters transfer to three-dimensional island. The structure transition from bcc (110) to fcc (111) of 3-D Pd clusters is shown. The quit complex transform behaviors of Ir clusters are also discussed.

SS-TuP36 Adsorption and Reaction of Oxygen and Hydrogen on Free Platinum Clusters*, **M. Andersson**, A. Rosen,* Chalmers University of Technology and Goteborg University, Sweden

In a cluster beam experiment metal clusters are produced with a pulsed laser vaporization source, kept at room temperature or liquid nitrogen temperature. The beam of neutral clusters passes two low-pressure collision cells and clusters and reaction products are detected with laser ionization and time-of-flight mass spectrometry. Thus, the reaction probability in a cluster-molecule collision can be determined.@footnote 1@ Stable reaction products with O@sub 2@ are detected for clusters with more than 6 atoms, and a high and relatively size-independent reaction probability of about 0.3 is measured. Also H@sub 2@ adsorbs readily on Pt@sub n@ but the exact number of adsorbed molecules is difficult to determine because of the Pt isotope distribution. If the clusters first react with O@sub 2@ and then with H@sub 2@ one can observe that the reaction of Pt@sub n@(O@sub 2@)@sub m@ with H@sub 2@ results in the removal of oxygen atoms from the cluster. This is interpreted as formation of water molecules, which subsequently desorb. The efficiency of the catalytic water formation is high on all cluster sizes measured (7-30 atoms), with only a weak dependence on cluster size.@footnote 2@ The configuration with two separate reaction cells enables reversing the order of interaction with the reactant molecules, and a high reaction efficiency is measured also when the Pt clusters first interact with H@sub 2@. @FootnoteText@ @footnote 1@ M. Andersson, J.L. Persson, and A. Rosen, J. Phys. Chem. 100, 12222 (1996).@footnote 2@ M. Andersson and A. Rosen, J. Chem. Phys. 117, 7051 (2002). .

SS-TuP37 Preperation of Ultra-thin Lattice Matched Multilayers of Cr@sub 0.63@Mo@sub0.37@ and MgO*, K.B. Gylfason,* Biopharmaceuticals, Iceland*; S. Olafsson, I. Meyvantsson,* University of Iceland, Iceland*; K. Johnsen,* Biopharmaceuticals, Iceland*; **J.T. Gudmundsson**,* University of Iceland, Iceland

We report on the preparation of a lattice matched hetheroepitaxial system in a magnetron sputtering discharge. Cr@sub 0.63@Mo@sub0.37@ thin films were grown on MgO(1 0 0) using a DC discharge, and an MgO overlayer was grown on top by reactive sputtering in a pulsed bipolar discharge. The composition of the binary metal alloy is chosen so that the film is lattice matched to the substrate when the direction of the film is parallel to the direction of the substrate. Ex situ X-ray diffraction (XRD) and low angle X-ray reflectivity measurements were performed to determine the film structure, film thickness, as well as the surface and interface roughness. The minimum thickness for continuity of the binary metal alloy film was determined using four point probe resistance measurements. The insulating properties of the MgO film as a function of thickness were assessed by measuring the tunnelling current I-V characteristics of a metal-insulator-metal structure.

SS-TuP39 O2-covered Reduced TiO2(110) Rutile: Dynamics and Chemistry*, **Y. Wang**, G.S. Hwang,* The University of Texas at Austin

The rutile TiO2(110) surface has been widely used as a catalyst for photochemical reactions and a support for transition metal catalysts. Molecular O2 adsorption plays an important role in determining the activity of TiO2 and supported metal catalysts. Surface bound oxygen species may directly influence chemical and photochemical processes occurring on TiO2. In addition, O2 exposure leads to significant structural changes of supported metal particles, which may in turn affect their catalytic activity. It has been found that molecular O2 adsorbs on TiO2(110) only when O-vacancies are present. Despite its importance, however the exact chemistry and dynamics of adsorbed O2 molecules on reduced TiO2(110) are still unclear. Using density functional theory calculations, we have investigated the adsorption and diffusion of oxygen species on the reduced TiO2 (110) surface. We have found that molecular O2 strongly binds not only to O-vacancies, but also to Ti(5c) neighbors, due to delocalization of unpaired electrons arising from removal of neutral bridging oxygen. Our results show that molecular O2 can jump across an oxygen vacancy and diffuse along a Ti(5c) row with moderate barriers. On the other hand, atomic O diffusion along a Ti(5c) row is rather unlikely at low temperatures (< 300K), because of the relatively higher probability of O-O formation by interaction with an adjacent bridging O(2c) atom. Based on our calculation results, we will discuss the diffusion and healing of O vacancies associated with O2 adsorption. We will also present the structure and energetics of higher coverage O2 adsorption and the chemistry of O2-covered reduced TiO2(110) surfaces.

SS-TuP40 Growth and Reactivity of Pt, Rh and Pt-Rh Nanoparticles on TiO@sub 2@(110)*, **S. Ma**, J.S. Ratliff, D.A. Chen,* University of South Carolina

Pt, Rh and Pt-Rh nanoparticles have been deposited on TiO@sub 2@(110) at room temperature and have been characterized by scanning tunneling microscopy (STM). The deposition of a small amount of Pt on the surface (0.12 ML) results in particles with an average diameter of 22.7+4.2 Å and height of 4.4+1.2 Å. In contrast to the growth of Cu and Ni on TiO@sub 2@(110), the Pt particles do not exhibit a preference to reside at the step edges. At higher Pt coverages (2 ML), the average size of the particles increases to 30.4+4.6 Å in diameter and 8.5+2.0 Å in height. Larger particles with roughly the same size distribution could be produced by depositing at room temperature and annealing to elevated temperatures. For example, after annealing the 2 ML coverage of Pt to 500 K, particles sizes ranged from 40-45 Å in diameter and ~10 Å in height. Further heating to 700 K increased the sizes of the particles to ~50 Å in diameter and 10-12 Å in height, and the largest particles were prepared by annealing at 1000 K (60 Å in diameter, 15 Å in height). Since Pt particles on TiO@sub 2@ are known to encapsulate with a TiO@sub x@ species upon annealing, X-ray photoelectron studies were carried out on the Pt particles annealed to 1000 K. However, there was no evidence for Ti@super +4@ reduction or Pt oxidation in the Ti(2p) and Pt(4f) regions. Possible encapsulation of the nanoparticles by TiO@sub x@ will be further studied by low energy ion scattering as well as grazing angle X-ray photoelectron spectroscopy experiments. The reduction of NO by CO on the monometallic and bimetallic clusters of different sizes will be investigated by temperature programmed desorption.

SS-TuP41 Adsorption of L-phenylglycine on Anatase TiO@sub2@(101) and (001): A NEXAFS and Photoemission Study*, **A.G. Thomas**,* University of Manchester, UK, U.K.*; C. Chatwin, W.R. Flavell, D. Tsoutsou,* University of Manchester, UK*; T. Johal, J. Purton,* CCLRC Daresbury Laboratory, UK

We present a study of the adsorption of L-phenylglycine from submonolayer to multilayer coverage on the (101)(1x1) surface of anatase phase TiO@sub2@. Photoemission is used to determine changes to the electronic structure of the substrate and adsorbate and the NEXAFS searchlight effect is used to determine the orientation of the phenylglycine on the substrate. NEXAFS spectra recorded from multilayers adsorbed from the vacuum show good agreement with solvent deposited thick films of glycine and phenylalanine@footnote 1@. From the intensity dependence of the ring @pi@* resonance on photon incidence angle in NEXAFS it appears that the molecule forms a disordered layer at all coverages studied here. Furthermore, again at all coverages studied, it appears that N is being lost from the amino acid molecule with time through a photon induced process. A similar result has been observed when glycine adsorbed on the rutile TiO@sub2@ (110)(1x2) surface is subjected to photons of energy 55 eV@footnote 2@. @FootnoteText@ @footnote 1@ J. Boese, A. Osanna, C. Jacobsen, J.Kirz. J. Electron Spectroscopy and Relat. Phenom. 85 (1997) 9.@footnote 2@ E. Soria, I. Colera, E. Roman, E.M. Williams, J.L. De Segovia. Surface Science 451 (2000) 188.

SS-TuP42 Deconvolution of the Fuchs-Kliewer Phonon Spectrum of Co@sub 3@O@sub 4@(110) Single Crystal Surfaces*, **E.M. Malone**, S.C. Petitto, M.A. Langell,* University of Nebraska-Lincoln

The Fuchs-Kliewer phonon spectrum of single crystal Co@sub 3@O@sub 4@(110) has been treated with a Fourier transform log deconvolution method which removes multiple scattering features from the single loss spectrum. Auger electron spectroscopy (AES), X-ray photoelectron spectroscopy (XPS) and low-energy electron diffraction (LEED) first characterized the Co@sub 3@O@sub 4@ crystal establishing the cleanliness, composition, and order of the (110) surface. High resolution electron energy loss spectroscopy (HREELS) was then used to obtain the phonon spectrum over the incident electron energy range of 2.25 to 14.25 eV. Due to the strong dipole cross section for the Fuchs-Kliewer phonon modes, intense multiple electron scattering was detected, which provided a complicated and overlapping combination of all possible loss modes. Deconvolution removed the multiple loss modes to produce well-resolved Fuchs-Kliewer fundamental phonon losses at 26.8, 47.5, 71.1 and 84.7 meV (216, 383, 573 and 683 cm-1). The series of multiple loss peaks were also identified using standard peak fitting procedures, which also confirmed the single loss energies obtained with the deconvolution procedure.

SS-TuP43 Kinetic Energy Dependent Oxidation Processes on Copper Surfaces*, **K. Moritani**,* Japan Atomic Energy Research Institute, Japan*; M. Okada,* Osaka University, Japan*; A. Yoshigoe, Y. Teraoka,* Japan Atomic Energy Research Institute, Japan*; T. Kasai,* Osaka University, Japan

The oxidation of Cu has been of great interest because of the important role of Cu oxides in material science, for example, high Tc superconductors of cuprates and solar cells. Thus, many experimental and theoretical studies have been performed to understand the oxidation of Cu. However, the oxide-formation processes have been little elucidated from kinetics and dynamics points of view. In the present work, we studied the oxidation of Cu surfaces with a hyperthermal O@sub 2@ molecular beam (HOMB) using high-resolution X-ray photoemission spectroscopy (XPS) in conjunction with a synchrotron radiation (SR) source. All experiments were performed with the surface reaction analysis apparatus (SUREAC 2000) constructed in BL23SU at SPring-8. The kinetic energy of incident O@sub 2@ can be controlled by changing the O@sub 2@, He and/or Ar gas mixing ratios and the nozzle temperature. The incident direction of the HOMB is along the surface normal of the sample. The surface temperature was kept at 300 K. After the irradiation of a proper amount of HOMB, high-resolution XPS spectra were measured at ~300 K using SR. We measured O-uptake curves, determined from the integration of O-1s XPS on the Cu(111), (100) and (110) surfaces spectra, after the HOMB irradiation and the exposure to the oxygen atmosphere. The kinetic energy of HOMB varied from 0.1 to 2.3 eV. The oxidation under 0.3 ML on the Cu(111) proceeded efficiently even with the ambient thermal O@sub 2@ gas, while further oxidation required the higher kinetic energy of O@sub 2@ molecules. The oxide structure above 0.3 ML changed to be a distorted Cu(100)-(@sr@2X@sr@2)R45°-O layer on the Cu(111). This reconstruction is induced by the additional incident energy. We will compare the data on Cu(111), (100) and (110) surfaces and discuss possible models of oxidation processes of Cu on the basis of the incident-energy dependence of the O-uptake curve.

SS-TuP44 The Adsorption of Benzene on Oxide Surfaces*, **M.-S. Chen**, A.K. Santra, D.W. Goodman,* Texas A&M University

The orientation and growth of benzene on various well-ordered oxide surfaces have been investigated with high resolution electron energy loss spectroscopy (HREELS), Auger spectroscopy (AES) and low-energy electron diffraction (LEED). Benzene on the Mo(112)-c(2x2)-[SiO4] surface is bound with its molecular plane parallel to the surface plane at submonolayer coverages. At intermediate coverages (1-3 ML), in contrast to benzene adsorption on metal surfaces, a layer-by-layer growth model where the benzene molecules bond parallel to the surface is observed. This is the first reported observation of benzene multilayer growth where the benzene molecules remain exclusively in a configuration parallel to the surface plane. In contrast, on SiO2 and TiOx thin films grown on the Mo(112), a tilted adsorption geometry with layer-by-layer grew up to 5-6 ML was found with a crystalline phase occurring at higher coverages. On a TiOx-SiO2 surface, where both parallel and tilted-up geometries coexist, crystalline benzene clusters formed at the second layer.

SS-TuP45 Competing Kinetic and Energetic Effects in the Adsorption of Ortho- and Para-H@sub 2@ on NaCl(001)*, J.P. Toennies,* Max-Planck-Institute für Strömungsforschung, Germany*; **F. Traeger**,* Ruhr-Universität Bochum and MPISF Göttingen, Germany*; C. Wöll,* Ruhr-Universität Bochum, Germany

Due to the electrostatic interaction of the hydrogen molecule's quadrupole moment with the electric field of the surface the ortho and para modifications experience slightly different molecule-surface potentials, which has been verified by scattering of n- and p-H@sub 2@ beams from the clean NaCl surface. A complementary way to study the molecule-surface interaction is to investigate the (1x1) monolayers of n-H@sub 2@ and p-H@sub 2@ on NaCl at 8 K with elastic and inelastic He atom scattering. The ortho-para differences result in 10-12 % higher frequencies for the external vibrations of o-H@sub 2@. Therefore, the relative intensities of the peaks in time-of-flight spectra of the scattered He atom provide information on the composition of the layer. Under steady-state conditions at H@sub 2@ gas pressures between 2.5 x 10@super -8@ mbar and 9.3 x 10@super -7@ mbar as well as during the desorption of the layer without gas pressure time-of-flight spectra have been recorded and are compared to desorption curves, i.e. the specular He intensity during desorption. Conflicting evidence regarding the adsorption probability for ortho- and para-H@sub 2@ is found, which is only partly in agreement with a model of thermodynamically and kinetically controlled adsorption proposed by Heidberg et al. from IR spectroscopy.

SS-TuP46 First Stages of Water Absorption on Alkali Halides Surfaces Studied by Scanning Polarization Force Microscopy*, **A. Verdaguer**, G.M. Sacha, M. Salmeron,* Lawrence Berkeley National Laboratory

Adsorption of water on sodium chlorite has been studied using scanning polarization force microscopy. A crystal is cleaved at low humidity (10% RH) and then humidity is increased as topography, contact potential and mobility of the ions is measured. At a critical humidity (40% for NaCl) important changes in the surface potential and ionic mobility occurred. Topographical changes occurred as well, in the form of step motion. We focused our study on the changes on the surface immediately before this critical humidity is reached. The evolution in the topographical and electrical properties and the ion mobility on the steps and the terraces as we approach to that point has been studied. An increase in the topographic contrast on the steps appears as we approach to the critical humidity. The increase in topographic electrostatic contrast is due to an increase in ionic mobility at step, indicative of ionic dissolution. As the mobility increases the difference between the local potential at the steps and on the terraces, measured from the Kelvin Probe signal, decreases. This supports the model deduced from the topography and indicates that the initial potential at the steps disappears due to the increased ionic mobility. The data obtained suggest us a model for the first stages of the dissolution of the crystal.

SS-TuP47 XPS and XAS Study of Water and Atomic Oxygen Co-absorbed on Pt(111)*, **L.-A. Naslund**, K. Andersson, T. Schiros,* Stockholm University, Sweden*; H. Ogasawara, A. Nilsson,* Stanford Synchrotron Radiation Laboratory

The chemical interaction between water and a metal surface is important in many practical fields, including corrosion, electrochemistry, molecular environmental science and heterogeneous catalysis. On hexagonal metal surfaces, like Pt(111), water molecules adsorb intact with strong intermolecular forces between the water molecules. A combined X-ray photoemission spectroscopy (XPS) and x-ray absorption spectroscopy (XAS) study shows that water (D@sub 2@O) co-adsorbed with atomic oxygen on Pt(111) stimulate dissociation of the water molecule and form a saturated hydrogen bonded network of OD and D@sub 2@O in the surface plane. The interaction with the Pt(111) surface is strong and give rise to a chemical shift of the Pt 4f orbital that is different from the results for water on Pt(111). XAS with polarized light shows that OD is standing up while D@sub 2@O is laying down. The amount of OD and D@sub 2@O are 0.28 ML and 0.55 ML, respectively, which gives an OD/D@sub 2@O ratio of 2. Upon heating D@sub 2@O desorbs and a reversible process gives back atomic oxygen.

SS-TuP48 XPS Study of Water on Cu(110)*, K. Andersson, A. Gomez,* Stockholm University, Sweden*; C. Glover,* MAXLab Lund University, Sweden*; L.G.M. Pettersson,* Stockholm University, Sweden*; **A. Nilsson**, H. Ogasawara,* Stanford University

The chemical interaction between water and a metal surface is important in many practical fields,including corrosion, electrochemistry, molecular environmental science and heterogeneous catalysis. On smooth metal surfaces, (e.g. fcc(111)), water molecules adsorb intact with strong intermolecular forces between the water molecules. This leads to the formation of a hexagonal two-dimensional ice lattice proposed as a "bilayer structure". The unit cell contains two water molecules, which are different in the interaction with respect to the metal surface. On the other hand, less is known about the behaviour of water on atomically rough surfaces (e.g. fcc(110)). An x-ray photoelectron spectroscopic (XPS) study was undertaken of the water/Cu(110)-system and we find that water adsorbs non-dissociatively on Cu(110) at temperatures below 165 K in contrast to a previous XPS study@footnote 1@. Above 165 K we find partial dissociation to take place. @FootnoteText@ @footnote 1@ Ch. Ammon, A. Bayer, H.-P. Steinruck and G. Held, Chem. Phys. Lett. 377 (2003) 163â?"169.

SS-TuP49 Water Dissociation on Ru(001): An Activated Process*, **H. Ogasawara**,* Stanford Synchrotron Radiation Laboratory*; K. Andersson,* Stanford Synchrotron Radiation Laboratory, Stockholm University, Sweden*; T. Schiros,* Stockholm University, Sweden*; A. Nikitin,* Stanford University*; L.G.M. Pettersson,* Stockholm University, Sweden*; A. Nilsson,* Stanford Synchrotron Radiation Laboratory

The chemical interaction between water and a metal surface is important in many practical fields, including corrosion, electrochemistry, molecular environmental science and heterogeneous catalysis. On Pt(111), it was shown that in the first layer all the molecules bind directly to the surface and to each other through the in-layer H-bonds without dissociation, creating a nearly flat overlayer. The water molecules are adsorbed through alternating metal-oxygen (M-O) and metal-hydrogen (M-HO) bonds@footnote 1@. On Ru(001), the water layer on Ru(001) shares similarities with the first water layer on Pt(111). We, however, obtained a dissociated state by irradiation of the adsorbed film by x-rays or heating the surface in water vapor above the desorption temperature. The latter shows a clear isotope effect between H20 and D2O indicating an activated dissociation process with a barrier slightly larger than the desorption channel. Previous theoretical and experimental disagreements can be explained in terms of electron or x-ray beam induced dissociation and under estimation of the dissociation barrier. We will also discuss about the bonding mechanism of water on Ru(001) based on DFT calculation. @FootnoteText@ @footnote 1@ H. Ogasawara et al, Phys. Rev. Lett. 89 (2002). .

SS-TuP50 Investigation of OH Desorption Energies and Reaction Paths within the H2/O2 Reaction on a Pd Catalyst using Kinetic Modelling and Laser-induced Fluorescence*, J.C.G. Andrae,* Royal Institute of Technology, Sweden*; A. Johansson,* Goteborg University and Chalmers, Sweden*; **P. Bjornbom**,* Royal Institute of Technology, Sweden*; A. Rosen,* Goteborg University and Chalmers, Sweden

A kinetic model for the H@sub 2@/O@sub 2@ reaction on a polycrystalline palladium catalyst has been constructed from experimental data. The aim was to obtain a deeper understand of the coverage-dependent OH desorption energy. The CHEMKIN software package was used in the modelling and each adsorbed oxygen atom was set to cover four Pd surface sites. The yield of OH and the water production were measured with laser-induced fluorescence (LIF) and microcalorimetry as a function of the relative hydrogen concentration, @alpha@@sub H2@. The temperature of the catalyst was 1300 K, the total pressure was 13 Pa and the flow was set to 100 SCCM. In fitting the model to the experimental data, the OH desorption energy E@super d@@sub OH@ was found to have a first-order coverage dependence according to: E@super d@@sub OH@ (@theta@)= E@super d@@sub OH@(0)-B@theta@, where @theta@ is the total coverage and B is a constant set to 92 kJ/mol. The desorption energy at zero coverage E@super d@@sub OH@(0) was determined to be 226 kJ/mol. The model could qualitatively and quantitatively reproduce the OH apparent desorption energy as a function of @alpha@@sub H2@ therefore it is believed that the coverage could be predicted by the model. It was found that the coverage on the Pd surface is in principle dominated by oxygen for all @alpha@@sub H2@. The values for E@super d@@sub OH@ (@theta@) were calculated as a function of @alpha@@sub H2@. Results of sensitivity analysis and rate of production calculations using this model imply that the main water-forming reaction on Pd at 1300 K is the hydrogen addition reaction H+OH ->H@sub 2@O.

SS-TuP51 What Can We Learn from Core Level Spectroscopy Studies of Ice?*, D. Nordlund,* Stockholm University, Sweden*; H. Ogasawara,* Stanford Synchrotron Radiation Laboratory*; M. Odelius, M. Cavalleri,* Stockholm University, Sweden*; P. Wernet,* BESSY, Sweden*; M. Nagasono,* Kyoto University, Japan*; B. Brena, M. Nyberg, L.G.M. Pettersson,* Stockholm University, Sweden*; A. Nilsson,* Stanford Synchrotron Radiation Laboratory

Core level spectroscopy is a powerful tool to obtain information on the unoccupied and occupied valence electron structure. The sensitivity of the valence electronic structure of water to different local H-bond situations is presented, where ice is used as a model system to approach important scientific aspects such as the local structure of liquid water, nature of the hydrogen bond, radiation induced ultrafast dissociation of water, and electron delocalisation and trapping processes. A number of experiments are presented together with spectral calculations based on density functional theory, revealing important information on the above listed aspects.

SS-TuP52 Self-Organized Growth of Nanopucks on 2D Pb Quantum Islands*, Y.P. Chiu,* National Taiwan Normal University, Taiwan*; H.Y. Lin, L.W. Huang,* Academia Sinica, Taiwan*; C.S. Chang,* Academia Sinica, Taiwan, Taiwan, ROC*; T.T. Tsong,* Academia Sinica, Taiwan

Self-organized growth is an attractive approach where a large number of structures can be formed simultaneously. The drawback for this approach involves the apparent difficulty in control of the structureâ?Ts size, their chemical homogeneity, and spatial arrangement. Several routes were taken to search for suitable templates on which the self-organized growth could be made tangibly practical. Regular strain-relief dislocations, periodic surface reconstructions, and Morie patterns have all been applied in attempt to improve the quality of self-organized growth. In this work, we employ the superstructures (electronic MoirÃ¨ patterns) found on 2D lead (Pb) quantum islands as a template to further grow self-organized 2D clusters (nano-pucks) of various materials. These patterns, originating from charge redistribution in the island in response to the lattice-mismatch-induced interfacial potential variation, thus differ from structure-driven templates. The boundaries of the periodic pattern are apparently repulsive for adatom diffusion. The activation energies for defining the template strength in trapping surface atoms have been obtained, which provide the practical parameters for controlling the size and spatial distribution of the nanopucks. A bi-layer complementary alternating behavior, similar to the confinement-induced phenomenon found in Pb quantum islands, also occurs in the growth of Ag nanopucks on the Pb islands of various thicknesses.

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