Surface Science Division
Room 4C - Session SS-TuP
Poster Session

SS-TuP1 Vacuum TPD from Traditional and Nano-fabricated Pt/Alumina Model Catalysts*, **E. Fridell**, T.R. Linderoth, B. Kasemo,* Chalmers University, Sweden

Temperature Programmed Desorption (TPD) is a valuable method to identify adsorbed species and investigate desorption kinetics. The usual method of performing TPD for (practical) catalyst samples is in a flow reactor under inert gas flow. The interpretation of the resulting spectra is hampered by complications associated with thermal gradients in the samples, re-adsorption of the desorbed species, gas phase transport under viscous flow conditions, etc.To remedy these problems, we have constructed an equipment allowing UHV-TPD from both model samples and "real" catalysts: The samples can be pre-treated at atmospheric pressures and high temperatures in a reactor cell mounted onto a UHV system. They are then exposed to the adsorbing gas before being translated to a position in front of a mass spectrometer for TPD in vacuum. The catalyst washcoat is applied directly onto, e.g., a metal foil which can be cooled or heated resistively providing precise temperature control. The equipment is intended primarily for catalysts made by traditional wet-deposition, but also for new "nano-fabricated" samples. To produce the latter, several methods are employed, for example we use colloidal particles adsorbed onto a surface as masks for sputtering of vacuum deposited metal/oxide films. After removing the colloidals the resulting 2D model catalysts consist, e.g., of Pt particles of uniform sizes and with controlled spatial separations on an alumina surface. In this presentation the equipment will be described and results of just initiated measurements concerning CO/oxygen adsorption on Pt/alumina catalysts will be presented.

SS-TuP2 Growth Mode of Au on SiO@sub 2@ Ultrathin Film*, **K. Luo**,* Texas A&M University*; D.Y. Kim,* Hallym University, Korea*; D.W. Goodman,* Texas A&M University

Au clusters supported on SiO@sub 2@/Mo(110) have been studied by x-ray photoemission spectroscopy(XPS), low energy ion scattering(LEIS), temperature programmed desorption(TPD) and low energy electron diffraction(LEED). At both 100 K and 300 K, the growth mode of Au at fractional monolayer coverages is quasi-two dimensional. With higher coverages, three dimensional growth of Au was found. No strong chemical interaction was observed between gold and silica. By annealing Au/SiO@sub 2@/Mo(110) to 1000 K, sintering of gold clusters was observed. The Au desorption activation energy was measured by temperature programmed desorption to be about 42 kcal/mol, lower than the sublimation energy of 90 kcal/mol for bulk gold.

SS-TuP3 Nucleation and Growth of Faceted Features on the Platinum Covered W(111) Surface*, **K. Pelhos**,* Rutgers, The State University of New Jersey*; J.B. Hannon, G.L. Kellogg,* Sandia National Laboratories*; T.E. Madey,* Rutgers, The State University of New Jersey

Low energy electron microscopy (LEEM) and scanning tunneling microscopy (STM) have been used to investigate the faceting of W(111) as induced by Pt. The atomically rough W(111) surface, when fully covered with a complete physical monolayer (1.7 x 10@super 15@ atoms/cm@super 2@) film of Pt and annealed to temperatures higher than ~750 K, experiences a significant morphological restructuring: the initially planar surface undergoes a faceting transition and forms three-sided pyramids with {211} faces. LEEM investigations show that when Pt is dosed onto the heated surface, the transition from planar to faceted structure proceeds through the nucleation and growth of spatially separated faceted regions starting at 2/3 physical monolayers coverage. STM reveals the atomic structure of the partially faceted surface, with large planar regions, dotted by clusters of pyramids of various sizes. On the other hand, when the initially planar sample is first completely covered with a physical monolayer of Pt and gradually heated, LEEM does not show any spatial separation in the faceting transition. STM observations of the initial stages of this transition show a continuous uniform roughening of the surface towards the faceted phase.

SS-TuP4 Adsorption of O@sub 2@ on Al(111) - No Evidence for "Hot Adatoms"*, M. Schmid, **P. Varga**,* Technische Universität Wien, Austria

Based on a scanning tunneling microscopy (STM) study,@footnote 1@ it has been suggested that adsorption of O@sub 2@ on Al(111) results in a high transient mobility of the two oxygen atoms created by dissociation of the oxygen molecule. It was suggested that these atoms move at least 80 Å apart before they come to rest at the surface.@footnote 1@ We have performed experiments under the same conditions. High-resolution STM images enable us to identify the features considered single O adatoms in ref. 1 as two O atoms in adjacent fcc hollow sites. We also find groups of three and four oxygen atoms, however. The dynamics of the O dimers point to an attractive interaction of O atoms in adjacent fcc hollow sites. These findings do not completely rule out the possibility of a large transient mobility and subsequent diffusion of individual O atoms, finally forming stable dimers. We consider it more likely, however, that only few O@sub 2@ molecules do not stay in adjacent hollow sites during adsorption and the single O adatoms created thereby diffuse until they coalesce with one of the dimers or larger O groups on the surface. With decreasing tunneling distance, Al atoms with three and two O neighbours appear as protrusions, explaining images with protrusions earlier attributed to single O adatoms. @FootnoteText@ @footnote 1@H. Brune et al., Phys. Rev. Lett. 68, 624 (1992); J. Chem. Phys. 99, 218 (1993).

SS-TuP5 Adsorption Dynamics of Oxygen on Al(111)*, **A.J. Komrowski**,* University of California, San Diego*; Y. Liu,* Syagen Technologies, Inc.*; A.C. Kummel,* University of California, San Diego

The interaction of oxygen with aluminum has become a prominent system in the study of metal oxidation. A previous study of Al(111) reacted with thermal O@sub 2@ at low coverages observed isolated features separated by >80 Angstroms which were attributed as dissociated O atoms.@footnote 1@ We have studied the oxidation of Al(111) using supersonic molecular beam techniques and scanning tunneling microscopy. The adsorption of monoenergetic O@sub 2@ on the Al(111) surface shows a change in the chemisorption site distribution (single reacted sites vs. doubles) with incident translational energy. We will contrast the O@sub 2@--Al(111) reaction against data from the reaction of supersonic oxygen atoms with Al(111) and compare the chemisorption results between activated and non-activated processes. @FootnoteText@ @footnote 1@ Brune, H. et. al. J. Chem. Phys. v99, 2128 (1993).

SS-TuP6 Water Dissociation on Boron-Doped Single Crystal Ni@sub3@(Al,Ti) (110) Surface*, **J. Wang**, B. Zhou, Y.W. Chung,* Northwestern University

Previous work demonstrated that water dissociates into hydrogen on Ni@sub3@(Al, Ti) (100) surfaces. There is clear evidence that this dissociation reaction results in the reduced ductility of many polycrystalline aluminum-based alloys in a moist environment. Ductility measurements further showed that addition of boron suppresses this moisture-induced embrittlement. To explore the effect of boron on water dissociation, we first dosed the surface of clean Ni@sub3@(Al, Ti) (110) with controlled amounts of boron, using a specially designed low-energy boron ion source, followed by low-temperature exposure to D@sub2@O and temperature-programmed desorption. Results indicated that water dissociates into atomic hydrogen on clean Ni@sub3@(Al, Ti) (110) boron-free surface, which was further verified by x-ray photoemission studies. This dissociation reaction is strongly suppressed by boron adsorption at a coverage of 0.5 monolayer. Auger studies on boron modified surfaces showed that boron is oxidized in this process. The chemical state of water was followed by x-ray photoemission. These studies indicated that addition of boron suppresses water dissociation into atomic hydrogen. By co-adsorption of D@sub2@O and oxygen on boron-modified Ni@sub3@(Al, Ti) (110) surfaces, the effect of oxygen was also investigated by temperature-programmed desorption. The significance of this observation will be discussed.

SS-TuP7 Ethene Adsorption on Cu(111), Cu@sub 3@Pt(111), CuPt@sub 3@(111), and Pt(111)*, **T. Pelster**,* Universität Bonn, Germany*; R. Linke,* Eindhoven University of Technology, The Netherlands*; J. Breitbach, A. Frey,* Universität Bonn, Germany*; M. Tanemura,* Nagoya Institute of Technology, Japan*; M. Grüne, R.-J. Linden, C. Becker, K. Wandelt,* Universität Bonn, Germany

The adsorption of ethene on Cu(111), Cu@sub 3@Pt(111), CuPt@sub 3@(111), and Pt(111) at 100K has been investigated using high resolution energy electron loss spectroscopy (HREELS), temperature programmed desorption (TPD), ultraviolet photoelectron spectroscopy (UPS), and work function change measurements. On Pt(111) ethene forms at 100K a well known di-@sigma@-complex, whereas on Cu(111) ethene adsorbs in a weakly bonded @pi@-complex which shows typical vibration spectra very similar to gaseous ethene. On Cu@sub 3@Pt(111) and CuPt@sub 3@(111) both species can be found, with higher intensity of the @pi@-complex on the Cu@sub 3@Pt(111) and the di-@sigma@-complex on the CuPt@sub 3@(111) surface, respectively. A full peak assignment in HREELS spectra gives a strong indication for a reduction of the C-C bond order of the di-@sigma@-species going from Cu@sub 3@Pt(111) to Pt(111). This can be attributed to an electronic effect due to the dilution of Pt by Cu. Both TPD and UPS support these results. Surprisingly, ethene does not dehydrogenate on the alloys when the surface is heated in contrast to ethene on Pt(111). This can be explained by the lack of appropriate sites on Cu@sub 3@Pt(111). On CuPt@sub 3@(111) the issue is more complex since on this surface such sites are available. On this surface the process might therefore be kinetically hindered.

SS-TuP8 HREELS and XPS Studies of Fe(C@sub 5@X@sub 5@)@sub 2@ / Ag(100) where X=H, D, or Me*, **C.M. Woodbridge**, D.L. Pugmire, M.A. Langell,* University of Nebraska, Lincoln

Although metallocenes show great potential as novel Chemical Vapor Deposition (CVD) source molecules, very little is known about how they bond to metal surfaces. Therefore, systematic investigation of ferrocene adsorption to different single crystal substrates are essential for understanding and controlling CVD processes involving metallocenes. We have used HREELS and XPS to study ferrocene, Fe(C@sub 5@H@sub 5@)@sub 2@, deuterated ferrocene, Fe(C@sub 5@D@sub 5@)@sub 2@, and its methylated derivative on Ag(100). HREELS was used to confirm the molecular nature of the adsorbed metallocene, determine the orientation and quantify interactions between ferrocene and the silver substrate. XPS was used to evaluate the chemical state of iron and carbon in the ferrocene films and to quantify the adsorbate surface concentration. Specific information about orientation and chemical shifts as a function of ferrocene exposure will also be presented.

SS-TuP9 Insertion Process of Conjugated Molecules into n-Alkanethiol Self-Assembled Monolayers on Au(111)*, **T. Ishida,*** JRCAT-NAIR and PRESTO-JST, Japan*; W. Mizutani,* JRCAT-NAIR, Japan*; U. Akiba,* Tokyo Institute of Technology, Japan*; N. Choi,* JRCAT-ATP, Japan*; M. Fujihira,* Tokyo Institute of Technology, Japan*; H. Tokumoto,* JRCAT-NAIR, Japan

Since conjugated molecules are a good candidate for the components of nanoscale devices, functions of organic molecules have been investigated in search of their potential applications. To analyze the property of such conjugated molecules, insertion of such a molecule into pre-assembled n-alkanethiol SAMs on Au(111) is attracted recently. We have investigated using STM insertion process of conjugated molecules, benzylmercaptane (BM), 4-biphenylmethanethiol (BP), and [1,1':4',1''-Terphenyl]-4-methanethiol (TP) into alkanethiol SAMs. These conjugated molecules were inserted into boundaries between structural domains of n-alkanethiol SAMs at the initial stage of insertion reaction. The insertion process rate increased with the number of phenyl rings of the conjugated molecule, i.e., the most of alkanethiols were replaced by BP and TP for 3-4 h and 2 h, respectively. On the other hand, BMs were inserted in the domain boundaries even after one day insertion reaction. These results suggested that the interaction energy difference between the conjugated molecules and alkanethiols strongly affected the insertion reaction.

SS-TuP10 Adsorption and Thermal Decomposition of 1,3-butadiene and 2-butyne on Ru(001)*, **M.J. Weiss**, C.J. Hagedorn, W.H. Weinberg,* University of California, Santa Barbara

The low temperature (80 K) molecular adsorption and subsequent thermal decomposition of 1,3-butadiene and 2-butyne are studied on Ru(001) using temperature programmed desorption and high resolution electron energy loss spectroscopy (HREELS). After heating to 300 K, the 1,3-butadiene decomposes to yield a (CH)@sub 4@ surface metallacycle. This result is particularly interesting in that the (CH)@sub 4@ species has been implicated as an intermediate in the production of 1,3-butadiene (and other molecules) during thiophene hydrodesulfurization. 2-butyne adsorbs at a coverage of 0.27 molecules for every surface ruthenium atom, a coverage which is equal to that observed for the adsorption of acetylene on this surface. The 2-butyne decomposes to yield surface hydrocarbon fragments whose HREEL spectra resemble those of vinylidene, acetylide, and methylidyne. Slight differences in the spectra, however, suggest that the fragments observed in the present work may actual be analogous species containing four carbon atoms.

SS-TuP11 A Study of Boron Effects on the Reaction of Co and SiGe at Various Temperatures*, **H.J. Huang**, K.M. Chen,* National Chiao Tung University, Taiwan, R.O.C.*; T.C. Chang, G.W. Huang, L.P. Chen,* National Nano Device Laboratory, Taiwan, R.O.C.*; C.Y. Chang,* National Chiao Tung University, Taiwan, R.O.C.

The boron effects on Co and SiGe interfacial reaction were studied with RTA from 500°C to 1000°C. The undoped and in-situ boron-doped strained Si@sub 0.91@Ge@sub 0.09@, Si@sub 0.85@Ge@sub 0.15@ layers were prepared at 550°C by ultra-high vacuum chemical vapor deposition system for silicidation. The resulting films were characterized by sheet resistance measurement, Auger electron spectroscopy, X-ray diffractometry, high resolution X-ray diffractometry, secondary ion mass spectroscopy, scanning electron microscopy, and transmission electron microscopy. Co(Si@sub 1-y@Ge@sub y@) cubic structure was formed from 500°C to 700°C RTA with different Ge content. For the boron-doped sample, Ge content (y = 0.064, 0.054) in Co(Si@sub 1-y@Ge@sub y@) was less than undoped sample (y= 0.12, 0.11) after 500°C RTA, which can be discovered by X-ray diffraction. This implied that boron atoms retarded the incorporation of Ge into the Co(Si@sub 1-y@Ge@sub y@) ternary phase. It also led to large piled-up of Ge at the reaction interface. On the other hand, according to the X-ray rocking curve, boron-doped sample led to less relaxation of strained SiGe layer. Furthermore, from sheet resistance measurement, the formation of CoSi@sub 2@ was a little slower in boron doped sample than in undoped sample. This may be due to the decrease of Co diffusivities, which was caused by the boron accumulation at the Co/SiGe reaction interface. At temperature above 800°C, CoSi@sub 2@ was formed and the underlying SiGe layer was almost totally consumed. From the AES and TEM analyses, Ge segregation to the surface and the CoSi@sub 2@ grain boundary was observed.

SS-TuP12 Vacancy Mediated Growth of Ga@sub 2@Se@sub 3@ Thin Films*, **Z. Qian**, Z. Dai, F.S. Ohuchi,* University of Washington*; K. Ueno, A. Koma,* University of Tokyo, Japan*; S. Meng, M.A. Olmstead,* University of Washington

Ga@sub 2@Se@sub 3@ thin films were grown on GaAs(100) and Si(111) substrates by molecular beam epitaxy (MBE). In spite of large differences in lattice and symmetry found in GaAs(100) and Si(111), reflection high energy electron diffraction (RHEED) showed that the Ga@sub 2@Se@sub 3@ thin films were epitaxially grown on both surfaces. Electronic structures were determined by ultraviolet photoelectron spectroscopy (UPS) and electron energy loss spectroscopy (EELS). For the Ga@sub 2@Se@sub 3@ thin films growth on GaAs(100) substrate, transmission electron microscopy (TEM) revealed that vacancies were distributed on one set of the [111] crystal planes of @alpha@-Ga@sub 2@Se@sub 3@ structure by forming a @sr@3x@sr@3 configuration, resulting in the formation of vacancy ordered @beta@-Ga@sub 2@Se@sub 3@ structure. In this structure, modulation periodicity along [110] crystal directions was three times larger than that of @alpha@-Ga@sub 2@Se@sub 3@, and the crystal structure was consistent to the model proposed by Lübbers and Leute for bulk material (J. Solid State Chem., 43 (1982) 339). Very different nature of the growth habit was observed on the Si(111). High population of planer defects observed in the thin film was regarded as the result of Ga vacancy ordering in the crystal structure of Ga@sub 2@Se@sub 3@. We claim that the vacancies play an important role in determining the thin film structure in addition to lattice and symmetry matching conditions in the heteroepitaxy.

SS-TuP13 Surface Morphology of Ge(111) and Ge(001) Etched by keV Xe Ions*, **J.C. Kim**, D.G. Cahill, R.S. Averback,* University of Illinois, Urbana-Champaign

In situ scanning tunneling microscopy (STM) was used to study the surface morphology and defects created by keV Xe@super +@ ion etching of Ge(111) and Ge(001). Starting surfaces were prepared by etching single crystal Ge wafers at ~ 510 @super o@C by 5 keV Xe@super +@ ions with ion flux of 2.7 x 10@super 13@ ions cm@super -2@s@super -1@ and fluence of 5 x 10@super 16@ ions cm@super -2@; the samples were subsequently cooled and etched at lower temperatures with various ion fluences and ion energies, and imaged at room temperature. Ge(111) and Ge(001) surfaces remain crystalline after being etched at T @>=@ 295 @super o@C. Crater-like surface features, which were not observed on the starting surfaces and will be called pits, were observed on both Ge(111) and Ge(001) surfaces etched at 295 @super o@C and 325 @super o@C. These pits are ~ 200 Å in diameter and are surrounded by closely spaced steps. Pits were observed on the Ge surfaces etched by Xe@super +@ ions with energies as low as 650 eV. Etching of a Ge(111) buffer layer, which was grown at ~ 365 @super o@C with the thickness of 1000 Å in an in situ

MBE chamber, at 295 @super o@ was performed to examine the interaction of 5 keV Xe@super +@ ions with the surface prepared without etching at high temperature and revealed no pits. These results that pits were observed following 650 eV Xe@super +@ ion etching and not observed following etching of an MBE buffer layer suggest that these large surface features are not the result of the individual surface cascades as has been observed for 20 keV Ga ions. The pits initially grow in size and number and eventually disappear after the samples were etched for approximately one hour, leading to different surface roughening morphologies at 295 @super o@C and 325 @super o@C. Rutherford backscattering spectroscopy (RBS) data show that Xe atoms are implanted below the starting surface, subsequent ion etching at lower temperatures causes a broadening of Xe peak in RBS spectra. Our data suggest that interaction of bulk defects, e.g. Xe bubbles or vacancy clusters, with surface can have a strong influence on the evolution of surface morphology during ion etching at keV energies.

SS-TuP14 Surface Core Level Shift on GaN(0001) Surface*, **Y. Yang**, S.H. Xu, H. Cruguel, G.J. Lapeyre,* Montana State University*; H.J. Ho,* TopoMetrix Co.

Synchrotron radiation photoelectron spectroscopy (SRPES) has been employed to investigate the electronic structure of clean wurzite GaN(0001) surface. The Ga 3d, N 1s and valence band emissions are measured by recording the energy distribution curves (EDC). A surface-shifted core level component is observed in the Ga 3d emission. It is located at 0.6 eV higher binding energy than the bulk component. The surface component is sensitive to atomic H adsorption. Experiment with deposition of ultra-thin Mg layer strongly support that it is attributed to the first layer Ga atoms. On the same sample, the surface core level shift of N 1s is identified at 1.0 eV lower binding energy side of the bulk component. The origin of the observed surface core level shifts will be discussed. Atomic-force-microscopy (AFM) image with line profiles are also acquired to determine the surface morphology.

SS-TuP15 Raman-scattering Study of In(As,Sb)/InSb Superlattices*, B. Marcos, R. Cuscó,* Institut Jaume Almera (CSIC), Spain*; R.A. Stradling,* Imperial College, U.K.*; **L. Artús**,* Institut Jaume Almera (CSIC), Spain

InAs@sub 1-x@Sb@sub x@ alloys display the smallest bandgap in the III-V group for x=0.6. By growing In(As,Sb)/InAs superlattices even smaller effective bandgaps can be obtained, making these layer structures very interesting for applications to mid- and far-infrared semiconductor lasers and light-emitting diodes operating at wavelengths from 4 to beyond 10 µm. In a previous paper@footnote 1@ we reported a Raman-scattering study of the optical phonon modes of InAsSb/InAs strained-layer superlattices(SSL) for different Sb compositions, but to our knowledge no study has been reported so far on the phonons of the other end system SSLs, namely the InAsSb/InSb SSLs. In the present work we report Raman measurements on InAsSb/InSb SSLs for several As concentrations below 20%. The InAsSb alloy displays a two-mode behaviour,@footnote 2@ and consequently the InSb-like and InAs-like LO modes of the alloy are expected. In fact, despite the low As concentration of the alloy, in the (Z|XY|-Z) Raman spectra we could observe not only the InSb-like LO mode of the alloy but also the InAs-like LO mode. The strain-induced relative shift of this peak is well accounted for by elastic strain calculations. In the (Z|XX|-Z) configuration an additional peak is observed below the InSb-like LO mode of the alloy that can be tentatively assigned to interface modes. @FootnoteText@ @footnote 1@ L. Artús, R. A. Stradling, Y. B. Li, S. J. Webb, W. T. Yuen, S. J. Chung, and R. Cuscó, Phys. Rev. B 54, 16 373 (1996). @footnote 2@ Y. B. Li, S. S. Dosanjh, I. T. Ferguson, A. G. Norman, A. G. de Oliveira, R. A. Stradling, and R. Zallen, Semicond. Sci. Technol. 7, 567 (1992).

SS-TuP16 The Adsorption and Thermal Decomposition of Monomethylamine Adsorbed on Si(100)*, **A.J. Dennis**, C.P.A. Mulcahy, S.M. Casey,* University of Nevada, Reno

Monomethylamine (MMA) adsorption on the Si(100)-(2x1) surface has been studied using Auger electron spectroscopy (AES), low-energy electron diffraction and temperature-programmed reaction spectroscopy (TPRS). It is shown that at room temperature MMA chemisorbs dissociatively on this surface. TPRS data show that the decomposition of the adsorbed MMA proceeds via two different mechanisms. The surface bound adsorbates can decompose via reactions that form gaseous hydrogen and hydrogen cyanide products; however, they may also decompose via a reaction channel producing gaseous ammonia. AES results show that repeated decomposition of MMA on Si(100) leads to the slow deposition of carbon- and nitrogen-based films. Kinetic analysis of the TPRS data will be discussed along with results from ab initio calculations modeling MMA adsorption on nine-atom silicon clusters.

SS-TuP18 The Formation of di-@sigma@ Bond in Chemisorbed Benzene and Chlorobenzene on Si(111)-7x7*, **Y. Cao**, G.Q. Xu,* National University of Singapore, Singapore

The adsorption of aromatics on Si surfaces has attracted great interests recently. In the present study, the adsorption of benzene and chlorobenzene on Si(111)-7x7 has been studied using high resolution electron energy loss spectroscopy (HREELS) and thermal desorption spectroscopy (TDS). Both chemisorbed and physisorbed benzene were observed at an adsorption temperature of 110 K. Chemisorbed benzene desorbs molecularly at 350 and 364 K while physisorbed molecules desorb at 180 K. In the HREELS studies, two separate energy losses at 2920 and 3025 cm@super -1@ were observed for chemisorbed benzene, attributable to the C-H stretching vibrations of sp@super 3@ and sp@super 2@ carbon atoms, respectively. In addition, the formation of Si-C bond is also evidenced at a vibrational frequency of 540 cm@super -1@. Our results clearly demonstrate that benzene is di-@sigma@ bonded to the adjacent adatom and rest-atom on Si(111)-7x7, forming a 1,4-cyclohexadiene-like structure. The adsorption behaviour for chlorobenzene is quite similar to that of benzene. However, due to the substitution effect of the Cl atom on ring of benzene, a regional-selective adduction of 2,5-sites in chlorobenzene on Si(111)-7x7 is observed, resulting the formation of 2,5-chlorocyclohexadiene like adduct.

SS-TuP19 Dissociative Adsorption of Molecular Hydrogen on Si(001): Energy Dependence, Angular Distribution and Reaction Mechanism*, **M. Duerr**, M.B. Raschke, U. Hoefer,* Max Planck Institut fuer Quantenoptik, Germany

The dissociative adsorption of molecular hydrogen on Si(001) surfaces was investigated by means of supersonic molecular beam techniques and optical second harmonic generation (SHG). Sticking on the flat surfaces shows strong activation with beam energy as well as surface temperature.@footnote 1@ Preparing single-domain surfaces by selectively passivating the step sites of vicinal Si(001) surfaces, polar and azimuthal distributions of the sticking coefficient could be measured. The polar distributions are found to be peaked towards the surface normal. However there is a strong azimuthal dependence, the distribution is considerably narrower (cos@super 12@) for incident angles perpendicular than parallel to the dimers (cos@super 3.5@). For multi-domain surfaces, the reduction of the sticking coefficients is more pronounced than it is to be expected by the reduction of normal energy. Therefore the energetic corrugation dominates the adsorption process. Temperature dependence of the sticking coefficient, deviation from normal energy scaling and azimuthal anisotropy result from the covalent bindings on the semiconductor surface, which lead to a strong corrugation of the potential energy surface and the strong influence of lattice vibrations on reaction dynamics. Proposed defect mediated mechanism, leading to an enhancement of sticking under glancing incidence can be excluded. @FootnoteText@ @footnote 1@ M. Duerr, M. B. Raschke, and U. Hoefer, J. Chem. Phys. (submitted).

SS-TuP20 Silicide Island Nucleation Behavior for Co/Si(111) Studied with STM and LEEM*, **T.H. McDaniels**, P.A. Bennett,* Arizona State University

We have measured the coverage and temperature dependence of island nucleation during deposition of Co on Si(111)-7x7 using STM for low temperature and LEEM for high temperature. Below 500C, 3 distinct structures occur: "lowered" regions mostly on the unfaulted half of the 7x7 unit cell, "raised" regions mostly on the faulted half, and flat island structures with a 2x2 pattern of silicon adatoms. Island density vs coverage follows a growth exponent near 1, suggestive of i=0 behavior (stable nucleus contains a single atom), and the temperature dependence is relatively weak. From 600-900C, the islands are atomically flat CoSi2, and they form only at step edges following completion of a 1x1-RC ("ring-clusters") layer. Island density is now much lower and strongly temperature dependent with an activation energy of approximately 2.0eV.

SS-TuP21 Nickel Graphite Intercalation Compound formed by High Temperature Deposition of Ni on SiC*, **K. Robbie**,* Linköping University, Sweden, Canada*; T. Jemander, N. Lin, R. Erlandsson, G.V. Hansson, L.D. Madsen,* Linköping University, Sweden

While studying the growth of sputter-deposited nickel on 6H SiC (0001) substrates, an unexpected islanded structure was formed. Nickel, deposited at room temperature and annealed to 950 C to form Ni@sub 2@Si, is the most common approach for forming ohmic contacts to n-type

SiC. In this study aimed at gaining understanding of the contact formation process, we sputter-deposited Ni layers of varying nominal thickness (sub- to 1000 monolayers) onto hydrogen-etched on-axis SiC substrates at temperatures ranging from ambient to 1000 C and subsequently annealed to 1000 C. In-situ analysis was performed with RHEED, LEED and/or STM. Unlike all previous experience with Ni deposited onto SiC, we observed the formation of islands of two types, one of which had very steep sidewalls (>60 degrees) and an extremely flat top with a peculiar "stitched" surface structure. Microspot AES analysis has shown that the islands are composed of Ni and C, or Ni, Si, and C, and that the carbon is bound graphitically in both types. Investigations with STM, AFM, and AES, and comparison to literature, has led us to believe that a new type of graphite intercalation compound was formed in the flat topped islands with a composition of approximately NiC@sub 12@, and that Ni on the top graphite sheet produced the "stitched" surface structure observed by STM. Previously, only alkali metals and transition metal chlorides have been shown to intercalate into the galleries of graphite, and the reactivity and instability of these compounds has limited their use in spite of their very exciting electronic, magnetic, and other physical properties.

SS-TuP22 Surface Modification in Heteroepitaxy : Laminar, Crystalline Silicon on CaF@sub 2@, ***B.R. Schroeder***, *S. Meng, A. Bostwick,* University of Washington*; E. Rotenberg,* Lawrence Berkeley National Laboratory*; M.A. Olmstead,* University of Washington

CaF@sub 2@/silicon heterostructures are strong candidates for obtaining visible light emission from silicon. However, the heteroepitaxial growth of laminar, crystalline silicon on CaF@sub 2@(111) substrates is hindered by two factors 1) CaF@sub 2@ surface energy is much lower than that of Si and 2) a strong etching reaction between Si and F. We have overcome these difficulties through surface modification 1) use of arsenic as a surfactant 2) electron irradiation to remove surface fluorine. Low energy (40 eV) electron irradiation removes fluorine (amount of F removed scales linearly with the electron dose) but the films become extremely reactive with oxygen and/or water vapor (even under UHV conditions). Arsenic termination stabilizes this surface and serves as a surfactant for the subsequent silicon growth. X-ray photoelectron spectroscopy shows Ca-Si bonds at the interface and As-Si bonds at the surface. The silicon surface has a bulk-like termination, characteristic of Si(111):As, as evidenced by the 1X1 LEED pattern. X-ray photoelectron diffraction shows that the grown silicon layer is crystalline, rotated 180@super o@ with respect to the CaF@sub 2@ substrate (Type B interface), and completely covers the CaF@sub 2@. Supported by DOE grant DE-FG03-97ER45646/A002.

SS-TuP23 X-ray Photoemission and Near Edge Absorption Studies of Rhenium (VII) Sorption onto Fe-bearing Materials*, **P. Liu**, W.W. Lukens, Jr., E.J. Moler, D.K. Shuh,* Lawrence Berkeley National Laboratory

Technetium (@sup 99@Tc) is a radioactive byproduct of nuclear fission, and its concentration may set the regulatory limit for disposal of nuclear wastes. Therefore, the high solubility and mobility of TcO@sub 4@@sup -@ needs to be addressed. A solution is to reduce Tc@sup 7+@ to Tc@sup 4+@, which is much less soluble and mobile. One method is by adsorbing Tc@sup 7+@ onto surfaces of reducing agents. While previous experiments demonstrated that Tc@sup 7+@ ions were sorbed on and reduced by some materials, the products and the mechanism of sorption and reduction are not fully characterized or understood. Rhenium (Re) has similar redox properties as Tc, and can be treated as a surrogate for Tc in selected systems. Since Re is non-radioactive, experiments are more efficiently performed. A class of possible reductants are Fe, Fe oxides, and sulfides. Sorption samples were prepared by immersing powders of Fe metal, FeO, FeS, and FeS@sub 2@, respectively, in 0.010M Re(VII) solution for 24 hours or longer, during which time the powder and the solution were constantly mixed. The reacted powders were extracted after the mixtures were centrifuged and the solutions decanted. The photoemission of Re 4d and 4f core levels, and NEXAFS of Re N@sub III@ experiments were carried out at the Advanced Light Source. The results reveal that the amount of absorbed Re decreases from Fe metal, through FeO, FeS, to FeS@sub 2@; and that different species of Re are sorbed on surfaces of different Fe-bearing materials, with more oxidized species tending to dominate on the less sorbed surfaces. Together with the pH measurements of the residual solutions, the results suggest that the sorption and reduction of Re on the surfaces of Fe-bearing materials are partially controlled by the final pH of the solution-particle mixture.

SS-TuP24 Epitaxial Growth of Thin Ag Films on Al(001) and Al(110) Surfaces@footnote 1@*, N.R. Shivaparan, M.A. Teter, **R.J. Smith**,* Montana State University

We report the results of a characterization of Ag films (0 to 60 Å thick), deposited onto Al(001) and Al(110) surfaces at room temperature, using high energy ion backscattering and channeling, x-ray photoelectron spectroscopy (XPS), and low energy electron diffraction (LEED). For the Al(001) surface, measurements of the backscattered ion yields from Al and Ag atoms show that the Ag atoms occupy fcc lattice sites and shadow Al substrate atoms. However, the ion scattering yields and photopeak intensities do not follow layer-by-layer model growth curves. Together with the evolution of the Ag 3d core level binding energies and the valence band shape as a function of Ag coverage, these results support a model of interface strain relief by means of Ag-Al alloy formation, with the interface ultimately covered by an ordered, epitaxial Ag film. For the Al(110) surface the observations are closer to those expected for layer-by-layer Ag growth, but still show evidence of some Al diffusion into the well-ordered Ag overlayer. @FootnoteText@ @footnote 1@ Work supported by NSF Grant No. DMR-9710092 and by NASA EPSCoR Grant NCCW-0058 .

SS-TuP25 The Reactivity of Short Chain Alcohols on VC (100)*, **R.L. Guenard**[1]*, University of Houston*; S.S. Perry,* University of Houston, US

The reactions of small chain alcohols on the nonpolar (100) surface of single crystal VC have been studied using temperature programmed desorption (TPD). The surface was prepared by argon ion sputtering followed by electron beam heating to 1400K. The sample was sputtered and annealed between coverages, as well, in order to insure the removal of any oxides formed in the reaction with an alcohol. The results of these experiments showed that VC exhibits selective reactivity towards alcohols including, dehydrogenation and alkene formation. In these TPD measurements, methanol adsorbed both molecularly and dissociatively onto VC. The products of temperature induced desorption being H@sub2@ and CH@sub4@. A molecular desorption reaction path was also observed. For ethanol and isopropanol, the resulting products of temperature induced desorption were notably different from that of methanol. A @beta@-hydride elimination mechanism results in the formation of water and an alkene. Ethylene and water are evolved from the surface when dosed with ethanol, while propene and water are the products evolved when isopropanol is dosed. In both cases the alkene product is separated from the surface at a temperature greater than water desorption. This reactivity of short chain alcohols, observed near room temperature on VC (100), illustrates potential pathways of lubricant degradation and highlights the possible need for passivating additives.

SS-TuP26 Extremely Efficient Electron Stimulated Desorption of Hydrogen from GaN(0001)*, **V.J. Bellitto**[2],* Georgia State University*; B.D. Thoms,* Georgia State University, US*; D.D. Koleske, A.E. Wickenden, R.L. Henry,* Naval Research Laboratory

To achieve high etch rates and anisotropy during etching of GaN, high temperatures, reactive chemicals, and/or high ion energies are required. The use of electron or photon stimulated processes for etching may be one method to avoid the use of reactive chemicals, damage produced by high ion energies, and materials limitations imposed by high temperatures. Electron stimulated desorption (ESD) of H from GaN(0001) has been observed and characterized using electron energy loss spectroscopy (ELS). Bombardment with 90 eV electrons produces a reversal of H induced changes in the ELS data at 3.5, 6.6, and 11.7 eV. We attribute the electron-stimulated desorption of hydrogen from surface Ga-H to be responsible for these reversals. The reversal of H induced changes to ELS was monitored versus electron exposure to determine the ESD cross section. We measured a cross section for ESD of H of 2 x 10 @super -17@ cm@super 2@ with a reduction of ~3 for the ESD of D to 7 x 10 @super -18@ cm@super 2@. The cross section for the ESD of H from GaN(0001) is 2 to 4 orders of magnitude greater than reported on Si surfaces. On GaN the cross section for ESD of D is ~3 times smaller than for H, while on Si(100) the ESD of D is ~50 times less than for H. Assuming the ESD of H from GaN(0001) occurs through an electronically excited state, as in the Menzel-Gomer-Redhead (MGR) model, the presence of a large cross section and small isotope effect would indicate slow quenching of the excited electronic state. In general, long-lived surface electronic excitations would result in enhanced efficiencies for electron- or photon-stimulated processes. This extremely fast ESD of H also has consequences for electron spectroscopies (LEED & ELS) of H/GaN using similar electron energies and current densities. For example, under the

---

[1] **Morton S. Traum Award Finalist**

[2] **Morton S. Traum Award Finalist**

conditions used in these experiments (90 eV, 33 µA/cm@super 2@), 34 % of the surface H is removed in the first minute of electron exposure. In essence, the H is removed from GaN(0001) more quickly than many electron spectroscopies can be performed.

Author Index

Bold page numbers indicate presenter