



# Tuesday Afternoon Poster Sessions, November 1, 2005

**SS-TuP7 Photoelectron Spectroscopy Studies of Potassium Deposition on Self-Assembled Monolayers**, *H. Ahn, J.E. Whitten*, The University of Massachusetts Lowell

The deposition of potassium in ultrahigh vacuum on alkanethiols self-assembled on gold surfaces has been investigated with X-ray and ultraviolet photoelectron spectroscopies (XPS and UPS). Several issues have been studied, including extent of penetration of the metal and chemical interaction with the organic layer. In the case of methyl-terminated alkanethiols, it is found that potassium penetrates and interacts weakly with the monolayer, as indicated by minimal changes in the valence electronic spectra, even for large metal doses. Angle-resolved XPS and changes in the areas of the K2p, C1s, S2p, and Au4f peaks with increasing potassium dose confirm penetration. Work function measurements, obtained from the widths of the UPS spectra, are consistent with metal diffusion through the methyl-terminated alkanethiols to the gold interface, and work function changes approaching -2 eV are observed for several atomic layers worth of potassium. These types of studies have been performed for a variety of chain lengths and at cryogenic and room temperature. In general it has been found that potassium-induced C1s core level shifts, using XPS when the spectra are referenced to the Fermi level, are a misleading indicator of chemical interaction and essentially disappear when the peaks are referenced to the vacuum level. On the other hand, the Au4f peaks do not shift with respect to the Fermi level. These data suggest that the C1s alkanethiol orbitals are pinned to the vacuum level, and angle-resolved XPS has been used to quantify and study this effect as a function of depth.

**SS-TuP8 Surface Nitridation of Terphenyl Methane Thiol Self-assembled Monolayer Using N@sub 2@ Neutral Beam Process**, *Y. Ishikawa*, Tohoku University, Japan; *T. Ishida*, AIST, Japan; *S. Samukawa*, Tohoku University, Japan

To realize the future molecular scale devices, a fine surface modification method is quite important for controlling surface properties of organic molecules, such as the electric properties. Generally, the plasma processes were widely used to modify the surface for not only semiconductor devices but also polymer surface. However, for the surface modification of organic monolayers that can be utilize molecular scale device, the plasma processes cannot be used because of radiation of VUV, UV photons and charged particles from plasma to surface. Namely, the organic monolayers are considered to be broken due to radiation of these particles. To eliminate these radiation damages, we have already proposed the neutral beam process.<sup>1,2</sup> This process could perfectly prevent the charged particles and ultraviolet photons to the surface and only the low energy neutral beam (accelerated atom and molecular beam) were irradiated to the substrates. In this paper, the pulse-time-modulated (TM) N@sub 2@ beam irradiation<sup>1</sup> was investigated to control the surface nitridation of terphenyl methane thiol self-assembled monolayer (TP1-SAM).<sup>3,4</sup> The N@sub 2@ neutral beam irradiation was modulated at a few tens microseconds to control the degree of surface nitridation. By using the novel modification method, we investigated the surface nitridation of TP1-SAM with maintaining the bulk structure. After the beam irradiation, we evaluated the amount of surface nitridation using the x-ray photoelectron spectroscopy. We found that the TM N@sub 2@ beam could precisely control the surface nitridation of TP1-SAM by changing the beam modulation period. <sup>1</sup>Samukawa et al.: *J. Vac. Sci. Tech.*, A22, 245 (2004) <sup>2</sup>Y. Ishikawa et al.: AVS 51st international symposium, PS+BI-FrM9 (2004) <sup>3</sup>T. Ishida et al.: *Langmuir*, 18, 83 (2002) <sup>4</sup>T. Ishida et al., *Langmuir*, 18, 10499 (2002).

**SS-TuP10 Reaction Site Selectivity of Analyte Gases on Metallophthalocyanines: A Density Functional Theory Study**, *N.L. Tran, S.R. Bishop, G.C. Poon, A.C. Kummel*, University of California at San Diego

Numerous studies have reported the use of metallophthalocyanines (MPcs) as thin film sensors for analyte gases, but a basic understanding of gas chemisorption onto these metal coordination complexes is lacking. Density functional theory was used to investigate the mechanism of chemisorption of two different analytes, NO and NH@sub 3@, onto two different MPcs, CoPc and FePc. Four analyte binding sites on the MPcs were investigated: (i) metal centers, (ii) inner ring nitrogen atoms, (iii) outer ring nitrogen atoms, and (iv) organic rings. For NO on FePc and CoPc, simulations show chemisorption onto the metal centers and physisorption onto the outer ring nitrogens and organic rings. In contrast, NH@sub 3@ chemisorbs onto the FePc metal center and physisorbs onto the Co metal. All other binding sites were not energetically favorable. Additionally, these calculations show a multi-step absorption mechanism in which NO initially binds to the inner

ring nitrogens and then undergoes a barrierless migration to the deep chemisorption well on the metal centers for FePc and CoPc. PDOS simulations reveal that the binding of NO and NH@sub 3@ to the FePc metal center significantly alters the electronic structure of the clean FePc. However the two systems have opposite charge transfer mechanisms: charge is accepted by the NO chemisorbate from the Iron metal but is donated from the NH@sub 3@ chemisorbate to the Iron metal. These different charge transfer mechanisms will differentially affect charge relaxation times and the photoconductivity threshold in an MPc film and therefore can be used to identify analytes instead of just measuring analyte concentration. Additionally, simulations are being performed to study the possibility of subsurface diffusion of the NO molecule into the bulk.

**SS-TuP11 Thermochromism Effects in Poly(3-hexylthiophene)**, *D.Q. Feng*, University of Nebraska-Lincoln; *P.A. Dowben*, University of Nebraska-Lincoln, US

We find evidence for a gradual semiconductor to insulator transition in poly(3-hexylthiophene), that appears to be mediated by a low density of defects states within the highest occupied molecular orbital to lowest unoccupied molecular orbital gap. The photoemission and transport measurements indicate that a loss of charge mobility occurs with decreasing temperature, while the molecular configuration also changes with temperature. Defects states have been identified in photoemission and these defects states are believed to be very heterogeneous.

**SS-TuP12 Adsorption and Decomposition of Triethylsilane on Si(100)**, *J. Lozano, D. Early, L. Bockewitz, J.H. Craig, Jr., P.W. Wang, K.R. Kimberlin*, Bradley University

The adsorption and decomposition of triethylsilane (TES) on Si(100) were studied using temperature programmed desorption (TPD), high resolution electron energy loss spectroscopy (HREELS), and x-ray photoelectron spectroscopy (XPS). Si(100) samples were dosed with TES at 100K. Desorption of mass 27 (attributed to ethylene) takes place at 750K, followed by desorption of hydrogen at 815K. This is indicative of a ???-hydride elimination process that results in at least partial removal of carbon species from the surface. At multilayer coverages, physisorbed species accumulate on the surface, as indicated by a low temperature desorption peak at 170K. At the highest TES exposures (~10L), a second low temperature TPD peak appears at 280K. This suggests that the second-layer physisorbed state is slightly more tightly bound than multilayer TES. In order to confirm this, HREELS and XPS data were obtained immediately following sequential thermal anneals to increasing temperatures, which were determined by landmark features in the TPD spectra. A model of the thermal evolution of TES on Si(100) based on the results obtained will be presented.

**SS-TuP13 Low Temperature Decomposition of Triethylsilane on Si(100) by Electron Irradiation**, *J. Lozano, D. Early, L. Bockewitz, P. Petrany, J.H. Craig, Jr., P.W. Wang, K.R. Kimberlin*, Bradley University

Electron-induced decomposition of triethylsilane (TES) on Si(100) at 100K was studied using temperature programmed desorption (TPD), high resolution electron energy loss spectroscopy (HREELS), electron stimulated desorption (ESD), and x-ray photoelectron spectroscopy (XPS). Si(100) samples were dosed with TES and then irradiated with 600-eV electrons for 5 minutes. During electron irradiation, ESD of neutral particles was monitored. Only a small hydrogen ESD signal was detected at all TES coverages. Following electron irradiation of multilayer TES/Si(100), TPD data exhibited decreased desorption of physisorbed species and a dramatic increase in mass 2, 27, and 59 desorption, compared to TPD from un-irradiated surfaces. This indicates that electron irradiation resulted in decomposition of TES and deposition of large fragments on the surface. Fragmentation of TES by electron irradiation was studied by obtaining HREELS and XPS data following sequential thermal anneals of the electron-irradiated surface to increasing temperatures.

**SS-TuP14 Molecular View of the Selforganization Processes on Silicon: Experimental and Computational Studies of Nitrobenzene and Hexafluoroacetylacetone on Si(100)-2x1**, *L.P. Méndez De Leo, L. Pirolli, A.V. Tplyakov*, University of Delaware

Molecular selforganization on semiconductor surfaces bears a variety of future applications: from deposition processes to molecular electronics. Here we present two different reactions on Si(100)-2x1 surface studied by an array of surface analytical techniques and by computational methods. The reaction of nitrobenzene on Si(100) surface is a prototypical model reaction for understanding the interaction of bifunctional molecules with the surface and for directing self-organization processes at cryogenic

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temperatures. The preferred reaction of the nitro-group has been studied previously and, along with the exceptional thermal stability of the resulting monolayer, provides an opportunity to manipulate surface reactions that have a long list of possible pathways. Computational analysis together with the vibrational studies suggest that only a few types of surface bonding are possible in this reaction and the interaction between the neighboring chemisorbed nitrobenzenes lay a groundwork for studies of electron transfer processes involving the  $\pi$ - $\pi$  interaction of the phenyl groups. Hexafluoroacetylacetone (hfac) is a common ligand in chemical vapor deposition processes of copper. The interaction of this ligand with the Si(100)-2x1 surface is of paramount importance for the deposition processes, at the same time, it possesses several functionalities and the utilization of the preferential binding of these functional groups to the surface can be used in the future not only to modify the interactions of the organometallic precursors with the substrate but also to understand the general rules in functionalization of the surface with complex multifunctional molecules. Just like in the case of nitrobenzene, computational methods were used in conjunction with the experimental studies to elucidate the mechanism of hfac interaction with Si(100)-2x1.

**SS-TuP16 Adsorption and Dissociation Studies of Tri-ethylgermane on the Si(100) Surface.** A. Brickman, P. Petrány, J. Lozano, J.H. Craig, Jr., P.W. Wang, Bradley University

Adsorption of tri-ethylgermane (TEG) on the Si(100) surface has been studied using temperature programmed desorption (TPD), electron stimulated desorption (ESD) in a time-of-flight mode, and high resolution energy loss spectroscopy (HREELS). Evidence for a beta-hydrogen elimination process will be presented in desorption spectra. Electron driven dissociation effects on the adsorbed TEG layer will be presented. The extent to which germanium is deposited on the Si(100) surface subsequent to TEG dissociation will also be discussed as characterized by X-ray photoelectron spectroscopy (XPS).

**SS-TuP17 The Adsorption Structure of Histidine on Ge(100).** S.J. Jung, S. Kim, Korea Advanced Institute of Science and Technology (KAIST), Korea; S. Hong, Sejong University, Korea

The adsorption of histidine molecule on the Ge(100)-2x1 surface was investigated using both scanning tunneling microscopy (STM) and the density functional calculation. Various adsorption features of histidine are founded to be formed under different conditions of temperatures and coverages. When histidine is exposed to a clean Ge(100) surface at 300 K, the histidine appears as round shaped bright protrusion in STM image, which is randomly distributed over the surface. After annealing the surface at 380 K, we found a short range ordering in molecular rows. When histidine is deposited onto Ge (100) at 380 K, histidine is found to form dumbbell shape protrusions that are located in either parallel or vertical direction to the dimer row. At the saturation coverage ( $\theta = 0.25$  ML), however, the STM image show globally ordered array consisted of dumbbell shape features without regard to the direction of dimer row of the Ge (100) surface. Such global ordering implies that the interaction between histidine molecules is much more significant than the interaction between the molecules and the surface dimer. The ab initio calculation also suggests that the surface at saturation coverage has an additional stability, induced by the lateral interaction, compared to that at low coverage. Based on the STM results and ab initio calculation, we will present the adsorption structures, inter-molecular interaction and ordering of histidine molecules on the Ge(100) surface.

**SS-TuP18 Chiral Attachment of Styrene Mediated by Surface Dimers on Ge(100).** Y.J. Hwang, Korea Advanced Institute of Science and Technology (KAIST), South Korea; A. Kim, Korea Advanced Institute of Science and Technology (KAIST), South Korea, Korea; E.K. Hwang, S. Kim, Korea Advanced Institute of Science and Technology (KAIST), South Korea

We determine the absolute chirality of adsorbed styrene using scanning tunneling microscope (STM) and demonstrate a novel method for the achiral molecule to produce dimeric enantiomers and diastereomers covalently bonded to the Ge(100) surface. On the Ge(100) surface, styrene adsorbs in a paired end-bridge between two neighboring Ge dimers within the same dimer row (PEB) as well as on the top of a single Ge-Ge dimer (OT). The OT configuration is classified into (S) and (R) OT chiral products according to the direction in which styrene molecule attacks the Ge dimer. Similarly, in case of paired adsorption, we found enantiomeric (R,R)- and (S,S)-trans-PEB and diastereomeric (R,S)-cis-PEB configurations through STM images. Temperature programmed desorption (TPD) spectra indicated that the desorption temperatures for the OT and PEB configurations are 320 K and 365 K, respectively. STM measurements

indicate that the OT configurations is converted into the thermodynamically more stable PEB configurations either by annealing a styrene-adsorbed Ge surface at 340 K or by scanning the Ge surface at high bias voltages. Such conversion of chiral configurations suggests the possibility of the controlled adsorption of chiral molecules on the surface. Therefore, we anticipate that the chiral structures prepared by paired adsorption will provide chiral organic hybrid systems on semiconductor surfaces for potential application to semiconductor-based molecular devices, chiral sensors, and heterogeneous enantioselective catalysis. @FootnoteText@ @footnote 1@ Hwang, Y. J.; Kim, A.; Hwang, E.; Kim, S. J. AM. CHEM. SOC. 2005, 127, 5016-5017

**SS-TuP19 Phonon-Activated Electron-Stimulated Desorption of Halogens from Si(100)-(2x1).** B.R. Trenhaile, V.N. Antonov, G.J. Xu, A. Agrawal, A.W. Signor, R.E. Butera, K.S. Nakayama, J.H. Weaver, University of Illinois at Urbana-Champaign

Spontaneous desorption of Cl, Br, and I from n- and p-type Si(100)-(2x1) was studied with scanning tunneling microscopy at temperatures of 620  $\pm$  825 K where conventional thermal bond breaking should be negligible. The activation energies and prefactors determined from Arrhenius plots indicate a novel reaction pathway that is initiated by the capture of electrons that have been excited by phonon processes into Si-halogen antibonding states. This configuration is on a repulsive potential energy surface, and it is sufficiently long-lived that desorption occurs, as in electron-stimulated-desorption. Surprisingly, the desorption rates for differently doped samples crossed and, above a critical temperature, the reaction with the largest activation energy had the highest rate. This is explained by large entropy changes associated with the multiphonon nature of the electronic excitation. For Cl desorption from p-type Si, these entropy changes amounted to 34 kB. They were 19 kB, 13 kB, and 8 kB for Br desorption from p-type, lightly-doped n-type, and heavily-doped n-type Si, respectively. The desorption rates for I were nearly three orders of magnitude larger than the rates observed for Cl and Br. Here, the Si-I antibonding states overlap the conduction band minimum, and we propose that electrons impinging on the surface with this energy can be captured by the Si-I antibonding states. Together, these results reveal that a complex relationship exists between phonons and electronic excitations during chemical reactions at surfaces.

**SS-TuP20 Water Etching of Hydrogen-Terminated Si(100): Implications for Oxidation.** S.K. Green, Smith College; M.F. Faggin, M.A. Hines, Cornell University; K.T. Queeney, Smith College

While it has been known for some time that deoxygenated H<sub>2</sub>O will etch hydrogen-terminated Si(100), our recent work shows that this etching generates a surface of surprising homogeneity. Transmission infrared spectroscopy is used both to examine the mechanism of this etching process and to decipher the surface termination of the structures formed. Analysis of both the stretching and bending modes of SiH<sub>x</sub> species reveals characteristic {100} and {111} facets that can be related to structures formed on extended (100) and (111) surfaces. Selective isotopic labeling reveals that the initial, H-terminated surface is completely removed within 10 minutes' immersion in room-temperature, deoxygenated H<sub>2</sub>O. The rate of this reaction is therefore fast compared to the rate of oxidation of H:Si(100) by O<sub>2</sub>(aq) that is normally present in air-equilibrated H<sub>2</sub>O, making the etching process a critical factor in the oxidation of Si(100) in neutral or basic aqueous solutions.

**SS-TuP21 Substrate-Bias-Dependent Orientation-Selective-Epitaxial Growth of CeO<sub>2</sub> Thin Films on Si(100) Substrates by Magnetron Reactive Sputtering.** T. Inoue, Iwaki Meisei University, Japan; D. Kukuruzyak, T. Chikyo, National Institute for Materials Science, Japan; K. Kato, Fukushima Technology Centre, Japan

Although many reports have been made on the growth of CeO<sub>2</sub>(110)/Si(100), orientation selective epitaxial (OSE) growth of CeO<sub>2</sub>(100) and CeO<sub>2</sub>(110) layers is found to be capable by controlling substrate bias and plasma power in reactive dc magnetron sputtering enhanced with an inductively coupled rf plasma. We adopted two step growth method; ultrathin metallic Ce layer deposition at room temperature using Ce metal target followed by silicidation process at several hundreds degree C, and subsequent reactive sputtering in an Ar/O<sub>2</sub> mixture environment at elevated temperature. Reactive magnetron sputtering is performed at rf power of 50 W for induction coil and 120 W for cathode dc plasma power under substrate bias ranging between -25 and +25 V varied by 5<sup>-</sup>V step. Growth rate is controlled in between 0.2 and 0.4 nm/s varying Ar gas flow between

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4 and 15 sccm. Oxygen gas flow for reactive sputtering is 1 sccm. CeO@sub 2@(100) layers grow under substrate bias around both +15 and -15 V with a width of approximately 10 V, otherwise CeO@sub 2@(110) layers grow. The orientation selection is found to be also dependent on plasma power, in other words the growth rate: upper limit in growth rate exists for (100) layer growth, above which (110) layer grow. Precise mapping of growth parameters for OSE, in terms of substrate bias and growth rate, for the growth of CeO@sub 2@(100) films are attained from a lot of growth experiments. In order to get insight into orientation selectivity depending on substrate bias, we are making systematic experiments to study orientation component changes with substrate bias in CeO@sub 2@ layers, which leads to a clue for understanding the relation between orientation of nuclei and substrate bias. We also demonstrate the experimental results indicating effectiveness of assistance by oxygen radical beams on reactive sputtering; successful epitaxial temperature lowering and crystalline quality improvements. Characterization of the epitaxial films are carried out using RHEED, XRD, XTEM and AFM. This orientation selective epitaxial growth (OSE) technology will be useful for sophisticated structure using multiple layer epitaxy. @FootnoteText@ @footnote 1@ T. Inoue et al., J. Vac. Sci. Technol. A 22(1), 46 (2004).

**SS-TuP22 Measurement of Surface States Above the Valence Band Maximum in n-type GaN(0001) Using Angle-Resolved Photoemission Spectroscopy, L. Plucinski, L. Colakerol, S. Bernardis, Y. Zhang, K.E. Smith, I. Friel, T.D. Moustakas, Boston University**

We have performed a high resolution angle-resolved photoemission study of N-polar GaN(000-1).@footnote 1@ We have observed sharp dispersive surface states extending approximately 2 eV above the valence band maximum (VBM). These states agree with those predicted for a N-polar GaN(000-1) 1x1 reconstructed surface. Samples were grown by plasma-assisted molecular beam epitaxy on c-plane sapphire. They were doped with Si and the free-carrier concentration was  $3 \times 10^{18}$  cm<sup>-3</sup> which resulted in a slightly degenerate n-type material at room temperature. Experiments were performed at the U5UA undulator beamline at the NSLS, using a Scienta SES100 electron energy analyzer. Clean surfaces were prepared in situ by sputtering with nitrogen ions and annealing in UHV. Samples were held at 120 K when recording spectra. We have found a full width at half maximum for the surface state feature of 400 meV at K-point of surface Brillouin zone. The width is limited by surface imperfections and the existence of reconstructions on the surface other than a simple 1x1. Our results are similar to those obtained for p-type GaN.@footnote 2@ However, in case of p-type GaN the surface likely contained 30 degree rotated domains.@footnote 3@ We show that in the case of n-type GaN the surface is free of domains. @FootnoteText@ @footnote 1@ Supported in part by the NSF DMR-0311792, by U.S. ARO 40126-PH, and by U.S. AFOSR. Our spectrometer system is funded by U.S. ARO DAAD19-01-1-0364. Experiments performed at the NSLS which is supported by the U.S. DOE, Divisions of Materials and Chemical Sciences.@footnote 2@ P. Ryan, Y. C. Chao, J. Downes, C. McGuinness, K. E. Smith, A. V. Sampath, and T. D. Moustakas, Surf. Sci. 467, L827 (2000).@footnote 3@ F.-H. Wang, P. Krueger, and J. Pollmann, Surf. Sci. 499, 193 (2002).

**SS-TuP23 Step Edge Diffusion in Strained Compound Semiconductors, C. Pearson, University of Michigan-Flint; J. Mirecki Millunchick, University of Michigan**

Understanding the growth of strained alloys films is an enduring problem in surface science. Models of strained film growth based on elastic strain energy predict unique morphologies for different strain: islands upon large terraces for compressive films and mesas separated by trenches for tensile films. Using a combined MBE-STM system, we have imaged 2 ML thick films both in compression (InAs or GaSb) and in tension (GaAs or AlAs) grown on InP(001) near T=480°C using a group III growth rate of ~0.2 ML/s with an approximate group V/III ratio of 5. A roughness analysis reveals that the skewness of the height distribution for InAs is positive, which is indicative of a morphology dominated by islands while for AlAs the skewness is negative, which is indicative of a morphology dominated by holes. These results agree with the previously described morphologies predicted using elastic strain energy considerations. The Ga containing compounds also follow this strain energy trend, except the terraces or mesas have significantly rougher steps and higher surface anisotropies. These observations suggest that in addition to the sign of the misfit strain, factors such as step edge diffusion contribute to surface roughness. From an analysis of the images we compute the step edge density (step edge length per unit area) versus deposition flux and use a recent level set model@footnote 1@ to extract values of step edge diffusion. These results

may explain the variety of microstructures observed in short period superlattice structures of these compounds that exhibit lateral composition modulation. @FootnoteText@ @footnote 1@ C. Ratsch, J. Garcia, and R. E. Caflich, submitted to Applied Physics Letters.

**SS-TuP24 Comparative Study of the Initial Oxidation Kinetics on Si(001) and Ti(0001) Surfaces by Real-Time Ultraviolet Photoelectron Spectroscopy, Y. Takakuwa, S. Ogawa, M. Ohira, IMRAM, Tohoku University, Japan; Y. Mizuno, Stanford University**

Oxidation on Si and Ti surfaces leads to growth of SiO@sub 2@ and TiO@sub 2@ layer, respectively. In order to clarify the behavior of adsorbed oxygen during growth of oxide, the initial oxidation kinetics on Si(001)2x1 and Ti(0001)1x1 surfaces was comparatively investigated by real-time ultraviolet photoelectron spectroscopy to measure the oxygen uptake and work function @phi@ simultaneously. On the Si surface at 357°C, the @phi@ increases gradually with increase of O@sub 2@ dosage after showing a dip due to negative charges, while the dip disappears with elevating temperature. The negative change of @phi@ means diffusion of adsorbed oxygen into the subsurface. On the other hand, a dip in @phi@ appears at temperatures above 300°C on the Ti surface. This suggests that adsorbed oxygen on the Ti surface can easily diffuse into the subsurface when elevating temperature, although such diffusion of adsorbed oxygen tends to occur on the Si surface when lowering temperature. The difference of adsorbed oxygen behavior between Si and Ti surfaces is discussed in terms of the O@sub 2@ dissociative adsorption kinetics and crystallographic nature of oxide, amorphous SiO@sub 2@ and crystalline TiO@sub 2@.

**SS-TuP25 Stress-induced Transformation between Si(5 5 12)-2x1 and Si(7 7 17)-2x1, S. Cho, J.M. Seo, Chonbuk National University, Korea**

From the reconstructed Si(5 5 12)-2x1, the area of locally-converted Si(7 7 17)-2x1 has been detected by scanning tunneling microscopy(STM). The atomic structure of Si(7 7 17)-2x1 has turned out to be the same as that of Si(5 5 12)-2x1 with missing one of (337) sections, namely D(337) with a dimer-facing-adatom(D/A) row. In this structural transformation from (5 5 12) to (7 7 17), neither the number of atoms nor the dangling-bond number changes, but the surface atoms simply rebond under the external stress originating from the (113) facet parallel to 1-D row. By the distribution of (7 7 17) domain, the direction and size of compressive surface-stress on Si(5 5 12)-2x1 can be deduced, implying that (7 7 17) can be utilized as a stress-indicator of nanometer scale on (5 5 12).

**SS-TuP26 Thermal Stability of Nickel Silicide Layer on Si, Relaxed-SiGe/Si, Strained-Si/relaxed-SiGe/Si Heterostructure, J.H. Ko, C.H. Jang, Sungkyunkwan University, Korea; S.H. Kim, Y.-J. Song, Electronics and Telecommunications Research Institute, Korea; N.-E. Lee, Sungkyunkwan University, Korea**

MOSFET device utilizing a strained-Si channel on relaxed SiGe buffer layer is one of the most promising structure for the next-generation CMOS integration scheme below 50 nm technology node because of its high channel mobilities compared to bulk Si and compatibility with conventional Si CMOS processes. Rapid thermal annealing was performed at 400 °C and then post thermal annealing was performed at of 600~800 °C as following process. Nickel silicide was formed on strained-Si/relaxed-SiGe/Si (001) and relaxed-SiGe/Si (001) and Si (001) using a sacrificial strained-Si layer and its morphological characteristics were investigated. Nickel silicide layers were grown by rapid thermal annealing of the samples with the structure of Ni (10.92 nm)/strained-Si (20 nm)/relaxed-SiGe/Si (001) at the annealing temperature (TA) range of 400~800 °C. And we deposited Ni at each 11nm and 21nm to know what is different. When we deposited 11nm Ni that it's interface roughness very bad but 21nm Ni deposited whose interface roughness improved. The phase formation, surface and interfacial morphologies, and electrical properties of the resulting sample were characterized by various measurement technique, including X-ray diffraction, scanning electron microscopy, cross-sectional transmission electron microscopy and the four-point probe method. As the result when we measured sheet resistance Ni 11 nm on strained-Si/relaxed-SiGe/Si (001) and relaxed-SiGe/Si (001) and Si (001) it were determined to be 9.778, 11.083, 8.464 @ohm@/sq. at 400 °C and it were determined 4.428, 5.453, 4.715 @ohm@/sq. at 400 °C 21 nm. Sheet resistance were determined 160.98, 78.79, 138.633 and 92.397, 65.857, 146.875 @ohm@/sq. at 800 °C 11nm and 800 °C 21 nm, respectively

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**SS-TuP27 Lithium Hydride and Lithium Amide for Hydrogen Storage, J. Engbaek,** Technical University of Denmark, Denmark; **G. Nielsen,** Technical University of Denmark; **I. Chorkendorff,** Technical University of Denmark, Denmark

Hydrogen storage is a serious showstopper for using hydrogen in the transport sector therefore this field has gained renewed interest. Lithium amide has a high hydrogen storage capability; 10.4wt.% hydrogen. In this study surface reactions of thin films of lithium with hydrogen and ammonia is studied under well controlled conditions with pure hydrogen and ammonia in a UHV-chamber. Thin well-characterized Lithium films from sub monolayer to several monolayers were grown on a nickel(111). The films of pure lithium and films reacted with hydrogen and ammonia were characterized with Auger, TPD and LEED. From the LEED patterns we have found that one monolayer of pure lithium form a stable 4x4 reconstructed surface with a coverage of 3 Li atoms to 4 Ni atoms. Lithium hydride was made by exposing a pure lithium film utilizing an atomic hydrogen source. TPD experiments were used to investigate the stability of the lithium / lithium hydride films and surprisingly we have found that lithium evaporate before lithium hydride. Similarly the stability of the lithium hydride / lithium amide was investigated by evaporating Lithium in an atmosphere of ammonia to make thin films of lithium amide. TPD experiments showed that lithium amide decompose at an even higher temperature than lithium hydride and lithium. This significantly complicates the use of lithium amide powder as a hydrogen storage system. The results made under UHV are compared to experiments on ball milled lithium hydride and lithium amide powders.

**SS-TuP28 Photoemission and Secondary Ion Mass Spectrometry Study of Uranium Passivation by Ion Implantation, A.J. Nelson, T.E. Felter, K.J. Wu, C. Evans, J.L. Ferreira, W.J. Siekhaus, W. McLean,** Lawrence Livermore National Laboratory

Implantation of C<sup>+</sup> ions into U<sup>238+</sup> produces a physically and chemically modified surface layer that prevents further air oxidation and corrosion. X-ray photoelectron spectroscopy and secondary ion mass spectrometry were used to investigate the surface chemistry and electronic structure of this C<sup>+</sup> ion implanted polycrystalline uranium compared to an unimplanted region of the sample, both regions exposed to air for more than a year. In addition, scanning electron microscopy was used to examine and compare the surface morphology of the two regions. High-resolution U 4f, O 1s and C 1s core-level and valence band spectra clearly indicate carbide formation in the modified surface layer. The time-of-flight secondary ion mass spectrometry depth profiling results reveal an approximately 200 nm thick UC layer with little or no residual oxidation at the carbide layer/U metal interface and a small amount of oxidation at the surface. This work was performed under the auspices of the U.S. Dept. of Energy by the University of California Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

**SS-TuP29 Surface Chemistry at a LiF-BeF Molten Salt / Beryllium Metal Interface: Probing the Structure and Composition of the Post-Reaction Interface with Microscopy and Electron Spectroscopy, P.J. Pinhero, G.R. Smolik, M.F. Simpson, R.A. Anderl, J.P. Sharpe, D.A. Petti,** Idaho National Laboratory

Molten FLiBe (2LiF:BeF<sub>2</sub>) is a candidate as a cooling and tritium breeding media for future fusion power plants. Neutron interactions with this salt will produce tritium and excess free fluorine ions. Beryllium metal has been demonstrated as an effective REDOX control agent to prevent the free fluorine from reacting with structural metal components. Simply-designed experiments were performed to measure the extent and rate of Be solubility in a FLiBe mixture that was continuously supplied with HF. This paper presents results from post-test examination of the reacted surfaces. This information provides a good link to understanding the reactions taking place at the interface between the molten salt solution and the Be rod. Potential influences of bi-metal exposures, some with direct coupling, e.g., Be to Ni and Be to Fe were examined. The impacts of the bi-metal contacts upon Be dissolution in the FLiBe and potential alloying with the transition metals are examined using scanning electron microscopy (SEM), atomic force microscopy (AFM), scanning Auger microscopy (SAM), and x-ray photoelectron spectroscopy (XPS).

**SS-TuP30 Tuneable Rough Surfaces: A New Approach for Elaboration of Superhydrophobic Films, L.M. Lacroix, M. Lejeune, L. Ceriotti, M. Kormunda, T. Meziani, P. Colpo, F. Rossi,** Joint Research Centre Ispra, European Commission, Italy

The hydrophobic and repelling solid surfaces have found a large utility on our daily lives. The present work describes the process enabling the

production of superhydrophobic surfaces by tailoring their surface topography and chemical properties. These surfaces have been developed using a simple plasma based techniques combining plasma etching and plasma polymerization on silicon substrates. These techniques have been chosen because they provide features such as large area processing and high reproducibility. The key step of this process is the modification of the surface topography of the substrate to create high roughness before deposition of fluorocarbon coating. The roughness on silicon wafer is induced by the over-etching of a photoresist layer by a SF<sub>6</sub> plasma treatment. The different layers obtained exhibit contact angles from 102 up to 180 depending of the preparation conditions. The observations of the topology by scanning electron microscopy reveal that the presence of dendrites on the surface of the substrate favors the superhydrophobicity of the films. The variations of the contact angle have been explained using the Wenzel's or Cassie's models.

**SS-TuP31 Friction Force Microscopy on Monolayer NaCl Films, P. Delage, T. Filleter, S. Maier, R. Bennewitz,** McGill University, Canada

Friction and wear on metal surface can be greatly reduced by solid lubricant layers. We have performed Friction Force Microscopy on a model system, ultra-thin films of NaCl on a Cu(100) substrate, in order to study the microscopic mechanisms of friction in solid lubricant films. The NaCl films were grown by means of molecular evaporation in ultra-high vacuum conditions. Large islands of monolayer films are covered with nanometer-scale rectangular islands forming the subsequent layers. The decay of island density close to the edge of the film suggests a low barrier for NaCl molecules diffusing from the first monolayer to the copper substrate. In regions where the film grows over substrate terraces, island density increases while islands size decreases. Stable friction experiments were possible even on single monolayers of NaCl, and atomic stick-slip processes have been recorded.

**SS-TuP32 Single Asperity Atomic Force Microscope Studies of the Chemical Mechanical Planarization of Silicate Glasses@footnote 1@, F. Stevens, S.C. Langford, J.T. Dickinson,** Washington State University

The Atomic Force Microscope (AFM) is not only an imaging tool, but also can be employed to apply highly localized stresses to a surface. In the presence of liquids, we can investigate a number of tribochemical processes. Here we present the results of fundamental studies of the simultaneous application of chemical agents and mechanical stress to amorphous sodium trisilicate. We show the consequences of combining highly localized mechanical stress (due to contact with the AFM tip) with exposure to aqueous solutions of known pH. This experiment incorporates many features of single-particle/substrate/slurry interactions in Chemical Mechanical Planarization (CMP). Importantly, we show quantitative, correlated data on the wear of both the AFM tip and the glass substrate. The significant modification of the tip during a single wear experiment has profound effects on the rate of material removal from the exposed surface. Such measurements allow us to determine how substrate wear depends on the stress applied by the tip. In addition, the temperature of the solution and substrate can be changed over a limited range. We examine solid surfaces of silicate glasses, inorganic single crystals, and silicon nitride. Quantitative models are presented to account for the observed nanometer-scale surface modification. @FootnoteText@ @footnote 1@This work was supported by the National Science Foundation.

**SS-TuP33 Non Contact Polishing Technique for Metal Foils, C.C. Chang,** Industrial Technology Research Institute, Taiwan, R.O.C., Taiwan; **C.J. Wu,** Industrial Technology Research Institute, Taiwan, R.O.C.

Non-contact polishing technique for surface treatment of metal foils has been studied. This paper presents a successful electropolishing technique to deal with the surface of stainless steel foils. This technique is capable of polishing large area(over 200mm width),ultra thin(below 50µm thick) metal foils to be with electric grade surface(Ra<0.02µm), and potential for mass production. The metal foils with electric grade surface could be used of a substrate of flexible electronic devices.

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