

Thursday Afternoon Poster Sessions

Surface Science

Room: Hall 3 - Session SS-ThP

Surface Science Poster Session

SS-ThP1 Ordered 2-D Structure of Si(337)-4×1 Induced by C Incorporation into Si(5 5 12)-2×1, H. Kim, O. Dugerv, G. Duvvir, H. Li, J.M. Seo, Chonbuk National University, Republic of Korea

Using STM, it has been found that Si(5 5 12)-2×1 composed of tetramer (T) / dimer-adatom (D-A) rows and π -bonded (π) / honeycomb (H) chains [Surf. Sci. **601**, 1831 (2007)] is transformed irreversibly to an ordered (337)-4×1 terrace with (113) facets through adsorbing C₂H₂ at 650°C followed by post-annealing at 750°C. The transformation from (5 5 12) to (337) starts from a T row and a π chain in the (5 5 12) surface, and simultaneously the rest part of (5 5 12) converts to T rows and π chains, which will be transformed to (337). By Si 2p and C 1s core-level photoemission studies using synchrotron radiation, it has been confirmed that such an irreversible structural transformation is due to subsurface C atoms. If the (337) terrace is only composed of T rows and π chains with a 2× periodicity, the compressive stress exists so that the (337) terrace becomes unstable. However, subsurface C atoms release this compressive stress through breaking 1-D structures and change to a stable surface composed of 4×1 dot structures. The detailed atomic structures of the 4×1 surface and the steps of transformation will be presented.

SS-ThP2 Surface Passivation by Sb Adsorption: Sb/Si(114)-2 × 2, O. Dugerv, H. Kim, G. Duvvir, H. Li, J.M. Seo, Chonbuk National University, Republic of Korea

Sb adsorption on the Si(114)-2×1 surface [composed of dimer (D), rebonded-atom (R), tetramer (T) rows] at 600 °C has been investigated by STM and synchrotron photoemission spectroscopy (PES). When the Sb coverage exceeds 0.25 ML, two periods of 2×1 [(D-R-T)-(D-R-T)] is transformed to 2×2 [D-R-D-R-R_{Sb}-D-R_{Sb}, where R_{Sb} means an R row replaced by deposited Sb atoms]. Such a transformation turns out to be nanofaceting to 2×(115) and 2×(113) and is originating from the stress balance between the tensile rebonded D_B-type D(6)-R(5)-D(6)-R(5) rings [Phys. Rev. Lett. **77**, 687 (1996)] and the compressive R_{Sb}(5)-D(7)-R_{Sb}(5) rings [Sur. Sci. **411**, 54 (1998)]. This Sb-adsorbed 2×2 surface has 37.5% less dangling bonds and 0.27 eV less band-bending than the clean surface. It has been found that the addimer adsorbs exclusively on the D(7)-R_{Sb}(5) ring site, which implies that the critical condition for addimer adsorption is the relative angle between dangling bonds of D(7)-R_{Sb}(5) rings.

SS-ThP3 In situ Attenuated Total Reflectance and Transmission Fourier Transform Infrared Spectroscopy of (tetrakis(dimethylamido)hafnium (IV) Decomposition and Adsorption Dynamics on H-Si(100) Surface, K. Li, N. Li, T.M. Klein, The University of Alabama

Low temperature atomic layer deposition (ALD) is favored for more uniform thin film. The authors have investigated the surface reaction mechanism of first step of Hf ALD agent tetrakis(dimethylamido)hafnium (TDMAH) reacting on the H-Si(100) surface for low temperature range 60-250°C by *in situ* ATR-FTIR. The formation H-Hf species was observed in the chemisorbed layer and a gas phase initiated adsorption mechanism was hypothesized by *ab initio* calculation. *In situ* transmission FTIR will be used to monitor the gas phase decomposition dynamics and products of TDMAH. Two most possible reactions: insertion and β -hydride elimination are expected to be observed. Deuterium water prepared background will be used to verify the Hf-H species on H-Si(100). Interfacial bonds of Hf-N and Hf-Si are to be of about 1:1.5 in concentration from thermodynamic calculation. Minor C-Si bond from silylation by product is expected to be observed during desorption. Experimental measurement of decomposition rate will be compared with the *ab initio* kinetic data.

SS-ThP4 Exploring Photomechanically Switching Molecules on Semiconductor Surfaces, J. Cho, L. Berbil-Bautista, N. Levy, D. Poulsen, J.M.J. Fréchet, M.F. Crommie, UC Berkeley

The photomechanical switching behavior of organic molecules changes dramatically when the molecules are placed on a surface. Metal surfaces, for example, often quench or slow photomechanical activity due to strong molecular interaction with continuum electronic degrees of freedom. Semiconductor surfaces are expected to induce very different molecular switching behavior due to the presence of a band gap, potentially resulting in longer excited-state lifetimes and enhanced control of photomechanical properties. We have explored the local structure and self-assembly of photomechanical molecules on the semiconducting GaAs(110) surface

using variable temperature scanning tunneling microscopy. We will report on the nanoscale response of azobenzene derivatives on GaAs to optical irradiation in the UV-vis spectral regime.

SS-ThP5 Photo-induced Reactions of Alanine Adsorbed on Permalloy: A Real Time X-ray Photoelectron Spectroscopy Study, V. Kalyanaraman, R.A. Rosenberg, Argonne National Laboratory, P.J. Ryan, Ames Laboratory, M. Abu Haija, Argonne National Laboratory

Recently it was demonstrated that chiral selective chemistry can be induced by spin-polarized electrons from a magnetic substrate. The C-O bond cleavage rate in adsorbed 2-butanol showed a 10% enhancement depending on the chirality of the molecule and spin polarization of the substrate secondary electrons(1). We have recently extended this research to alanine (CH₃CHNH₂COOH), the simplest chiral amino acid. Our initial work examined the x-ray induced photolysis of alanine adsorbed on a thick Permalloy film by monitoring changes in the C1s and N1s photoelectron spectra as a function of irradiation time. Alanine was shown to adsorb in both zwitterionic (~2/3) and neutral (~1/3) forms on Pd(111)(2). C1s and N1s x-ray photoelectron (XP) spectra of alanine adsorbed on Permalloy at 200 K indicate similar adsorption behavior. Irradiation of the adsorbate with x-ray photons results in changes in both the C1s and N1s XPS data, which we attribute to C-C bond fission at the chiral carbon desorbing CO₂ and/or CO from the COO- moiety, and leaving behind ethylamine and/or HCN. Strong support for this assignment comes from similar intensity variations in the C 1s and N 1s XP spectra from D-alanine on Pd(111) as the substrate temperature was increased above room temperature(2). Future work will be devoted to determining if the observed x-ray induced reaction rates are sensitive to the alanine chirality and the polarization of the secondary electrons from the underlying substrate.

This work was performed at the Advanced Photon Source and was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-06CH11357.

References

- (1) R. A. Rosenberg et al., Phys. Rev. Lett. **101** (2008) 178301.
- (2) Feng Gao et al., Surf. Sci. **601** (2007) 3276.

SS-ThP6 Trajectories and Neutral Fractions of Alkali Ions Scattered from Au(788), R.E. Lake, M.P. Ray, C.E. Sosolik, Clemson University

Stepped metal surfaces are natural systems for studying lateral quantum confinement [1]. Au(788) is a surface vicinal to the (111) plane that reconstructs and forms stable 3.8 nm wide periodic monatomic steps with (111) orientation. Step edges terminate in {111} microfacets. Electron wave functions are confined laterally in a direction perpendicular to the steps and contribute a 1D-like quantum well state to the Au(111) electronic structure. To probe this structure-property relationship we scatter hyperthermal energy alkali ions from the surface and measure the energy and neutral fraction of the scattered ions. By analyzing our data with the classical trajectory simulation SAFARI, ions scattered from the steps can be clearly distinguished from the step edge scattering events. The neutral fraction of scattered alkali ions is sensitive to the electrostatic potential directly above a scattering site and can detect quantum confined states [2]. Measured neutral fractions for different species of alkali ions are interpreted with a model of multi-state resonant charge transfer.

- [1] A. Mugarza, A. Mascaraque, V. Perez-Dieste, V. Repain, S. Rousset, F. J. Garcia de Abajo and J. E. Ortega. Phys. Rev. Lett. **87**, 107601 (2001).
- [2] G. F. Liu, Z. Sroubek and J. A. Yarmoff. Phys. Rev. Lett. **92**, 216801 (2004).

SS-ThP7 Probing Diffusivity in Nanoscale Supercooled Liquid Films using Rare-Gas Atoms, J. Matthiesen, R.S. Smith, B. Kay, Pacific Northwest National Laboratory

Molecular beams, temperature programmed desorption, and infrared spectroscopy were used to study the diffusivity in nanoscale supercooled liquid films of alkanes and alcohols. Amorphous films were grown on top of a layer of rare-gas atoms on a Pt(111) substrate at 25 K in UHV. As the films are heated they transform from amorphous to supercooled liquid films around the glass transition temperature. The rare-gas atoms were found to diffuse through the films in the supercooled liquid state. In a series of experiments, the layer thickness and heating rate were varied to extract diffusivities over a range of different temperatures. Numerical simulations of the rare-gas atoms diffusing through the supercooled films were used to quantitatively model the experimental results. Mixing of initially layered isotopically labeled alcohol and alkane films were also performed. The extracted diffusivities for the rare-gas atoms were in good agreement with the self-diffusion coefficients extracted from the experiments with

isotopically labeled species. The details of the experiment and the interpretation of the results will be discussed in detail.

The research described here was performed in the Environmental Molecular Sciences Laboratory, a national scientific user facility sponsored by the Department of Energy's Office of Biological and Environmental Research and located at Pacific Northwest National Laboratory.

SS-ThP8 Adsorption of Metal Phthalocyanines on Cu(111) and Cu(100): A STM Study. S. Chang, J. Brede, J. Schwöbel, S. Kuck, G. Hoffmann, R. Wiesendanger, University of Hamburg, Germany

The temperature dependent adsorption behavior of 4-fold symmetric metal phthalocyanines (MPcs) on metals with commensurate and incommensurate symmetries was investigated by means of scanning tunneling microscopy. On the 4-fold symmetric Cu(100) surface, planar and 4-fold molecular structures in two equivalent orientations were found for MPcs when prepared at room temperature. In addition, two metastable orientations were identified when prepared at low temperature which can be depopulated upon annealing. MPcs adsorbed on the 6-fold symmetric Cu(111) surface showed a disturbed molecular appearance. The symmetry of molecular structures changed from 4-fold to 2-fold which is discussed in terms of molecule-substrate interaction.

This work was supported by the DFG within the GrK 611 and the SFB 668-A5 and by the European Union in the project "SPiDMe".

SS-ThP9 Iron Phthalocyanine on the Ag(111) Surface: Structure and Electronic States. K.W. Higgs, T. Takami, C.E. Carrizales, Washington State University

Epitaxial growth of iron phthalocyanine on a silver (111) surface has been studied with scanning tunneling microscopy in ultrahigh vacuum. Commensurate two-dimensional ordering with parallelogram unit vectors (**b**₁, **b**₂) where **b**₁ = 5**a**₁ + 2**a**₂ and **b**₂ = 5**a**₂, where **a**₁ and **a**₂ are unit vectors of Ag(111) surface, were observed. The parallelogram structure was more commensurate than those of FePc on Au(111) or graphite and of CuPc on Ag(111), and the surface density is greatest on Ag(111). The orbital mediated tunneling spectra showed a first ionization potential at 5.1 eV, similar to that in cobalt phthalocyanine on Au(111) surface.

SS-ThP10 Adsorption, Self Assembly, and Electronic States of Corrole Molecules Adsorbed on Different Copper Facets. L. Lichtenstein, S. Kuck, G. Hoffmann, R. Wiesendanger, University of Hamburg, Germany

A new member of the metalloporphyrinoid class is the one-carbon short corrole which is a very accessible, easily tunable compound with many potential applications in material science and catalysis. These molecules differ from the parent porphyrin molecules [1] mainly by their lower inherent symmetry and the smaller cavity. In this study using STM we address the conformation (orientation and chirality) and self assembly of iron-triphenylcorrole (FeTPC) molecules on Cu(100) and Cu(111). At low coverage FeTPC molecules show restricted symmetry and can be controllably switched among different conformations [2]. At higher coverage formation of regular aggregates can be observed. We will present the results of the growth study in dependence of surface geometry and coverage and discuss results of scanning tunneling spectroscopy investigations of these systems.

[1] W. Auwärter et al., "Molecular nanoscience and engineering on surfaces", Int J. Nanotechnology Vol. 5, 1171 (2008).

[2] S. Kuck et al., "Naked" Iron-5,10,15-triphenylcorrole on Cu(111): Observation of Chirality on a Surface and Manipulation of Multiple Conformational States by STM, J. Am. Chem. Soc., 130, 14072 (2008).

This work was supported by the DFG within the GrK 611 and the SFB 668-A5 and by the European Union in the project "SPiDMe".

SS-ThP11 One and Two Dimensional Structures of Water on Cu(110) and O/Cu(110)-(2x1) Surface. B.Y. Choi, Y. Shi, M. Salmeron, Lawrence Berkeley National Laboratory

The interaction of water molecules with single crystalline surfaces provides a model for a fundamental understanding of the wetting properties of metals. We investigate one and two dimensional water structures on a clean and on an oxygen precovered Cu(110) surface using scanning tunneling microscopy and non-contact atomic force microscopy. In previous work it has been proposed that at sub-monolayer coverage water forms pentagon based chain-like structure on the clean Cu(110) surface at low temperature. Water pentagons have a strong water-metal interaction as well as a minimal strain in hydrogen bond¹. On an oxygen precovered Cu(110) surface, hexagonal based honeycomb structures are preferred to form along the Cu-O stripes. However, it is not clear whether the hexamers are composed of intact or half-dissociated water molecules². We will discuss how the Cu-O

stripes affect the formation of the honeycomb structures and chains of water pentamers.

¹J. Carrasco et.al Nature Mater. 8, 427 (2009)

²J. Ren et.al Phys. Rev. B 77, 054110 (2008)

SS-ThP12 Evaporation and Sliding of Water Droplets on Hydrophobic Coatings with Nanoscale Roughness. T. Furuta, A. Nakajima, Tokyo Institute of Technology, Japan, M. Sakai, KAST, Japan, T. Isobe, Tokyo Institute of Technology, Japan, Y. Kameshima, Okayama University, Japan, K. Okada, Tokyo Institute of Technology, Japan

Hydrophobic coatings have been used widely to apply for various engineering products. For assessing these properties, static wettability such as the contact angle or sliding angle is not always a useful criterion for materials design. Recently, the recognition of the importance of dynamic wettability such as droplet's sliding velocity or acceleration on a tilted surface has been growing gradually.

Water droplets are known to slide down on the hydrophobic solid surface by a caterpillar-like rolling motion with or without slippage at the solid-liquid boundary; a direct observation method for internal fluidity of sliding water droplets was established recently using particle image velocimetry (PIV). The contribution ratio of rolling and slipping motions to overall sliding acceleration reportedly depends on nanoscale roughness and chemical heterogeneity of the hydrophobic coatings.

On the other hand, evaporation is a fundamental phenomenon for liquids. Various studies have been conducted in relation to this phenomenon for liquid droplets on solid surfaces. Ultra-small, e.g. nanoliter-scale, droplets are evaporated and disappeared in a short time, which corresponds to a situation of large volume change ratio per unit period. It might possess similar dependence against nanoscale surface heterogeneity as well as dynamic wettability.

We prepared fluoroalkylsilane coatings with different nanoscale roughness. This study examined evaporation (including nanoliter-scale droplets) and sliding behaviors of water droplets on these coatings using an automatic microscopic contact angle meter and PIV method.

Evaporation and sliding behaviors of water droplets were investigated on smooth and rough coatings. Evaporation behaviors for these two coatings differed when nanoliter-scale droplets were used, although they were nearly identical for microliter-scale droplets. The droplets on the smooth coating exhibit greater sliding acceleration and a larger slipping velocity ratio than those on the rough coating. Both the evaporation behavior of nanoliter-scale droplets and sliding velocity of microliter-scale droplets were affected by nanoscale surface heterogeneity.

Moreover, considering power balance around the three phase contact area, line tension was measured for microliter-scale and sub-nanoliter-scale droplets of an ionic liquid on a highly smooth and homogeneous fluoroalkylsilane coating. Values for microliter-scale droplets were two orders larger than those for sub-nanoliter-scale droplets despite their identical combinations of solid surfaces and liquid. Scale factors related to this measurement and from the liquid play an important role in the discrepancy.

SS-ThP13 Passivation of Al(111) with Organic and Inorganic Adlayers. T. Yamada, RIKEN, Japan, M. Kawai, The University of Tokyo, Japan

Passivation of clean Al(111) has been attempted against oxidation in O₂ or air at room temperature by various kinds of adlayers prepared on the surface. The goal of this attempt is to block the growth of oxide layer by introducing a covering monolayer or thin multilayer, whose thickness is smaller than 1 nm. Metallic aluminum surfaces stored in air are usually covered with more than a few nm of Al oxide layer, which prevent us from fabrication of nanostructures and nanoparticles of pure metallic Al. If an ultrathin passivation layer, composed of inorganic or organic materials in a controlled manner, can inhibit oxidation of Al substrate, it will help enhancing the accuracy and precision of nano-scale fabrication. This approach was successful in passivating Si wafer surfaces [1]. When a clean Al(111) surface was exposed to pure O₂ gas at room temperature, the surface was covered with an amorphous oxide layer observed by low energy electron diffraction (LEED) and X-ray photoelectron spectroscopy (XPS) [2]. The thickness of oxide layer was calculated from XPS signal intensities, with referring to spectra of a cleaned sapphire (γ -Al₂O₃) surface. The process of oxide accumulation was once saturated below $\sim 10^{-1}$ Torr of O₂ pressure, at which the thickness of oxide layer was <0.5 nm. Formation of such oxide layers was blocked with various kinds of thin adlayers, such as fluoride thin layers, alkanethiol monolayers etc., similarly to the formerly reported C₆₀ layer [3]. At O₂ pressures higher than 10⁻¹ Torr, another sort of rigorous oxidation process took place. The thickness of oxide layer was approximately proportional to the logarithm of O₂ exposure, reaching a few nanometers. Most of the monolayers from small precursor compounds

could not block this process of oxidation. This process seems to involve penetration of O atoms deeply into the Al substrate. Practically, it is desirable to inhibit this rigorous process of oxidation. In this talk, we will present our attempts using monolayers including long linear molecules anchored on Al(111). The oxidation process was examined in the air up to the atmospheric pressure, involving O₂ and H₂O. Some kinds of adlayers on Al(111) were vulnerable in contact with H₂O. It is probably important to involve hydrophobic compounds to build a firm, oxidation-resistant monolayer.

[1] T. Yamada et al., *J. Electroanal. Chem.* **532** (2002) 247, T. Yamada et al., *J. Chem. Phys.* **121** (2004) 10660.

[2] H. Brune et al., *J. Chem. Phys.* **99** (1993) 2128, V. Zhukov et al., *Surf. Sci.* **441** (1999) 251.

[3] A. V. Hamza et al., *Surf. Sci.* **318** (1994) 368.

SS-ThP14 Reduction of Friction Drag by Superhydrophobic / Superhydrophilic Coatings, M. Sakai, Kanagawa Academy of Science and Technology, Japan, A. Nakajima, Tokyo Institute of Technology, Japan Recently, the importance of controlling wettability on the solid surface is recognized in various industries. In the current paper, we evaluated friction drag of water on various surfaces including superhydrophobic / superhydrophilic coatings. The amount of friction drag was evaluated by the decrease of hydrostatic pressure during flowing in the tubes coated by various materials. When Reynolds number is smallest, superhydrophobic coating provides small friction drag. On the other hand, a superhydrophobic coating provided smallest friction drag when Reynolds number is 6000. The mechanism of this difference was discussed from the viewpoints of fluid mechanics and surface materials science.

SS-ThP15 Dynamic Solid-liquid Interaction on Hydrophobic Surfaces, N. Yoshida, The University of Tokyo, Japan, M. Sakai, Kanagawa Academy of Science and Technology, Japan, A. Nakajima, Tokyo Institute of Technology, Japan, T. Watanabe, The University of Tokyo, Japan Dynamic solid-liquid interaction as a liquid droplet-movement on inclined hydrophobic~superhydrophobic surfaces was investigated. The liquid droplet movement was affected by a surface energy, roughness, and homogeneity of the solid surface, and furthermore it is revealed that the internal fluidity detected by Particle Image Velocimetry method changed the movement. On hydrophobic surfaces, the movement simply depended on contact angle if the solid surface had chemically and physically homogeneity. Surface inhomogeneity caused increases of contact angle hysteresis and internal fluidity, and then the droplet movement was observed to be decreased. In this presentation, we will discuss about the detail of relations among them.

SS-ThP16 Surface Reaction of Ozone with Alkali Halide Salts, T. McIntire, J. Taing, University of California, Irvine, P. Ashby, Lawrence Berkeley National Laboratory, R.L. Grimm, A. Margarella, M.H. Cheng, University of California, Irvine, Z. Liu, Lawrence Berkeley National Laboratory, J.C. Hemminger, University of California, Irvine

Heterogeneous reactions involving the oxidation of the halide components of sea-salt aerosols with trace atmospheric gases (e.g., ozone, hydroxyl, and NO_x) have been proposed to be responsible for the release of active halogen species into the gas phase. While such halogen containing species have been observed in the marine boundary layer by field studies, the detailed mechanisms of the heterogeneous reactions leading to halogen release from sea salt aerosols are not well understood. In this work, reactions of gas phase ozone with alkali halide single crystals were studied at varying ozone and water vapor concentrations. Changes in the alkali halide salts were measured using transmission FTIR, x-ray photoelectron spectroscopy (XPS), and atomic force microscopy (AFM). While previous investigations found single crystals of KI oxidize to form a passivating layer of KIO₃ crystallites, the present study notes the loss of reactants with no observed surface-phase oxidized species, AFM experiments show that ozonolysis of KBr single crystals leads to roughening of step edges and the formation of etch pits which appears to depend on the amount of water vapor present. XPS spectra show a decrease in interfacial bromide believed to be concomitant with the etching observed in the AFM studies. Implications for the role of water on the reaction of gases such as ozone with alkali halide single crystals are discussed.

SS-ThP17 Evolution of Microscopic Surface Deformation on Si(111) due to Low Energy Ion Bombardment, P. Piercy, J.M. David, D. Pohl, University of Ottawa, Canada

Low energy ion bombardment of a crystalline solid may cause a variety of surface and subsurface damage. At moderately elevated sample temperatures to prevent amorphization, the sputtering process may leave a step-and-terrace morphology, but surface reconstruction may be disordered

and a distribution of ion-induced defects may remain in a shallow, inhomogeneously strained, subsurface layer. After low energy argon ion bombardment on Si(111), we use a spot profile analysis of low energy electron diffraction data at in-phase conditions to measure a low amplitude, continuous distribution of surface height, which occurs in addition to atomic-height steps and other short-range atomic disorder at the surface. Measurements over a range of ion dose, ion energy, and sample temperature, are attributed to surface deformation due to strain around subsurface defects. For bombardment of the Si(111) surface at 600K by 230 eV argon ions with dose increasing in the range 10¹⁵-10¹⁶ cm⁻², we find a continuous surface height distribution, whose contribution to the interface width increases from hundredths of an Angstrom up to ≈ 0.1 Å, correlated laterally over tens of Angstroms. These results may be interpreted in terms of an elastic continuum model of the solid, with defects created below the surface by independent ion bombardment events modeled simply by a distribution of small inclusions. At a higher surface temperature of 800 K, the surface deformation after the same ion energy and doses as above gives interface width contribution *w* increasing to 0.07 Å; with further bombardment to a dose of 10¹⁷ cm⁻², *w* grows to 0.15 Å. At a higher ion beam energy of 730 eV, *w* increases to a saturation value of 0.18 Å after an argon ion dose of ≈ 2·10¹⁶ cm⁻². Implications for the evolution of the buried defect distribution will be discussed.

SS-ThP18 Ordering Mechanisms of Stripe Arrays on B-doped Si(100), I. Ermanowski, N.C. Bartelt, G. Kellogg, Sandia National Laboratories

We have used low energy electron microscopy (LEEM) to study in real time the self-assembly of periodic stripe arrays on atomically flat Si(100) with high boron doping. Stripes consist of extremely elongated vacancy islands of single atomic height, formed at ~900°C, confined in micrometer-sized pits. We have been able to create highly ordered arrays of straight, parallel stripes (in pits of up to ~8 μm in size) formed by allowing various defects to heal over relatively long periods of time. To allow this equilibration to occur, sublimation was compensated for by an external Si doser, allowing observation of stripe evolution over the course of hours, with no net loss or gain of Si from the area of interest. Equilibrium stripes are very uniform in width and periodicity, and exhibit the greatest stability at 0.5 monolayer coverage. Observed stripe formation and ordering mechanisms include spontaneous nucleation and growth of new stripes, longitudinal splitting, as well as coarsening due to surface diffusion. Stripe periodicity depends on temperature, allowing for control of this property. Stripes form in a temperature range of ~100C, outside of which they assume the familiar shape of elongated islands. Stripe order can be preserved to room temperature by quenching.

Work supported by the U.S. DOE, Office of BES, DMSE. Sandia is operated by Sandia Corporation, a Lockheed Martin Company, for the U.S. DOE's NNSA under Contract No. DE-AC04-94AL85000.

SS-ThP20 Degradation of Semiconductor Photoelectrode Surfaces in Aqueous Environments from *ab-initio* Molecular Dynamics, B. Wood, T. Ogitsu, E. Schwegler, Lawrence Livermore National Laboratory

Among currently known approaches for hydrogen production, catalytic splitting of water molecules using semiconductor-based photoelectrochemical (PEC) devices has garnered particular interest, with reasonably high efficiencies already demonstrated in laboratory conditions. Unfortunately, these materials often evidence extremely facile surface corrosion, severely limiting their practical use in real-world devices. Currently, a clear understanding of this corrosion process at the water-semiconductor interface and its damaging effect on catalytic activity is lacking. Although certain theoretical efforts have attempted to address this issue, these studies have generally focused on zero-temperature gas-phase molecular adsorption, forgoing a realistic model of the liquid-solid interface. Accordingly, we have performed extensive *ab-initio* molecular dynamics simulations to probe the structure, chemistry, and dynamics of the water-electrode interface for model semiconductor systems in a realistic aqueous environment. Our work has focused on InP and GaAs, which, although structurally and functionally similar, exhibit substantial differences in terms of stability in an aqueous environment and in surface reactivity. These calculations are able to provide a unique in-depth understanding of surface

structure and transport. As such, they promise to provide a crucial first step towards understanding the complexities of the atomistic processes involved in hydrogen evolution and PEC corrosion.

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