

## Surface Science

Room 310 - Session SS1-ThM

### Patterned Growth and Etching of Semiconductors

Moderator: A.C. Kummel, University of California, San Diego

8:20am **SS1-ThM1 Self-Assembly of Atomic Chains on Stepped Silicon**, *F.J. Himpsel*, University of Wisconsin, Madison **INVITED**

It is now possible to systematically engineer one-dimensional chain structures of metal atoms on silicon using self-assembly. Stepped Si(111) templates offer the opportunity to vary the chain spacing with atomic precision and to control the electron count, including fractional band filling. Two applications of chain structures are explored: 1. An atomic scale memory is constructed using self-assembled, 5-atom wide tracks that form on Si(111)5x2-Au. Extra Si atoms in lattice sites on top of the tracks are used to store data, one bit per atom with an empty buffer space of 5x4 atoms. The density is comparable to that in DNA (32 atoms/bit). This memory serves as test structure for finding the fundamental limits of data storage density and readout speed. They are given by the correlation between adjacent atoms and the shot noise in STM. 2. One-dimensional electrons in metallic chains are characterized by mapping their band structure and Fermi surface. While metallic surface electrons are completely decoupled from the Si substrate, the metal atoms are locked into Si lattice sites which makes a Peierls transition to an insulator unfavorable. The dimensionality is varied between 1D and 2D via the chain spacing. R. Bennowitz, et al., Atomic scale memory at a silicon surface, *Nanotechnology* 13, 499 (2002). A. Kirakosian, et al., Correlations in a one-dimensional lattice fluid on Si(111)5x2-Au; *Phys. Rev. B*, in press. R. Losio, et al., Band splitting for Si(557)-Au: Is it spin-charge separation?, *Phys. Rev. Lett.* 86, 4632 (2001); K. N. Altmann, et al., Electronic structure of atomic chains on vicinal Si(111)-Au, *Phys. Rev. B* 64, 035406 (2001); J. N. Crain, et al., Fermi Surfaces of Surface States on Si(111) + Ag, Au, *Phys. Rev. B* 66, 205302 (2002); J. N. Crain, et al., Fractional band filling in an atomic chain structure, *Phys. Rev. Lett.*, in press.

9:00am **SS1-ThM3 Length Scale Dependence of Evolution of Corrugations During Sublimation from Patterned Vicinal Si(111) Surfaces\***, *T. Kwon, H.C. Kan, R.J. Phaneuf*, University of Maryland

We describe the results of a combinatorial approach toward controlling the evolution of topography during sublimation from silicon. Arrays of lithographically-patterned cylindrical pits on vicinal Si(111) surfaces interfere with the motion of "straight" steps at temperatures near 1200C. On each substrate, pit diameters are varied from 0.7 microns to 8 microns, with the pit-spacing equal to twice the diameter. Within this range, a critical length scale is found, above which straight steps wrap around pits, leaving a pronounced corrugation within the surface plane, but beneath which the evolution is quickly to straight step bunches, with a pronounced corrugation perpendicular to the surface plane. In the simplest model, this critical length scale is set by the competition between the sublimation induced spreading pressure on the steps and their intrinsic stiffness. Preliminary observations on vicinal Si(111) surfaces also indicate the importance of step-step interactions in the evolution of the topography, with a pronounced inward relaxation of the pit wall on the "uphill" side, and an inward bowing of otherwise straight steps on the "downhill" side. \*Work supported by the Laboratory for Physical Sciences and an NSF-MRSEC.

9:20am **SS1-ThM4 Current-Induced Pattern Formation on Vicinal Surfaces**, *T. Zhao, J.D. Weeks*, University of Maryland

Vicinal surfaces can exhibit a number of different morphological instabilities that may be important in crystal growth and nano-scale device fabrication. Particularly interesting step bunching and step wandering patterns arise from electromigration on Si(111) surfaces; these patterns are observed depend on both the current direction and the temperature. We develop a new two-region diffusion model where adatoms in a small region near a step are assumed have different diffusion rates from those on terraces due to different surface reconstruction or bonding configurations near the step. A linear stability analysis of this theoretical model yields both the bunching behavior and the most unstable wavelength for in-phase wandering. We find good agreement with existing experiments. Moreover, to account for the long time behavior of such surfaces, we use a geometric representation of the interface to derive a nonlinear

evolution equation for a step in the presence of anisotropic diffusion arising from the electric field. The evolution of the step resulting from fields oriented with different angles off the z-axis bears strong resemblance to the experiments. See M. Degawa, K. Thürmer, I. Morishima, H. Minoda, K. Yagi, and E.D. Williams, "Initial stage of in-phase step wandering on Si(111) vicinal surfaces," *Surf. Sci.* 487, 171 (2001). See M. Degawa, H. Minoda, Y. Tanishiro, and K. Yagi, "In-phase step wandering on Si(111) vicinal surfaces: Effect of direct current heating tilted from the step-down direction," *Phys. Rev. B* 63, 045309/1 (2001).

9:40am **SS1-ThM5 Effects of Diffusion and Chemical Reactivity on Step Bunching: The Formation of Macrosteps During Etching**, *S.P. Garcia, H. Bao, M.A. Hines*, Cornell University

The chemical production of macroscopic features on etched silicon surfaces was investigated using scanning tunneling microscopy and atomistic, kinetic Monte Carlo simulations. Macroscopic features arise when atomic steps bunch together into enormous macrosteps with heights on the order of microns. In aqueous silicon etching, step bunching is driven by spatial inhomogeneities in the etchant, as demonstrated by experiments in which diffusive transport is controlled. Under conditions of step-flow etching, inhomogeneities can be enhanced when random fluctuations bring some steps close together. The inhomogeneities can influence the etch rate locally. For example, etchant depletion can lead to local deceleration of step etching, whereas heat released by the etching reaction can lead to local acceleration. This coupling of chemical reactivity to diffusion-controlled processes may cause closely spaced steps to speed up or slow down. To understand how atomic-scale chemical processes and mesoscale diffusion produce step bunching, we have developed a simulation that combines an atomically realistic, two-dimensional model of etching with a continuum model of diffusion. Simulations generated by this technique show that step bunching can give rise to a variety of etch morphologies, all of which are strongly affected by the site specificity of etching and by the effect of diffusion on local reactivity.

10:00am **SS1-ThM6 Equilibrium Morphologies for Cl-roughened Si(100) at 700 - 750 K: Experiments and Monte Carlo Modeling**, *G.J. Xu, K.S. Nakayama, B.R. Trenhaile, C.M. Aldao, J.H. Weaver*, University of Illinois at Urbana-Champaign

Adsorbed halogen atoms on Si(100)-(2x1) can induce roughening at temperatures where material removal (etching) is minimal. Variable temperature scanning tunneling microscopy was used to follow roughening at 700 - 750 K for surfaces with 0.1 - 0.99 ML of Cl. Dimer vacancies and Si adatoms were observed at short times, and at longer times the progression toward a state of dynamic equilibrium was traced. Once dynamic equilibrium was reached, the appearance of individual pits and regrowth islands changed but their densities and mean sizes did not. The results show that the roughness depends non-linearly on Cl coverage with surfaces having 0.3 ML being nearly ten times rougher than those with 0.1 ML. The importance of Cl-free dimers is stressed, and the role of Cl as an impediment for vacancy and adatom diffusion is demonstrated. Roughening is attributed mainly to adsorbate-adsorbate repulsive interactions. Further insight can be gained from Monte Carlo simulations, where the consequences of adsorbate-adsorbate interactions are explored and the resulting morphologies are compared with those experimentally observed. While adsorbate-adsorbate interactions may be the main driving force responsible for roughening, contributions from other interactions cannot be ruled out.

10:20am **SS1-ThM7 Adsorbate Interactions and Roughening of Sub-monolayer Halogenated Si(100) Surfaces**, *D. Chen*, University of North Carolina at Chapel Hill; *J.J. Boland*, Trinity College Dublin, Ireland

Spontaneous roughening of halogen terminated Si(100) surfaces was previously shown to arise from steric repulsions between adsorbates. However, more recent studies have shown that significant roughening occurs even for coverages that are substantially below a monolayer and calls into question the role of steric repulsions. Here, we present a comprehensive study of the roughening process on a sub-monolayer chlorinated Si(100) surface, and in particular its correlation with both the surface coverage and spatial distribution of adsorbates. We find the roughening is due to steric repulsions and this interpretation is supported by DFT calculations. A new model is developed to describe the dependence of roughening on halogen coverage. C.F.Herrmann, D.Chen, J.J.Boland, *Phys. Rev. Lett.* 89, 096102 (2002)

# Thursday Morning, November 6, 2003

10:40am **SS1-ThM8 Atomistic Modeling of Morphological Evolution During Active and Passive Oxidation of Si(100)**, *M.A. Albao, D.-J. Liu*, Iowa State University; *C.H. Choi*, Kyungpook National University, South Korea; *M.S. Gordon, J.W. Evans*, Iowa State University

Prolonged exposure of Si(100) surfaces to oxygen produces: etching at high temperatures (T) characterized by the formation of monolayer-deep elliptical etch pits in successive layers (active oxidation); simultaneous etching and formation of oxide-capped Si-nanoprotrusions at moderate T (transition regime); and coverage of the substrate by an oxide layer at low T (passive oxidation). We develop a simple atomistic model with the goal of describing evolution of the complex far-from-equilibrium surface morphology for a broad range of temperatures across the transition regime. Model development is guided by experimental observations, by general concepts from nucleation theory for the formation of etch pits and oxide islands, and by input from ab-initio quantum chemistry (e.g., indicating different SiO desorption barriers for perfect and defective surfaces).

11:00am **SS1-ThM9 Oxygen Etching of Low- and High-Index Si Surfaces**, *J.L. Skrobiszewski, A.A. Baski*, Virginia Commonwealth University

When Si surfaces are exposed to O@sub 2@ at elevated temperatures, both oxide nucleation and etching can occur, with etching dominating at higher temperatures. We have used scanning tunneling microscopy (STM) to study the transition regime where both processes occur on the low-index (001) and (111) surfaces, as well as on the high-index (5 5 12) and (113) surfaces. All of these surfaces were exposed to O@sub 2@ at sample temperatures of 675 to 750°C, pressures on the low 10@super -7@ Torr scale, and exposures of 5 to 400 Langmuirs. On the low-index surfaces, the surface morphology can be significantly disrupted in this transition regime by etch pits, as well as monoatomic height islands caused by etching around oxide-induced pinning sites. The original terrace-plus-step morphology is only maintained for temperatures above 750°C, where only step-flow etching occurs. For the transition regime on the high-index Si(5 5 12) surface, no etch pits are found on the terraces, but three-dimensional pyramidal or linear islands are observed on terraces and along step edges. These islands presumably form at oxide nucleation sites and grow in size as the surrounding surface is etched away. Interestingly, both the pyramidal and linear islands incorporate (113) facet planes, indicating an enhanced stability of this orientation against etching. When the Si(113) surface is exposed to O@sub 2@ under similar conditions, the resulting morphology also shows no etch pits and incorporates 3D islands, but without any well-defined facet planes. The etching behavior of the high-index surfaces in the transition regime is therefore qualitatively different from that observed for the low-index planes.

11:20am **SS1-ThM10 Growth of Gd on the High-Index Si(113) and Si(5 5 12) Surfaces**, *E. Morris, J.W. Dickinson, A.A. Baski*, Virginia Commonwealth University

The growth of rare earth metals on the low-index Si(001) surface has been of recent interest due to the appearance of silicide "nanowires."@footnote 1@ This nanowire formation is presumably due to a close lattice match between the rare earth silicide and Si lattice along the [1bar10] row direction, and poor match perpendicular to it. In this study, we have used scanning tunneling microscopy (STM) to examine the growth of the rare earth metal Gd on two high-index Si surfaces: Si(113) and Si(5 5 12). These two surfaces are oriented 25.2° and 30.5° down from (001) towards (111), respectively. When very low coverages of Gd are deposited onto these surfaces and annealed at 600°C, (113) terraces with a well-ordered 2x2 reconstruction are formed. In the case of Si(5 5 12), the reconstructed (113) terraces are opposed by other facet orientations. When the coverage is increased to approximately 0.5 ML, isolated nanowires nucleate at step edges and extend along the [1bar10] direction. These nanowires are 5 to 15 nm wide, 1 to 2 nm tall, and grow up to 0.5 micron in length. Because the lattice periodicity along the nanowire direction is identical for the (001), (113), and (5 5 12) surfaces, the appearance of such nanowires on the high-index surfaces provides further evidence for a lattice mismatch mechanism. Interestingly, the anisotropic structure of these high-index surfaces results in nanowire growth that causes fewer disruptions to the initial step morphology than observed for (001). @FootnoteText@ @footnote 1@ C. Ohbuchi, J. Nogami, Phys. Rev. B 66, 165323 (2002) and references therein.

11:40am **SS1-ThM11 Attempts on Synthesizing Linear Atomic Metal Chains on GaN(0001)**, *C. Lung, C. Chang*, National Taiwan University, R.O.C. The continuing advances in miniaturization of semiconductor devices have seriously challenged the fields of materials processing and circuit designs.

This work explores the chemical reaction involved in the possible formation of nanowires using a pyridylamino chelate that contains a linear atomic chain of chromium for CVD. The adsorption, surface reaction, and thermal pyrolysis of this metal string chelate on GaN(0001) were characterized using synchrotron radiation-induced core-level photoelectron spectroscopy, secondary ion mass spectrometry, and temperature-programmed desorption. Secondary ion mass spectrometric studies showed that pyridylamino trinuclear chromium complex may react with the GaN(0001) surface to produce pyridine and pyridylamino fragments even at a very low substrate temperature of less than 150 K. Upon increasing exposure of the trinuclear chromium metal-chain complex on GaN(0001), the Cr3p photoelectron profile altered substantially, revealing an evolution in bonding configuration of the chromium metal-chain chelate on the surface. At low exposures, the Cr3p profile contained three features, peaked at different binding energies, of equal areas. The number of distinguishable features in the Cr3p spectrum increased to five as the chelate coverage on GaN(0001) was increased to more than one monolayer. Increasing the substrate temperature not only caused a change of the bonding geometry of the chromium string on the surface but also induced decomposition of the chromium chelate in two different stages. Desorption of the dipyridylamino ligand took place at a substrate temperature of 340 K, while disruption of the chromium string occurred at about 540 K. Results of this work point to the possibility of forming chromium nanospecies on the semiconductor surface through vacuum chemical deposition using organometallic metal strings. The fundamental aspects and the formation of nanowires involved in the nano-contact technology will be discussed.

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