

Surface Science

Room: 208 - Session SS1+NC-WeM

Surface Structure and Morphology

Moderator: A.A. Baski, Virginia Commonwealth University

8:00am **SS1+NC-WeM1 Short vs. Long-Range Interactions: Consequences of Distributions**, *T.L. Einstein*, University of Maryland, A. Pimpinelli, University Blaise-Pascal, France and University of Maryland, K. Kim, A. BHadj Hamouda, R. Sathiyarayanan, University of Maryland

In computing terrace-width distributions on vicinal surfaces, one commonly assumes a long-range repulsion between steps as the inverse square of the step separation. In many cases there may be a different short-range interaction, or the steps might be able to locally form double-height steps (inconsistent with the fermion analogy). We show that such effects can alter the apparent strength of the interaction, leading to flawed predictions of the strength of the long-range elastic repulsion while still offering a good fit by the generalized Wigner distribution. Since these are finite-size effects, we show how to deal with this problem by measuring several misorientation angles of the vicinal surface. More generally, the range of the interaction affects the form of the distribution in a remarkable way; we discuss the limiting forms and the crossover between them. We apply these ideas to other surface phenomena, such as the distribution of capture zones in island growth. Work at UMD supported by the MRSEC, NSF Grant DMR 05-20471. Visits to UMD by AP supported by a CNRS Travel Grant.

8:20am **SS1+NC-WeM2 Studies of Plasma Nitridation of Ge(100) by Scanning Tunneling Microscopy**, *J.S. Lee, E. Chagarov, A.C. Kummel*, University of California, San Diego

Several recent reports on Ge MOSFET have shown the benefit of having either GeON or GeN interfacial layer between Ge and the high-k gate oxide. We have performed scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) experiments to understand the bonding and electronic structure for Ge-O and Ge-N surface species. For Ge-O, a Ge(100) surface was exposed to O₂ and annealed to form order structures. The O₂ dosing pins the Fermi level at high local coverage. Formation of Ge-N adsorbates is more challenging since N₂ nor NH₃ readily dissociate on clean Ge(100). We performed the direct nitridation on Ge(100) using an electron cyclotron resonance plasma source, and investigated the submonolayer structures of the surface using STM. The nitrided surface was annealed between 200°C and 500°C to differentiate the various adsorbate sites. By annealing the surface above the oxygen desorption temperature but below the nitrogen desorption temperature, our preliminary data is consistent with our being able to prepare Ge-N adsorbates. We are also performing STM experiments and DFT calculation to determine the electronic structure of the Ge-N adsorbates and explain why they might be superior interfacial passivants compared to pure GeO₂.

8:40am **SS1+NC-WeM3 Atom-Wide Co Wires on Vicinal Cu(111)**, *N. Zaki, D.V. Potapenko, R.M. Osgood, P.D. Johnson*, Brookhaven National Laboratory

Due to stronger electron-electron interactions, 1-D systems are predicted and, in some cases, have been shown to exhibit unique and exotic electronic physical properties, such as spin-charge separation, spin-splitting in a nonmagnetic metal,^{1,2} and fractional-charge phase solitons.³ One route to the formation of 1-D systems is by self-assembly using low-index vicinal crystal surfaces. In this regard, we have successfully formed 1-atom wide Co wires using Cu(775), a 7-atom wide stepped array with (111) terraces. Contrary to a recently reported DFT prediction, the Co wires are not laterally encapsulated but are positioned exactly at the step edge. Furthermore, the wires can be relatively long; in one case, a wire measured 160 Co atoms. We will present STM studies of this system performed at room temperature and under UHV. While vicinal Cu(111) does exhibit "frizz" at the steps when scanning above cryogenic temperatures, the Co wires pin the edges, visually accentuating their presence under STM. Furthermore, we observe a lower density of states for the Co wires as compared with the Cu steps, which also serves to differentiate the two metals. Cu(111) possess a surface projected bandgap which may electronically decouple the wire electrons that reside in this gap. Correspondingly, STS measurements of these atom-wide wires will be discussed.

¹D. Sanchez-Portal, S. Riikonen, and R. M. Martin, PRL 93, 146803 (2004)

²I. Barke, Fan Zheng, T. K. Rugheimer, and F. J. Himpsel, PRL 97 226405 (2006)

³P.C. Snijders, S. Rogge, and H. H. Weitering, PRL 96, 076801 (2006)

9:00am **SS1+NC-WeM4 Surface Self-Diffusion and Structural Evolution of Pd/Cu(100) Surface Alloys**, *E. Bussmann, I. Ermanoski, G.L. Kellogg*, Sandia National Laboratories

Ultra-thin films of Pd on Cu(001) are of interest both as model systems for metal-metal surface alloy formation and as potential electromigration inhibitors for Cu interconnect applications.¹ To determine how alloyed Pd, residing in the atomic layer below the surface, affects Cu surface self-diffusion, we are using low energy electron microscopy (LEEM) to study the decay of 2-D Cu islands as a function of temperature and second-layer Pd concentration. These studies are enabled by previous investigations, in which the distribution of Pd in the top three Cu layers was determined from multiple-scattering-theory fits to LEEM-IV spectra.² Here, we use LEEM-IV spectra in a "fingerprinting" mode to monitor the Pd concentration during deposition and island decay. Measurements of the decay rates as a function of temperature show that the activation energy for island decay increases from 0.82±0.04 eV to 1.02±0.07 eV when 0.06±0.03 ML of Pd is alloyed into the second layer. As the Pd concentration is further increased, up to 0.5 ML, we observe a monotonic decrease in the island decay rates at temperatures less than 240°C. These measurements confirm that Pd, alloyed into the second layer, slows Cu surface transport and suggests a mechanism by which Pd could reduce the detrimental effects of electromigration. A full Arrhenius analysis was not possible at higher Pd concentrations because a significant fraction of the Pd is lost from the second layer during the measurements. We are currently using LEEM to investigate the mechanism of this Pd dissolution, which appears to involve Pd diffusion into the bulk and Cu diffusion to the surface. 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.

¹C. K. Hu, et al., Appl. Phys. Lett. 81, 1782 (2002).

²J. B. Hannon, J. Sun, K. Pohl, and G. L. Kellogg. Phys. Rev. Lett. 96, 246103 (2006).

9:20am **SS1+NC-WeM5 Additive-Enhanced Mass Transport on Metal Surfaces: Hunting Elusive Agents of Change**, *P.A. Thiel, M. Shen, C.J. Jenks, J. Evans, D.-J. Liu*, Iowa State University **INVITED**

Sulfur is well known to enhance dynamic rearrangements of single-crystal metal surfaces for the coinage metals (Ag, Cu, and Au). It has been proposed that the associated enhanced surface mass transport of metal is due to the formation and diffusion of stable metal-sulfur clusters or complexes. From scanning tunneling microscopy (STM) images of a Ag(111) surface with adsorbed sulfur below room temperature, we have been able to "see" clusters that probably contribute to enhanced transport. We propose that the imaged clusters are Ag₃S₂.¹ Our ability to see these trimeric clusters derives from the feature that they self-organize into a distinctive dot-row structure. The dot-rows are very robust, in the sense that they exist over a coverage range that spans an order of magnitude (0.03 to 0.5 monolayers). The dots are assigned as Ag₃S₂ clusters, based on DFT calculations of their energetic stability, on the calculated and measured dimensions of the dots in STM, and on experimental evidence that they incorporate Ag. We have also explored the effect of S on Ag surface dynamics by measuring the stability of Ag adatom islands produced by vapor deposition and subsequently exposed to S. By varying both surface temperature and S-coverage, we identify three regimes: At high S-coverage where a dense row-dot structure forms, the Ag islands are stable or "frozen" over long periods of time. At intermediate coverage, S serves to destabilize the Ag islands. At very low coverage (0.01 monolayer), S has no effect because it passively decorates step and island edges. Thus, S is not universally effective in accelerating mass transport, but rather exhibits complex dependencies upon temperature and coverage.

¹M. Shen, D.-J. Liu, C.J. Jenks, and P.A. Thiel, J. Phys. Chem. C, 112, in press (2008).

10:40am **SS1+NC-WeM9 Growth and Evolution of Au/Ge(111) Studied by LEEM and STM**, *J. Giacomo, S. Chiang, C. Mullet, A.M. Durand*, University of California Davis

The clean Ge(111) surface has a c(2x8) reconstruction at room temperature. Au growth on Ge(111) above 300°C occurs via nucleation. The first layer is an epitaxial ($\sqrt{3}\times\sqrt{3}$)R30° phase with a coverage of 1ML. Further Au coverage results in the formation of islands. When heated to about 620°C, the ($\sqrt{3}\times\sqrt{3}$)R30° Au transitions to a disordered phase. In LEEM videos, we observed domains fluctuating between the ordered and disordered phases at the transition temperature. For 2 to 10 ML of Au coverage, we have observed three dimensional islands in the LEEM images, as expected for the Stranski-Krastanov growth mode. Surprisingly, the LEEM movies show concerted hopping of islands of approximately 100 nm diameter near 300°C. Preliminary data measured by STM show additional evidence for the Stranski-Krastanov mode.

11:00am **SS1+NC-WeM10 Si Adatoms Atop the Si(111)5x2-Au Surface Diffuse in One Dimension by a Defect-Mediated Hopover Process**, *E. Bussmann*, Sandia National Laboratories, *S. Bockenhauer*, Stanford University, *F.J. Himpsel*, University of Wisconsin-Madison, *B.S. Swartzentruber*, Sandia National Laboratories

The Si(111)5x2-Au surface has provided new understanding of the properties of one-dimensional electronic states.¹ The reconstruction includes an overlayer of Si adatoms which partly determine the surface electronic properties.² The chainlike surface structure naturally confines the adatoms to tracks, similar to bits in existing digital media, and previous workers have used the individual adatoms as bits in a model atom-scale memory.³ We have characterized the thermal 1-d diffusion of the adatoms by scanning tunneling microscopy. The statistics of motion are inconsistent with diffusion by a random walk. Instead, correlations between sequential adatom jumps in both direction and time imply that the diffusion is defect-mediated. We show that the unique character of the statistics of the diffusion is consistent with a model in which each adatom diffuses by hopping over a defect localized nearby. Specifically, the measured (nonbinomial) jump length distribution, the (nonexponential) wait-time distribution, and the observed correlations are all modeled accurately over a range of temperatures (145-215° C) using a Monte Carlo implementation of our model. The effective activation barrier for adatom diffusion is found to be 1.24 ± 0.08 eV. Intuitively, defect-mediated hopover diffusion is unexpected in a strictly 1-d system, because sequential diffusion events arising from adatom jumps back-and-forth over the defect are always in opposite directions leading to zero net displacement. 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.

¹ I. Barke, R. Bennowitz, J. N. Crain, S. C. Erwin, A. Kirakosian, J. L. McChesney, and F. J. Himpsel, *Solid State Comm.* 142, 617-626 (2007).

² H. S. Yoon, S. J. Park, J. E. Lee, C. N. Whang, and I.-W. Lyo, *Phys. Rev. Lett.* 92, 0986801 (2004).

³ R. Bennowitz, J. N. Crain, A. Kirakosian, J.-L. Lin, J. L. McChesney, D. Y. Petrovykh, and F. J. Himpsel, *Nanotechnology* 13, 499-502 (2002).

11:20am **SS1+NC-WeM11 Influence of Si Deposition on the Phase Transition Temperature of Si(111)-7x7**, *I.A. El-Kholy*, *H. Elsayed-Ali*, Old Dominion University

Reflection high-energy electron diffraction (RHEED) during the Si(111)-(1x1)_h to (7x7) phase transition shows that Si deposition lowers the transition temperature. A Ti-sapphire laser (100 fs, 800 nm, 1 kHz) was used to ablate a Si target on Si(111)-(1x1)_h during quenching from high temperature. To measure the transition temperature during quenching with and without Si deposition, the experiment was performed as follows: Initially, in the absence of the laser ablation plume, the Si(111) was kept at a temperature above the phase transition temperature to ensure the uniformity of the temperature throughout the surface area of the sample. The heating current was switched off and the RHEED pattern was recorded. Then, in the presence of Si laser ablation plume, the sample was kept at the same high temperature as was done without an ablation plume. The RHEED intensity was observed as the substrate was exposed to the Si plume and the Si(111) substrate was quenched at a rate of ~40°C/s. The RHEED patterns when the Si plume was present showed a shift in the transition temperature from 840°C without the plume to 820°C with the plume. We interpret this result based on the effect of adatom mobility on the nucleation of the (7x7) structure. In the vicinity of the transition temperature, the two phases coexist on the surface. When the surface temperature is lowered below the transition temperature, the reconstruction starts to grow at the step edges then expand across the terraces. Since the high temperature (1x1)_h phase has higher density than the (7x7), the excess atoms, found on large terraces after quenching, are released when the lower density (7x7) is formed. The quenching process results in the cooling of the surface at a lower rate than the time needed for adatoms to diffuse across the terraces; consequently the adatoms are trapped on the surface forming secondary (7x7) nuclei on terraces, thus reducing the observed (1x1)_h to (7x7) transition temperature.

11:40am **SS1+NC-WeM12 Vanadium Adsorption on Si(111)-7x7 Surface: A Combined DFT and STM Investigation**, *F. Stavale*, Nat'l Inst. of Metrology & Federal U. of Rio de Janeiro, Brazil, *M.M. de Araújo*, Nat'l Inst. of Metrology, Brazil, *A.A. Leitão*, Nat'l Inst. of Metrology & Federal U. of Juiz de Fora, Brazil, *R.B. Capaz*, Nat'l Inst. of Metrology & Federal U. of Rio de Janeiro, Brazil, *H. Niehus*, Nat'l Inst. of Metrology & Humboldt-U. zu Berlin, Germany, *C.A. Achete*, Nat'l Inst. of Metrology & Federal U. of Rio de Janeiro, Brazil

The development of superlattices of nanodots and nanomagnetism, metals on Si substrates are of great scientific and technological importance. Consequently metal deposition on Si(111) 7x7 has been studied intensively by the surface science community. The surface diffusion energies and diffusion pathways of the adsorbates are important subjects to understand the growth mechanism of nanostructures. In this sense the scanning tunneling microscopy (STM) appeared to be a powerful technique for the

study of adatom diffusion on the Si(111) 7x7 surface. In general the transition metals expose a high reactivity usually due to the formation of silicide nanostructures. Although several reports on V-Si(111)-7x7 surface system are already available a detailed and complete study of the vanadium from the very beginning adsorption stages up to high coverage cluster and island coalescence on the Si(111)-7x7 substrate has not been yet performed. In this work, we report about an investigation from the low-coverage regime up to few monolayers of vanadium deposition on Si(111)-7x7 in the range of 100K up to 850K substrate temperature. A combination of STM, density-functional theory (DFT) adsorption energy calculations and simulated STM images has been applied. In the low coverage and temperature regime we identify the most common STM signatures in this system to be: (1) substitutional vanadium atoms at silicon adatom positions and (2) interstitial vanadium atoms between silicon adatoms and rest atoms. At higher temperatures the diffusion of adatoms and clusters promote cluster coalescence into specifically shaped nanoclusters which occupy very special unit cell positions of the substrate. Such clusters are composed by vanadium and silicon atoms into an initial silicide formation. Finally, at high coverage, depending on the initial vanadium coverage and the post-annealing temperature well shaped (faceted) VSi₂ clusters are formed. In conclusion a model for the adsorption, diffusion and reaction of vanadium on the Si(111)-7x7 surface is proposed.

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