Surface Science Division
Room 604 - Session SS3+NS-WeA
Islands, Clusters, and Steps

Moderator: J.C. Hamilton, Sandia National Laboratories

2:20pm **SS3+NS-WeA2 The Phase Diagram of a Self-Organizing Nano-Array*, K. Pohl*,** *J. de la Figuera, M.C. Bartelt, N.C. Bartelt,* Sandia National Laboratories*; J. Hrbek,* Brookhaven National Laboratory*; R.Q. Hwang,* Sandia National Laboratories

Recent experiments show that in a submonolayer silver film on Ru(0001), a perfectly ordered array of nanometer-sized vacancy islands forms upon exposure to sulfur. By measuring the thermal vibrations of this equilibrium structure the forces responsible for the observed self-organization were identified and the elastic constants of the lattice derived.@footnote 1@ In order to develop a better understanding of the formation and ordering processes of this structure, we have explored the complete phase diagram of the vacancy island lattice. Via scanning tunneling microscopy we follow in real time the assembly of the hole lattice at different temperatures and S-Ag coverages. We find the hole lattice to be very robust against annealing cycles to 500 K. The final periodicity of the vacancy island lattice seems to be independent of the periodicity of the initial dislocation network in the strained silver film. This network only determines the initial etching sites for the S adatoms. The periodicity of the dislocation network in the clean Ag film depends on the Ag coverage. Beyond a threshold S-coverage, the array undergoes a phase transition to a periodic array of stripes. We will present a detailed study of the stability of these various novel equilibrium phases and identify the driving forces behind their formation. This work is supported by the Office of Basic Energy Sciences Division of Materials Sciences of the U.S. DOE (DE-AC04-94AL85000). @FootnoteText@ @footnote 1@K. Pohl et al., Nature 397, 238 (1999)

2:40pm **SS3+NS-WeA3 Tunneling on Ag and Au: Surface State Spectroscopy and Magic Molecular Clusters*, R. Berndt,*** RWTH Aachen, Germany **INVITED**

We use low-temperature scanning tunneling microscopy (STM) to investigate geometric and electronic properties of nanoscale structures. In this presentation, we discuss various aspects of the Ag(111) surface state such as surface state confinement to nanometer-sized islands, its interaction with isolated magnetic impurity atoms, and the first study of lifetimes effects on Shockley surface state electrons using low-temperature STM spectroscopy. Moreover, we report on observations of two-dimensional supramolecular clusters and chains which self-assemble upon deposition of 1-nitronaphthalene (NN) onto Au(111). NN molecules become 2D-chiral upon adsorption. Their handedness is determined from from high-resolution STM images and local density calculations. Modeling shows that hydrogen bonds cause the observed self-assembly. Clusters and chains mutually interact via electrostatic repulsion.

3:20pm **SS3+NS-WeA5 Step Energetics of Pb(111) Vicinal Surfaces from Facet Shape*, H.P. Bonzel,*** *K. Arenhold, A. Emundts, S. Surnev,* Forschungszentrum Jülich, Germany*; P. Wynblatt,* Carnegie Mellon University

The formation energies of steps and kinks, the step stiffness and the step interaction energy of B-steps vicinal to (111) have been derived quantitatively from the equilibrium shape of small three-dimensional Pb crystallites supported on a Ru(001) surface. The crystallites were imaged by scanning tunneling microscopy and show (111) and (100) facets.@footnote 1@,@footnote 2@ The boundary of these facets is well defined in the STM images and was used to determine also the azimuthal dependence of the step free energy for vicinal (111) surfaces by employing an "inverse" Wulff construction. Taking the accepted value for the surface free energy of Pb, absolute step energetic quantities can be quoted for both A- and B-steps. The step stiffness is derived from the step curvature and the step energy. The entropic step interaction energy of B-steps at 440 K is calculated from the step stiffness. Furthermore, by taking into account the curved portion of the vicinal (111) surface normal to the direction of B-steps, which shows a Prokovsky-Talapov behavior,@footnote 2@ the total step interaction energy of B-steps is also obtained. The entropic and total step interaction energies of B-steps at 440 K are thus 2.3 meV/Å@super2@ and 7.9 meV/Å@super2@, respectively.@footnote 3@ The difference is largely attributed to the elastic dipole-dipole interaction. Calculations of the step and elastic step interaction energies using the embedded atom potential of Pb@footnote 4@ are currently underway and will be compared with the experimental data. @FootnoteText@ @footnote 1@ S. Surnev et al., J. Vac. Sci. Technol. A 16(1998)1059. @footnote 2@ K. Arenhold et al., Surf. Sci. 417(1998)L1160. @footnote 3@ K. Arenhold et al., Surf. Sci. 424(1999)271. @footnote 4@ H.S. Lim, C.K. Ong, F. Ercolessi, Surf. Sci. 269/270(1992)1109.

3:40pm **SS3+NS-WeA6 Control of Monolayer Island Vacancies on Pt(111) and their Impact on Surface Chemistry*, K. Nafisi,*** *J. Samu, J.C. Hemminger,* University of California, Irvine

Michely and Comsa@footnote 1@ have demonstrated that argon ion sputtering Pt(111) at elevated temperature will create ordered monolayer deep island vacancies. We show, by varying the surface temperature parameter, that it is possible to control the size of these vacancies over the range of 30Å to 400Å. We have used a variable temperature, scanning tunneling microscope (STM) to quantify the formation of the island vacancies. We have also used the STM to investigate the dehydrogenation of a series of mono-olefins to form carbon particles at 700 K. The carbon particles were formed both on a clean, annealed, and on sputtered Pt(111) surfaces. The carbon particles are randomly distributed over the surface, and show no preference for formation at particular surface features such as step edges. Also, the formation of the carbon particles is not influenced by large monolayer island vacancies. However, on a surface, where smaller island vacancies have been formed, the carbon particles show a preference of forming on the terraces and not inside of the island vacancies. The difference in behavior between large vacancy islands and small vacancy islands (d @<=@ 40Å) can be explained if molecular diffusion across steps is slow and dehydrogenation products initially decorate the walls (steps) of the vacancy islands. We have also studied the impact of sputtering the sample prior to olefin adsorption with the incident ion beam at an angle away from the surface normal. The carbon particles formed on such surfaces are highly spatially aligned. @super *@This work was supported by the US Department of Energy, Office of Basic Energy Sciences. @FootnoteText@ @footnote 1@ T. Michely and G. Comsa, Nucl. Instr. and Meth., B82, 207 (1993).

4:00pm **SS3+NS-WeA7 Coalescence Dynamics of Small Pt Clusters on Pt(111) Surfaces: A Molecular Dynamics Study*, V. Chirita,*** *E.P. Münger, L. Hultman,* Linköping University, Sweden*; J.E. Greene,* University of Illinois, Champaign-Urbana

The diffusion and coalescence of small clusters are fundamental intralayer mass transport processes, playing a crucial role during the early stages of thin film deposition and crystal growth. We use embedded-atom method molecular dynamics simulations to follow the kinetics characterizing these processes for compact, 2D Pt@sub 5@ and Pt@sub 6@ clusters on Pt(111), at 1000 K. Investigations are carried out for configurations consisting of clusters initially separated by a distance equal to that between second neighbors, in statistically independent runs of 10 ns each. Prior to coalescence, we observe that the intercluster separation distance is reduced via two pathways: net cluster diffusion, involving mechanisms which preserve cluster shape, and repeated cluster reshaping. Cluster diffusion occurs primarily via concerted gliding and reptation, a recently proposed diffusion mechanism for 2D clusters on (111) metallic surfaces. Cluster reshaping involves edge-diffusion and/or concerted dimer/trimer gliding. Our simulations reveal that cluster coalescence is achieved via complex dynamics. Clusters preserving their initial compact shape can coalesce via concerted gliding and form clusters with a high number of intracluster bonds. These larger clusters maximize the number of intracluster bonds in relatively short times, primarily via edge-diffusion. We observe for the first time, that during the fusion process, cluster-cluster interactions can induce cluster translations via sequential atom motion, through fcc/hcp bridge sites, within clusters. For clusters that reshape prior to coalescence, we observe that cluster-cluster interactions induce the transfer of single atoms, from either cluster, to sites neighboring both clusters, and thus create a "bond" between clusters. Once formed, we did not observe dissociation. In this case, the newly formed clusters have elongated shapes with narrow middle sections (1 to 2 atoms thick) and, as a result, the transition toward compactness is achieved over considerably longer times. Moreover, these clusters exhibit a variety of reconfiguration and migration events. Edge-diffusion, reptation and dislocation propagation are the competing diffusion mechanisms observed for clusters in this range.

4:40pm **SS3+NS-WeA9 Spontaneous Island Formation on the GaAs(001) 2x4 Reconstructed Surface***, **P.M. Thibado**, V.P. LaBella, M. Anser, Z. Ding, D.W. Bullock,* University of Arkansas

Given the growing use of III-V semiconductor materials in wireless and high speed communication devices the preparation of atomically flat single crystal GaAs(001) surfaces was examined, since these devices are primarily fabricated using epitaxial methods . To achieve this, a state of the art molecular beam epitaxy (MBE) system with a novel temperature measurement system accurate to within ±2 @super o@C, has been combined, in situ, with a scanning tunneling microscope (STM). Surprisingly, when the GaAs(001) 2x4 reconstructed surface is annealed above a critical temperature (570 @super o@C), under a constant As@sub 4@ flux, it spontaneously forms one monolayer high islands covering one half of the otherwise flat terraces. This process is reversible and when fit to a free energy model yields information about the surface bonding energies. This work was funded in part by the National Science Foundation (DMR-9733994) and the Office of Naval Research (N00014-97-1-1058).

5:00pm **SS3+NS-WeA10 TiN(001) Epitaxy: An in-situ Temperature-Dependent STM and Level-Set Modeling Study***, S. Kodambaka, **P. Desjardins**, A. Vailionis, I. Petrov, J.E. Greene,* University of Illinois, Urbana*; D. Chopp,* Northwestern University

We have used in-situ temperature-dependent STM measurements during deposition and post-annealing combined with modeling to provide atomic-scale insights into surface morphological evolution during TiN growth. Epitaxial TiN(001) layers were grown by reactive evaporation onto MgO(001) at 700-950 @super o@C. Partial TiN monolayers (0.1-0.4 ML) were then deposited and in-situ high-temperature STM used to follow the coarsening and decay kinetics of single and multiple islands (Ostwald ripening) on flat terraces and in single-atom deep vacancy terraces. From these results, combined with finite-element solutions of the Gibbs-Thompson and diffusion equations, we obtain the activation energy for surface diffusion, the Ehrlich barrier energy, and the island line tension. We have also derived and implemented a level-set method for simulating the dynamics of island decay on time scales not accessible to experiment. Level-set methods are numerical techniques for computing the position of propagating fronts that can easily handle topographical changes as well as singularities including corner and cusp development. Our model includes geometry-dependent surface and edge diffusion, step-edge dynamics, and attachment/detachment rates. We compare our numerical results to in-situ STM time-sequence experiments under the same conditions. The results of the level-set calculations serve as a basis for a robust quantitative and predictive model for both microstructural and surface morphological evolution as a function of deposition conditions during polycrystalline TiN growth.

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