Wednesday Morning, October 27, 1999

Surface Science Division
Room 606 - Session SS1-WeM

Surface Structure
Moderator: J. Hinch, Rutgers University

8:20am **SS1-WeM1 Temporal Diffraction: A New Method for Studying Surface Kinetics*, E.H. Conrad,*** The Georgia Institute of Technology **INVITED**

An understanding of surface kinetics is crucial to many areas of 2D and 3D film growth. A variety of techniques are currently available to extract surface kinetics parameters such as diffusion coefficients, atom attachment rates to islands and steps, etc. Most of these techniques, however, are limited to low coverages (i.e., single atom kinetics) and a limited temperature range (usually far from equilibrium). We have been developing a new technique, Temporal LEED Spectroscopy (TLS), that should be applicable over a much larger range of temperatures and up to densities where hydrodynamic diffusion equations are applicable.@footnote 1@ This technique uses the inherent intensity fluctuations, @delta@I(t) = I(q,t)-*, in a surface diffraction experiment that are caused by the motion of steps, atoms, grain boundaries, etc. From these fluctuations a self auto-correlation function, G(@tau@)) = <@delta@I(t)@delta@I(t+@tau@)>, is constructed that contains the essential kinetics information. I will present a short discussion of how the technique works and the limits on its sensitivity and time resolution. As a specific example, I will show how kinetics information from a system of fluctuating steps on a vicinal surface can be extracted. Data will be presented for two systems where the step motion is governed by different rate limiting kinetics: stepped W(430) and stepped Si(111) surfaces. @FootnoteText@ @footnote 1@ E.H. Conrad, A. Menzel, S. Kiriukhin and M.C. Tringides, Phys. Rev. Lett. 81, 3175 (1998).*

9:00am **SS1-WeM3 Similarities in Tensile and Compressive Strain Relief in Growth of Cu and Ag on Ru(0001)@footnote 1@*, A.P. Baddorf,*** Oak Ridge National Laboratory*; H. Zajonz,* Brookhaven National Laboratory*; D.M. Zehner,* Oak Ridge National Laboratory*; D. Gibbs,* Brookhaven National Laboratory

Growth and dynamics of strained films of Cu and Ag on Ru(0001) have been studied at temperatures between 300 and 925 K using x-ray diffraction. A diverse series of structures are observed, which appear to be prevalent in heteroepitaxial growth on hexagonal surfaces. Thin films of both Cu and Ag are initially strained, in the first case from tensile stress of a 5.8% lattice mismatch and in the second from compressive stress of a 6.3% mismatch. Both Cu and Ag form stripe phase reconstructions, in which strain is reduced by uniaxial contraction or expansion along the [100] direction of the film. In Cu films, the stripe phase appears during formation of the second layer, the first being pseudomorphic, while in Ag films the first layer forms the stripe phase. For Cu, the stripe phase undergoes an abrupt incommensurate/commensurate transition to a registry dependant on temperature. Differences in thermal expansion may explain this temperature dependence. A second registry is correlated with third layer growth of Cu, however the third layer is metastable. At higher coverages, both Cu and Ag stripe phases coexist with (111) oriented 3-dimensional islands. For Cu, island formation follows stripe phase development, however for Ag, unstable islands appear first and participate in formation of the stripe phase. Structures grown in equilibrium at high temperature are compared with those grown at room temperature and imaged with scanning tunneling microscopy as well as with results from semi-empirical calculations. @FootnoteText@ @footnote 1@ORNL is managed by Lockheed Martin Energy Research Corp. under US DOE contract DE-AC05-96OR22464. BNL is supported by US DOE DE-AC02-98CH10886.

9:20am **SS1-WeM4 Step-Step Interactions on TaC(910)@footnote 1@*, J.-K. Zuo,*** Oak Ridge National Laboratory and Southwest Missouri State University*; T.-J. Zhang,* University of Tennessee and Oak Ridge National Laboratory*; **J.F. Wendelken**, Z. Zhang, D.M. Zehner,* Oak Ridge National Laboratory

TaC, an ionic crystal with an extremely high melting point of ~3983 C, exhibits a strong faceting behavior for (n10) surfaces after heating to ~2000°C.@footnote 2@ These facets are very regular when n = 1, 2 or 3 but become less regular when n = 9. Through a scanning tunneling microscopy based study of the step distribution and structure on TaC(910), we determine that the observed morphology results from the interplay of a step-step repulsive interaction with both short- and long-range attractive interactions. The surface is dominated by bunched double-height steps where the bunches are separated by relatively long intervening (100) terraces having irregular widths. The step-separation distribution is highly skewed and sharply peaked at 13 atomic rows, the average spacing within a step bunch, while the (910) orientation is maintained with an average step-separation of about 18 rows. A Monte Carlo simulation shows that a weak, long-range, attractive interaction, -B/x@super a@, must be added to a strong, medium-range, repulsive interaction, A/x@super 2@, to fit the measured distribution. In addition, a short range attractive interaction is required for the creation of multiple-height steps that are oriented in the [010] direction. Possible physical origins for each of these interactions will be discussed. @FootnoteText@ @footnote 1@ ORNL is managed by Lockheed Martin Energy Research Corp. under U.S. DOE Contract No. DE-AC05-96OR22464. @footnote 2@ J.-K. Zuo, J. M. Carpinnelli, D. M. Zehner and J. F. Wendelken, Phys. Rev. 53, 16013 (1996).

9:40am **SS1-WeM5 Phosphide Phases on Cu(001): a Helium Atom Scattering Study*, L.V. Goncharova, J. Braun, A.V. Ermakov, B.J. Hinch,*** Rutgers University

PF@sub 3@ and PH@sub 3@ adsorbs molecularly on Cu(001) at low surface temperatures. As these molecules are susceptible to electron induced decomposition; helium atom scattering proves to be a powerful diagnostic tool. On raising the surface temperature competition between desorption and decomposition occurs. Decomposition is complete after annealing to room temperature. A low coverage of phosphorous induces a poorly ordered c(6x8) phase. Subsequent annealing to 500K substantially improves the long range ordering of this structure. For PF@sub 3@ exposures at room temperature, no adsorption is observed. In contrast, PH@sub 3@ adsorbs dissociatively. Under these exposure conditions a c(6x6) phase is observed. Both c(6 x 8) and c(6 x 6) phases display low rainbow angles implying phosphorus incorporation into the surface plane. We shall discuss possible structures for these low-corrugation, phosphorus-in-copper phases.

10:00am **SS1-WeM6 Ordered Alloying of Pd with the Mo(001) Surface*, D. Wu, Z.Q. He, M.S. Altman, W.K. Lau, C.T. Chan,*** Hong Kong University of Science and Technology, P.R. China

The interaction of Pd with the Mo(001) surface has been studied with low energy electron microscopy (LEEM) and diffraction (LEED), and first principles total energy calculations. A significant change of surface morphology is revealed by LEEM during the development of a Pd-induced c(2x2) periodic structure. The creation of a large number of islands upon Pd deposition is consistent with the formation of a subsitutional alloy. Accommodation of Pd in excess of the ideal c(2x2) coverage leads to the formation of a c(2x8) structure, although with no apparent change of surface morphology. The c(2x8) structure is stable at the interface between Mo and thicker Pd overlayers. Theoretical calculations demonstrate that the substitutional alloy is energetically favored compared to an overlayer structure at half monolayer coverage. Proliferation of antiphase domain walls in the c(2x2) subsitutional alloy is proposed to explain the c(2x8) periodic structure. Theoretical calculations indicate that a pseudomorphic Pd overlayer is more stable than substitutional alloys at one monolayer coverage, and that the Pd-covered Mo(001) surface would be unstable with respect to faceting to the (112) orientation if the pseudomorphic growth can be realized. However, experiment reveals that there is a kinetic limitation to the formation of the pseudomorphic structure and that faceting is preempted by the formation of more complex surface alloy structures.

10:20am **SS1-WeM7 Alkali-Metal-induced 3x1 Reconstruction of the Ge(111) Surface*, G.S. Lee,*** Korea Research Institute of Standards and Science, Korea*; J. Kim,* Korea Advanced Institute of Science and Technologies*; I. Chizhov, H. Mai, R.F. Willis,* The Pennsylvania State University

We present the scanning tunneling microscopy (STM) images of the 3x1 reconstruction of the Ge(111) surface induced by the adsorption of Na and Li. Both filled- and empty-state images of Ge(111)3x1-Na consist of double-row zigzag chains. For Ge(111)3x1-Li, the filled-state image shows single-width rows with sparsely distributed block features between the rows, while the empty-state image is characterized by double rows of dimer-like features. For both surfaces, the dual-polarity images taken simultaneously reveal lateral shift and phase reversal of the rows upon polarity reversal. The apparent dissimilarity of the STM images is contradictory to the expectation that the Ge(111)3x1 surface, like the Si(111)3x1 surface, is a substrate reconstruction which is not specific to the kind of alkali metals. The interpretation of the images of both Ge(111)3x1 surfaces will be

discussed by comparing with those of the Si(111)3x1 surfaces, and the recently proposed structural model for the Si(111)3x1 reconstruction.

10:40am **SS1-WeM8 High-Resolution Structural Analysis of Te/Ge(001)**, ***B.P. Tinkham***, Northwestern University; *P.F. Lyman,* University of Wisconsin, Milwaukee; *O. Sakata, D.A. Walko,* Northwestern University; *M.J. Bedzyk,* Northwestern University, Argonne National Laboratory

We propose models for the surface structure of Te/Ge(001). Te has proven to be an effective surfactant for Si/Ge heteroepitaxy.@footnote 1@ Thus, the study of Te/Ge(001) will determine more precisely the method of surfactant action. Our group has performed high-resolution XSW (X-Ray Standing Wave) and LEED (Low-Energy Electron Diffraction) studies at Te coverages of 1 and .5 monolayer. We are presently investigating these structures with surface x-ray diffraction in order to allow us to fully describe the surface structure, including the composition and structure of the Te dimers. STM will also be used to verify the competing models suggested by the x-ray measurements. @FootnoteText@ @footnote 1@ H.J Hosten, J. Klatt, G. Lippert, E.Bugiel, and S. Higuchi, J. Appl. Phys. 74, 2507 (1993).

11:00am **SS1-WeM9 A Novel STM Imaging Mechanism Used to Resolve the Atomic Structure of the As-Rich GaAs(001)-(2x4) Surface**, ***V.P. LaBella***, *D.W. Bullock, P.M. Thibado,* University of Arkansas; *P. Kratzer, M. Scheffler,* Max-Planck-Gesellschaft, Germany

Motivated by the importance of GaAs in the compound semiconductor device market. The atomic arrangement of the technologically important GaAs(001)-(2x4) reconstructed surface is determined using scanning tunneling microscopy (STM) and first-principles, electronic structure calculations. The bias-dependent STM images reveal the relative position and depth of atomic-scale features within the trenches between the top layer As dimers, which are in agreement with the @beta@2 (2x4) structural model. The bias-dependant simulated STM images reveal that a retraction of the top most dangling bond orbitals is the unique mechanism that enables the STM tip to image the trench structure. This work was funded in part by the National Science Foundation (DMR-9733994) and the Office of Naval Research (N00014-97-1-1058).

11:20am **SS1-WeM10 Dislocations, Phason Defects, and Domain Walls in a One-dimensional Quasiperiodic Superstructure of a Metallic Thin Film**, *Ph. Ebert,* Forschungszentrum J@um u@lich, Germany; *K.-J. Chao, Q. Niu,* ***C.K. Shih***, University of Texas, Austin

We investigated disorder and structural defects in a one-dimensional quasiperiodic superstructure of a thin Ag film on GaAs(110) surfaces by scanning tunneling microscopy. The superstructure forms sequences with long and short separations exhibiting a self-similarity. We demonstrate that the modulation can be described best with a Fibonacci sequence and deviations are due to structural defects. We identify dislocations, phason defects, and domain walls. The static stress field of dislocations is found to be a source of phason defects.

11:40am **SS1-WeM11 The Surface Reconstructions of InP(001)**, ***Z. Ding***, *V.P. LaBella, D.W. Bullock, P.M. Thibado,* University of Arkansas

Motivated by the increasing use of InP in high speed opto-electronic devices that are fabricated using molecular beam epitaxy (MBE), the surface reconstruction phases of the technologically important InP(001) surface are studied. This study is performed in a combined ultrahigh vacuum MBE and scanning tunneling microscopy (STM) multi-chamber facility that incorporates a solid source phosphorus evaporation source and a novel temperature measurement system accurate to within ±2 @super o@C. Both reflect ion high energy electron diffraction (RHEED) and STM are used to map out the InP(001) surface reconstruction phase's dependence upon substrate temperature and phosphorus pressure. A c(4x4), a (2x1), and a (2x4)/c(2x8) reconstruction are all observed. Thi s work was funded in part by the National Science Foundation (DMR-9733994) and the Office of Naval Research (N00014-97-1-1058).

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