Surface Science Division
Room 606 - Session SS1+EM+NS-ThA

Metal/Metal Growth

Moderator: R.Q. Hwang, Sandia National Laboratories

2:00pm **SS1+EM+NS-ThA1 Dislocation Structures of Submonolayer Films near the Commensurate-Incommensurate Phase Transition: Ag on Pt(111)**, ***J.C. Hamilton***, *R. Stumpf,* Sandia National Laboratories*; K. Bromann, M. Giovannini, K. Kern, H. Brune,* EPF Lausaane, Switzerland

We provide a theoretical explanation@footnote 1@ for unusual experimental observations@footnote 2@ of submonolayer Ag film growth on Pt(111). These films exhibit parallel partial dislocations with narrow hcp regions separated by much wider fcc domains. Using a 2D Frenkel-Kontorova (FK) model we show that this unusually large difference is primarily due to proximity to the commensurate-incommensurate phase transition, and only secondarily to stacking fault energies. We next consider the relationship between island energy, island dislocation structure, and island shape. Using the FK model we calculate the stability of islands with no dislocations, a single dislocation pair across the island, two parallel dislocation pairs across the island, and a "Y" shaped dislocation structure. The model is in excellent agreement with experiment in predicting the onset of dislocation structures in growing islands. It also suggests that the dislocations have little or no effect on the equilibrium island shape. Finally we discuss the relationship between these calculations and related experiments@footnote 3@ on the structure of the clean Pt(111) surface which reconstructs above 65% of the melting point. @FootnoteText@ @footnote 1@ J. C. Hamilton, R. Stumpf, Karsten Bromann, Marcella Giovannini, Klaus Kern and Harald Brune, Phys. Rev. Lett., in press@footnote 2@ Karsten Bromann, Harald Brune, Marcella Giovannini, and Klaus Kern, Surf. Sci. V388, L1107 (1997). @footnote 3@ A. R. Sandy, S.G.J. Mochrie, D.M. Zehner, G. Grubel, K.G. Huang and Doon Gibbs, Phys. Rev. Lett. 68, 2192 (1992).

2:20pm **SS1+EM+NS-ThA2 Non Capillarity Driven Grain Growth in a Strained Cu Ultrathin Film**, ***A.K. Schmid***, *T. Giessel, N.C. Bartelt, J. de la Figuera, R.Q. Hwang,* Sandia National Laboratories

Properties of metal films are crucially influenced by details of their grain structure. To determine basic mechanisms of grain evolution we have investigated a prototypical granular thin film using LEEM and STM. In two monolayer thick films of Cu on Ru(0001) a uniaxial relaxation relieves the misfit strain (5.5%) with the substrate, leading to a two-dimensional grain structure consisting of three orientationally different domain types. We observed in-situ grain growth using LEEM in dark field imaging mode and took STM snap shots at several stages of the grain evolution. While on large scale of both time and area the total length of grain boundary decreases in order to reduce the free energy of the system an increase of boundary length has been observed locally and on smaller time scale. The observed behavior can not be described within the framework of a Q-state Potts model which has been widely used for the description of grain growth. We show that the long-ranged lateral interactions between the surface atoms in the strained Cu film which are not considered in Potts model are responsible for the observed behavior.

2:40pm **SS1+EM+NS-ThA3 Exchange Processes in Metal on Metal Growth Studied with High-resolution STM**, ***M. Schmid***, Technische Universitaet Wien, Austria **INVITED**

In the early 1990's, after the first atomic-scale studies by field ion microscopy and related simulation calculations it became apparent that many processes in growth of thin films involve exchange of substrate and deposited atoms. It was concluded that interlayer diffusion at steps, the key process determining the growth mode, often occurs by replacing a substrate atom with a deposited atom, pushing the substrate atom onto the lower terrace. A new way to study such phenomena is scanning tunneling microscopy (STM) with atomic resolution and chemical contrast@footnote 1@. We have deposited a small amount of Co on a Pt(111) surface with a high density of steps. In the resulting structure, we can distinguish between substrate (Pt) and deposited material (Co) on an atom-by-atom basis. An analysis of the STM data shows that Co atoms do not descend Pt steps by diffusing over the step, but descend from the upper terrace to the lower by an exchange diffusion process at the step edge with the Pt atoms. The Co atoms descend a Pt step edge by this process neither at straight A nor at B steps, but rather at the corners or kinks of the vacancy islands. These results are in qualitative agreement with simulations based on embedded atom method (EAM) potentials. Other examples of exchange processes can lead to subsurface growth of the deposited material, with substrate atoms floating on top of it. Such phenomena were observed to occur already at or near room temperature when Co was deposited on the Pt(111) and Pt(110) surfaces. @FootnoteText@ @footnote 1@ E. Lundgren, B. Stanka, G. Leonardelli, M. Schmid, and P. Varga, Phys. Rev. Lett., accepted.

3:20pm **SS1+EM+NS-ThA5 Self-diffusion on Pt(110)-1x2: Ab-initio Barriers vs. Experiment@footnote 1@**, ***P.J. Feibelman***, Sandia National Laboratories

Because it requires breaking more bonds, dimer diffusion by dissociation and recombination on clean Pt(110)-1x2 should cost more energy than the recently discovered@footnote 2@ "leapfrog" mechanism. Since cohesion per bond decreases with increasing coordination, the leapfrog mode should also have a lower barrier than monomer diffusion. Though first-principles calculations confirm these deductions, they are at odds with experiment, possibly signalling the influence of low-level surface contamination. @FootnoteText@ @footnote 1@ Work supported by the U. S. Department of Energy under Contract No. DE-AC04-94AL85000. Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy @footnote 2@ T.R. Linderoth, et al., Phys. Rev. Lett. 82, 1494(1999); F. Montalenti and R. Ferrando, Phys. Rev. Lett. 82, 1498(1999).

3:40pm **SS1+EM+NS-ThA6 Novel Temperature Dependence of the Morphology of Deposited Multilayer Ag/Ag(100) Films**, ***C.R. Stoldt***, *A.R. Layson, C.J. Jenks,* Iowa State University*; M.C. Bartelt,* Sandia National Laboratories*; K. Caspersen, J.W. Evans, P.A. Thiel,* Iowa State University

Metal(100) homoepitaxy provides a natural testing ground for recently developed ideas on kinetic roughening and "mound formation" due to step-edge barriers. Non-monotonic variation of roughness with deposition temperature (T) has been predicted,@footnote 1@ but not observed. Here, we report comprehensive VT-STM studies for growth of Ag/Ag(100) films between 130K and 300K which reveal this behavior. Roughness of 25ML Ag/Ag(100) films at first increases "classically" below 300K due to inhibited downward transport, but then decreases below 220K, achieving a low plateau value below 170K. Unlike Pt/Pt(111) and Rh/Rh(111) growth, non-monotonic behavior is not associated with a dramatic change in 2D island morphology, but rather with enhanced downward funneling from (the more prevalent) step edges at lower T. We also characterize the mound morphology, noting the steepness of the mound sides and small lateral dimension at lower T. A breakdown of kinematic scattering behavior of the intensities observed in our HRLEED studies of these films is attributed to this feature. Monte Carlo simulations of a realistic model for growth@footnote 1@ are consistent with and elucidate observed behavior. @FootnoteText@ @footnote 1@M.C. Bartelt and J.W. Evans, Surf. Sci. 423 (98) 189; Phys. Rev. Lett. 75 (95) 4250.

4:00pm **SS1+EM+NS-ThA7 Edge Diffusion During Growth: Kink Ehrlich-Schwoebel Effect and Resulting Instabilities@footnote 1@**, *O. Pierre-Louis,* Univ. J. Fourier (CNRS), France*;* ***T.L. Einstein***, University of Maryland

In addition to the usual step Ehrlich-Schwoebel effect (SESE) on typical metal and semiconductor surfaces, there can also be a kink Ehrlich-Schwoebel effect (KESE), associated with asymmetries in barriers at kinks/corners encountered by atoms during transport along step edges.@footnote 2@ We take into account both phenomena to study the evolution of arbitrarily oriented surfaces during molecular beam epitaxy. We find that the heretofore rarely discussed@footnote 3@ KESE has a profound effect on growth morphology. Under the usual growth conditions, KESE induces a new instability of vicinal surfaces, supplanting the familiar Bales-Zangwill instability@footnote 4@ due exclusively to SESE. The possibility of stable kink flow growth is analyzed; fluctuations can shift the stability threshold. For some orientations, KESE can stabilize steps. KESE can also induce mound formation. @FootnoteText@ @footnote 1@Work supported by NSF MRSEC grant DMR 96-32521. @footnote 2@ O. Pierre-Louis, M. R. D'Orsogna, and T. L. Einstein, Phys. Rev. Lett. 82 (1999) 3661; note also M. V. Ramana Murty and B. H. Cooper, preprint. @footnote 3@ See, however, I. L. Aleiner and R. A. Suris, Sov. Phys. Solid State 34 (1992) 809; Z. Zhang and M. G. Lagally, Science 276 (1997) 377; J. G. Amar, Bull. Am. Phys. Soc. 43 (1998) 851 and to be published. @footnote 4@ G.S. Bales and A. Zangwill, Phys. Rev. B 41 (1990) 5500.

4:20pm **SS1+EM+NS-ThA8 Atom-by-Atom Growth: Bonding and Rebonding on Metal Surfaces**, ***A. Bogicevic***, Sandia National Laboratories

The bond-order--bond-length concept put forth by Pauling almost 70 years ago has greatly added to our intuitive understanding of atomic-scale bonding in molecules. The basic idea is that the more bonds an atom makes, the weaker and longer each becomes [rebonding]. This concept has been extensively tested, and is routinely used in molecular chemistry today, so one would assume that a similar model for the gas-surface interface would prove useful. In an early first-principles study of Al/Al(100), strong and observable rebonding effects were predicted. Unfortunately, these results are an artifact of some severe modelling compromises imposed by computational limitations. New, fully converged (160-180 atom unit-cells, 36 k-points), first-principles density-functional calculations for a wide variety of homogeneous and heterogeneous metal systems show that, contrary to rebonding theory, addimers (adsorbed atom pairs) do not have longer surface bonds than adatoms, do not reside farther above the surface, and do not meet the rebonding arguments for augmented mobility. Rebonding does contribute to destabilize addimers, but does not explain inherently weak adatom-adatom interactions. I explain the absence of rebonding effects in terms of elastic and electronic contributions to the rebonding energy, and present an alternative explanation for the adatom-adatom bond weakness based on bond frustration. Implications for nucleation and growth of metals will be discussed.@footnote 1@ @FootnoteText@ @footnote 1@ Work at Sandia National Laboratories is supported by the U.S. Department of Energy under Contract DE-AC04-94AL85000. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy.

4:40pm **SS1+EM+NS-ThA9 Diffusion of Lead on the Au(111) Surface Studied by Scanning Tunneling Microscopy and Embedded-Atom Method Molecular Dynamics**, ***M.C. Robinson***, Trent University and Queen's University, Canada; *K. De'Bell,* University of New Brunswick in Saint John, Canada; *A.J. Slavin,* Trent University and Queen's University, Canada

Low coverages of Pb deposited on the reconstructed Au(111) surface have been studied with STM and show that the reconstruction strongly influences diffusion and film morphology. Nucleation sites for Pb adatoms are found at the kinks of the reconstruction. For higher coverages, Pb atoms concentrate in the fcc and hcp regions; the elevated transition regions are much less populated. The reconstruction is lifted for some coverage between 0.05 and 0.3 monolayers (ML). For comparison, the Embedded Atom Method-Molecular Dynamics (EAM-MD) method has been used to study diffusion of Pb on both the unreconstructed (flat) and reconstructed surfaces. EAM-MD simulations show that diffusion is complicated by the reconstruction. Using both static and dynamic methods, the diffusion energies have been determined. They show that, for an adatom moving perpendicular to the compression direction, the energy barrier is 1.7 times greater than for motion in the parallel direction. Diffusion is slowed on the fcc part of the reconstructed surface, as compared to the unreconstructed, by a factor of about 2. No greater coverage than 0.07 ML could be forced onto the EAM-modelled reconstructed surface. However, the flat surface could be fully covered, suggesting that the reconstruction is not energetically stable at higher coverages, as has been observed experimentally.

5:00pm **SS1+EM+NS-ThA10 Low Energy Electron Microscope Investigation of Pb Overlayers on Cu(100)**, ***G.L. Kellogg***, Sandia National Laboratories

Pb overlayers on Cu substrates provide a model system for investigating epitaxial films exhibiting large lattice misfits and for studying two-dimensional phase transitions (e.g., disordering and surface melting). On Cu(100), room-temperature deposition of Pb follows classical Stranski-Krastanov growth with three well-defined overlayer structures forming at submonolayer coverages.@footnote 1@ In this investigation, low energy electron microscopy (LEEM) is used to (1) characterize the changes that occur to these structures resulting from annealing to various temperatures and (2) monitor the subsequent growth of 3-D islands. The low-coverage c(4x4) and high-coverage c(5@sr@2x@sr@2)R45 phases, both of which consist of rotationally inequivalent domains, are observed to disorder at temperatures of 270C and 215C, respectively. By forming images using selected low energy electron diffraction beams (i.e., dark-field LEEM), the domain structure that forms upon cooling from above the transition temperature is imaged directly with a spatial resolution of ~10 nm. Dark-field LEEM is also used to characterize the c(4x4) - c(2x2) co-existence structure that forms upon desorption of excess Pb from the high-coverage phase. The growth of three-dimensional Pb islands on top of the high-coverage phase and the coarsening of these structures at temperatures from 100-150C are measured to derive fundamental energetic parameters involved in the melting of 3-D Pb clusters. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the U. S. DOE under Contract DE-AC04-94AL85000 @FootnoteText@ @footnote 1@ J. Henrion and G. E. Rhead, Surface Sci. 29(1972)20.

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