Surface Science Division
Room 308 - Session SS1-WeA

Electromigration and Surface Transport

Moderator: T.L. Einstein, University of Maryland

2:00pm **SS1-WeA1 Quantifying Surface Electromigration: Si(111) as a Model System@footnote 1@*, E.D. Williams,*** University of Maryland, College Park **INVITED**

Electromigration induced changes in structure result from a diffusion bias caused by an imposed external electric field. The mechanisms by which the diffusion bias is induced (wind force or direct force) are similar in the surface and the bulk. Thus in temperature regimes where surface diffusion is more readily activated than bulk diffusion, surface electromigration should play an important role in changes in morphology of a current-carrying structure. Surface electromigration occurs on Si(111) surfaces at elevated temperatures. The signature is the spontaneous evolution of non-equilibrium configurations of the steps with one direction of the current, and the return to equilibrium with the opposite direction of current with respect to the "down-hill" step direction. Quantification of the nature of the surface electromigration force has been performed by STM-measurement of the shapes and rates of the evolving non-equilibrium morphologies, and by comparison of the rates of decay in the presence and absence of the stabilizing direct current. The basic mechanism of both formation and decay is the motion of individual steps, which occurs with a rate governed by the rate of equilibrium fluctuations of the steps. During formation of non-equilibrium structures, individual fluctuations couple to the external field, yielding single-point step collisions which then "zip" up to form step bunches. The curvature at the "zip" point has been quantified in terms of the competing effects of energetic costs of step bending and the electromigration force. During decay, steps move in a nearly one-dimensional mode which has been quantified in terms of the step-step repulsions and the electromigration force. The results are consistent with an effective charge less than 0.01 electron units. The applications of this approach to studying broader problems in electromigration will be discussed. @FootnoteText@ @footnote 1@Supported by the U. of MD NSF-MRSEC

2:40pm **SS1-WeA3 Electromigration and Cluster Motion@footnote 1@*, O. Pierre-Louis,*** *T.L. Einstein,* University of Maryland, College Park

We describe the fluctuations, dynamics, and instabilities of adatom and of vacancy single-layer islands during electromigration, generalizing earlier work on straight steps without driving forces.@footnote 2@ We emphasize the dependence on the mass-transport mechanism: periphery diffusion (PD), terrace diffusion (TD), or evaporation-condensation (EC).@footnote 3@ In particular, we find non-circular steady states and derive the cluster diffusion constant D@sub c@. Analytical calculations using Langevin formalism are corroborated by both Monte Carlo simulations and numerical integration. We determine the cluster drift velocity, which in the 3 limiting cases has the size dependence of cluster-area x D@sub c@. In EC, clusters elongate perpendicular to the drift axis. Differences exist in this novel behavior for atom and vacancy clusters. In PD a morphological instability leads to cluster splitting.@footnote 4@ We show that adatom diffusion across the terrace induces a new morphological instability for vacancy clusters and discuss the threshold. Shape fluctuations and D@sub c@ are studied in our Langevin framework. For weak electromigration the cluster responds isotropically for TD or PD but not EC. Fluctuation behavior close to the instability threshold is characterized analytically and numerically. An electric current can also alter attachment/detachment probabilities; novel consequences on cluster dynamics (drift velocity, shape, etc.) are investigated. We discuss experimental relevance of our results. New phenomena should be observed on metal surfaces, and implications for voids in electric lines are discussed. @FootnoteText@ @footnote 1@Work supported by NSF MRSEC grant DMR 96-32521. @footnote 2@O. Pierre-Louis and C. Misbah, Phys. Rev. Lett. 76, 4761 (1996); Phys. Rev. B 58, xxx (1998). @footnote 3@S. V. Khare and T. L. Einstein, Phys. Rev. B 57, 4782 (1998); 54, 11752 (1996). @footnote 4@W. Wang and Z. Suo, J. Appl. Phys.79, 2394 (1996); M. Schimschak and J. Krug, Phys. Rev. Lett. 80, 1674 (1998).

3:00pm **SS1-WeA4 Theory of Surface Electromigration on Metals*, P.J. Rous,*** *D.N. Bly,* University of Maryland, Baltimore County, US

We describe the application of layer-KKR theory to the calculation of the driving force for adatom electromigration on metallic surfaces. We find that the dominant component of the force arises from momentum transfer to the adatom from the charge carriers; the so-called wind force. We have computed the direction and magnitude of the driving force for electromigration along typical migration pathways on low Miller index surfaces. Averaging the force felt by an adatom traversing these paths permits the calculation of the effective wind valence Z@sub w@. By comparing Z@sub w@ for impurity and self-electromigration on various substrates we have correlated the magnitude of the driving force with the local carrier density and the adatom transport cross-section. For migration of isolated adatoms, we find that the ballistic model, appropriately modified for the effect of the substrate provides a reasonable qualitative description of the calculated effective valence. @FootnoteText@ This work is supported by the National Science Foundation under Grant No. DMR-9632521

3:20pm **SS1-WeA5 Theory of Surface Electromigration on Stepped and Islanded Surfaces.*, J. Cheng,*** *P.J. Rous,* University of Maryland, Baltimore County, US

We have applied multiple scattering theory to explore the variation of the electromigration wind force experienced by an adatom in the vicinity of steps and islands on a metal surface. We find that the electromigration wind force felt by a migrating adatom is strongly perturbed as it approaches a step or island edge. This is a result of multiple scattering of the carriers between the adatom and step/island which alters the local current density. The implications of this inhomogeneity in the electromigration driving force for current-induced changes in surface morphology are discussed. Since the calculated wind valence may be directly related to the surfaceinduced resistivity of an adatom we discuss the how the scattering interactions between steps and adatoms may be manifest in the resistivity of a metallic surface. @FootnoteText@ This work is supported by the National Science Foundation under Grant No. DMR-9632521

3:40pm **SS1-WeA6 Surface Electromigration Processes on Gold and Copper Films*, N. Shimoni,*** *O. Biham, O. Millo,* The Hebrew University, Israel

Electromigration processes on the surfaces of gold and copper films are studied using scanning tunneling microscopy (STM). We perform time-lapse STM scans under controlled sample temperature conditions, both with and without current stressing. We shall present results regarding the following issues: 1. The evolution of monolayer islands, voids and terraces on the surface of polycrystalline gold films. 2. The appearance and evolution of surface dislocations on flame-annealed gold films. 3. Grain boundary migration, and elongation of surface grains in the direction of the applied current in copper films. Our results will be discussed in context of the various possible surface dynamic processes, including the affect of the sub-surface layer on these dynamics. We will also address differences between thermally activated and electromigration induced processes.

4:00pm **SS1-WeA7 Molecular Dynamics Studies of Interlayer Mass Transport and Dendritic-to-Compact Morphological Transitions during Submonolayer Growth on Pt(111) Surfaces*, V. Chirita,*** *E.P. Münger, J.-E. Sundgren,* Linköping University, Sweden*; J.E. Greene,* University of Illinois, Urbana

We use embedded-atom method molecular dynamics simulations to investigate the kinetics of two processes which are critical in achieving the layer-by-layer growth mode: interlayer mass transport and dendritic-to-compact morphological transitions. The former investigation is carried out by following the dynamics of adatoms, vacancies and adatom-vacancy pairs within hexagonal Pt@sub 19@ clusters on Pt(111) at 1000 K, for simulation times totalling ~ 135 ns. The latter study concentrates on the dynamics of Pt dendrites containing up to 25 atoms on the same surface at the same temperature. The mapping of adatoms motion on top of the clusters shows that prior to incorporation, adatoms are trapped near the cluster edge for ~ 80% of the total simulation time. Cluster configurations with central vacancies are found to be quite stable. Adatom incorporation is observed to occur mainly via the two well known mechanisms of hopping and push-out/exchange with edge atoms. However, our simulations for adatom-vacancy pairs within clusters, bring the first direct evidence that both mechanisms can be active in the central region of the cluster, i.e. monovacancies are filled by adatom hopping or via exchanges with one of the atoms adjacent to the vacancy. We carry out minimum energy path calculations to examine the energetics of the two mechanisms. The results show that activation barriers are comparable to the corresponding interlayer mass transport mechanisms observed at the outer edge of the cluster. We have also followed the dynamics of Y-shaped Pt dendrites for simulations times in excess of 100 ns. The results show that, in agreement

with previously proposed models, the dendritic-to-compact morphological transition proceeds via diffusion around branch corners,as well as edge diffusion. Our simulations reveal however, the presence of a new diffusion mechanism, in which the entire corner of a dendritic branch translates to adjacent terrace sites via a concerted motion of the atoms forming the corner. The process has an activation barrier similar to that of two-fold coordinated atoms diffusing around the corner.

4:20pm **SS1-WeA8 Edge Barriers and Mass Transport on Metal (100) Surfaces@footnote 1@**, ***W.W. Pai,*** The University of Tennessee*; J.F. Wendelken,* Oak Ridge National Laboratory

Since epitaxial growth is subject to kinetic limitations, epitaxial growth morphology is usually thermodynamically unstable. These kinetic limitations, in particular the Schwoebel barrier in homoepitaxial systems, often result in a rough, multilevel morphology which begins during deposition of the first monolayer. Post-deposition equilibration of the resultant morphology occurs through several avenues of mass transport. When the starting condition consists of monolayer height islands following a submonolayer deposition at room temperature, coarsening is observed to result from island diffusion and coalescence on Cu(100) and Ag(100) surfaces, where the island diffusion occurs via rapid edge diffusion.@footnote 2@ When a multilevel system results from higher depositions, islands may still diffuse, but this diffusion is inhibited at downhill step edges due to an edge barrier just as the Schwoebel barrier inhibits downhill transport of adatoms. On the (100) surface, this barrier is found to be very high when the step edge is in the close-packed [110] direction, but very low, or even non-existent, when the edge is oriented in a non-close-packed direction. If a diffusing island encounters an edge with such a low barrier, the island may very quickly descend to the lower level with its atoms being incorporated into the step edge in a manner similar to that which has been reported for Cu(111).@footnote 3@ These low barrier sites, in combination with island diffusion and edge diffusion are found to provide the main pathway for smoothening at room temperature on Cu(100) and Ag(100). This is in contrast to the evaporation-condensation mechanism implied by the line tension driven smoothening at higher temperatures on Cu(100).@footnote 4@ @FootnoteText@ @footnote 1@Research performed at ORNL, which is managed by Lockheed Martin Energy Research Corporation for the U.S. DOE under Contract No. DE-AC05-96OR22464 @footnote 2@Woei Wu Pai, Anna K. Swan, Zhenyu Zhang and J. F. Wendelken, Phys. Rev. Lett.79, 3210 (1997).@footnote 3@M. Giesen, G. Schulze Icking-Konert, and H. Ibach, Phys. Rev. Lett. 80, 552 (1998).@footnote 4@J.-K. Zuo and J.F. Wendelken, Phys. Rev. Lett. 70, 1662 (1993).

4:40pm **SS1-WeA9 Metal Row Growth on a High-Index Silicon Surface***,* ***H.H. Song****, K.M. Jones, S.R. Blankenship, J.A. Carlisle, A.A. Baski,* Virginia Commonwealth University

Recent STM studies of high-index silicon surfaces have revealed unique morphologies not found on their low-index counterparts.@footnote 1@ For example, Si(5 5 12) forms a single-domain reconstruction composed of row-like structures, primarily pi-bonded chains. This highly anisotropic surface is expected to provide a unique template for the growth of metal overlayers, particularly in the formation of one-dimensional nanometer-scale structures. Our STM studies show that Ag deposited onto Si(5 5 12) and annealed to moderate temperatures does form row-like overlayer features. At coverages as low as 0.05 ML, rows appear on top of the most prominent pi-bonded chains, resulting in a 5.4 nm inter-row spacing. These rows have high aspect ratios (up to 40:1) and a mean length of 20 nm. As the Ag coverage is increased, the overlayer rows grow in length and number until the surface forms a periodic array of such rows at ~0.25 ML. Above this coverage, Ag appears to be incorporated into other structures on the surface and the long-range ordering becomes disrupted. A statistical analysis of the row lengths reveals the expected increase in mean row length as a function of coverage (0.05 to 0.2 ML) and annealing temperature (400 to 550°C). At annealing temperatures above 550°C, however, the deposited Ag causes local faceting of the Si surface, disrupting the ordered arrays of Ag rows. The metal rows must therefore be a metastable arrangement of the surface. @FootnoteText@ @footnote 1@A.A. Baski, S.C. Erwin, L.J. Whitman, Surf. Sci. 392, 69 (1997).

5:00pm **SS1-WeA10 One Dimensional Growth Behavior of Xe Atoms on Step Edges of Cu(111)***,* ***J.-Y. Park****, Y. Kuk,* Seoul National University, Korea*; K. Miyake, H. Shigekawa,* University of Tsukuba, Japan

A rare gas atom adsorbed on graphite or various metal surfaces has been extensively studied as a model two dimensional system because of its weak interaction with the substrate. In this study, we used a low temperature scanning tunneling microscope to understand the interaction of Xe atom with Cu(111) surface in the temperature range of 10K ~ 30K. Quite different one dimensional wetting behavior was observed at the lower and upper side of Cu surface steps. Xe atoms first adsorb at lower side of steps, but they reveal repulsive interaction among themselves. The Xe adsorbates then modify the Ehrlich-Schwoebel barrier, resulting in the wetting at upper side of steps. A model is proposed to explain the 1D growth behavior. As observed earlier,@footnote 1@ standing waves, caused by reflection of surface state electrons at step edges and impurities, were observed. It was also observed that the surface state energy is shifted in the presence of the Xe overlayer. @FootnoteText@ @footnote 1@M. F. Crommie, C. P. Lutz, and D. M. Eigler, Nature 363, 524 (1993).

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