Wednesday Morning, October 31, 2001

Surface Science
Room 120 - Session SS1-WeM
Surface Diffusion

Moderator: G.L. Kellogg, Sandia National Laboratories

8:20am **SS1-WeM1 Diffusion on and in Surfaces: The Atomic Slide Puzzle***,* ***J.W.M. Frenken****, R. Van Gastel, E. Somfai, S.B. Van Albada, W. Van Saarloos,* Leiden University, The Netherlands **INVITED**

Usually, surface mobility is thought to be restricted completely to the steps and kinks on crystal surfaces. These sites form the natural locations for atoms to come and go. Atoms in the close-packed terraces are often considered to be completely static, since they are tightly packed by their neighbors. In this talk, measurements will be shown that have been obtained with the scanning tunneling microscope, that show that a close-packed terrace of a metal surface can be far from static, even at temperatures as low as room temperature! We make the motion visible of the atoms in a Cu(001) terrace, by embedding a low density of In atoms in the first Cu layer. The peculiar characteristics of the motion of the In show that the diffusion of surface vacancies is responsible for a continual reshuffling of all the (In and Cu) atoms in the first layer.@footnote 1@,@footnote 2@ @FootnoteText@ @footnote 1@ R. van Gastel, E. Somfai, W. van Saarloos and J.W.M. Frenken, Nature 408 (2001) 665. @footnote 2@ R. van Gastel, E. Somfai, S.B. van Albada, W. van Saarloos and J.W.M. Frenken, Phys.Rev.Lett. 86 (2001) 1562.

9:00am **SS1-WeM3 Nothing Moves a Surface: Probing Surface Vacancy Dynamics with a Surface Alloy***,* ***R. Van Gastel****, E. Somfai, S.B. Van Albada, W. Van Saarloos, J.W.M. Frenken,* Universiteit Leiden, The Netherlands

Indium atoms that are deposited on the Cu(001) surface at room temperature rapidly diffuse to steps where they are incorporated into the first layer of the crystal surface. We use the In/Cu(001) surface alloy to probe the dynamics of surface vacancies. The motion of embedded indium atoms enables us to use these atoms as `tracer' particles for the direct visualization of vacancy mediated diffusion of surface atoms.@footnote 1@ Steps on the surface act as sources and sinks for surface vacancies. This crucial role of steps is exposed as the mobility of embedded indium atoms is spatially mapped out. The temperature dependence of the diffusion of embedded indium atoms is investigated through high speed STM movies. The temperature dependence provides us with a direct measurement of the surface vacancy mobility, and yields the sum of the vacancy formation and migration energies. In addition to this, we present first results from experiments, in which monatomic surface vacancies are artificially created. From these the vacancy migration energy can be obtained so that we can experimentally separate out the formation and migration energies. @FootnoteText@ @footnote 1@R. van Gastel et al., Phys. Rev. Lett. 86 (2001), 1562.

9:20am **SS1-WeM4 Surface-diffusion Mechanism vs. Electric Field: Pt/Pt(001)****,* ***P.J. Feibelman,*** Sandia National Laboratories

Identifying macroscopic variables that affect the rates and mechanisms by which surface atoms move should enhance our ability to control surface morphology. The search for new "knobs to turn" is at the root of the decade-long effort to modify thin-film growth by depositing appropriately chosen "surfactant" species. It also motivates the work reported here, in which ab-initio total energy calculations are used to understand how an externally imposed electric field should affect the mechanism and rate of adatom self-diffusion on Pt(001), a surface for which Field Ion Microscopy experiments@footnote 1@ suggest that the low energy process, concerted substitution, is supplanted by hopping when the external field is high enough. The result is that theory agrees with FIM that the barrier to concerted substitutional diffusion of a Pt atom on Pt(001) varies linearly with external electric field (slope ~0.1eÅ), increasing for fields oriented to push electrons into the surface. But, with a computed hopping barrier remaining >0.5 eV higher than that for substitution, the calculations contradict the idea that a change in FIM site visitation at fields of 1.5-2 V/Å and temperatures ~265-284K can be attributed to the onset of hopping. @FootnoteText@ @footnote *@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 U. S. Department of Energy. @footnote 1@G. L. Kellogg, Phys. Rev. Lett. 70, 1631(1993).

9:40am **SS1-WeM5 Temperature-Dependent Surface Diffusion Parameters on Amorphous Materials***,* ***E.G. Seebauer****, D. Llera-Hurlburt, A. Dalton,* University of Illinois, Urbana

Diffusion on amorphous surfaces represents a little-studied physical phenomenon that controls several important kinds of material processing. To elucidate some general features of this phenomenon, we have determined Arrhenius parameters for the surface self-diffusion of amorphous silicon (a-Si) by measuring the formation kinetics of hemispherical grained silicon. The results exhibit significant temperature dependence in the activation energy for total mass transport. We develop a physical model and associated mathematical formalism to show that this behavior should characterize diffusion on amorphous surfaces in general. Adatom formation on amorphous surface can arise from a near-continuum of structures and energy states. The formation energy for mobile atoms is therefore described by a continuous distribution function f(E). The breadth of f(E) on a-Si and related surfaces contrasts sharply with the sum of delta functions corresponding to kinks, steps and terraces on crystalline surfaces. Thus as T increases on amorphous surfaces, the average formation energy for mobile adatoms increases continuously, and the Arrhenius plot for total mass transport bends upward. The sharpness of the curvature depends upon the breadth of f(E); a broader distribution yields more gentle curvature.

10:00am **SS1-WeM6 Hopping Induced by the Vibrational Excitation of Adsorbed Molecule through Inelastically Tunneled Electrons***,* ***M. Kawai,*** *T. Komeda, Y. Kim,* RIKEN, Japan

There is a rising interest for the phenomena caused by inelastic tunneling in the experiments using scanning tunneling microscope (STM).@footnote 1@ In this report, we show surface-diffusion of adsorbate is induced by inelastic tunneling of electron for the molecules of CO and ethylene on Pd(110) at 4.8K. When a certain amount of tunneling electron is dosed on a single adsorbate, the change of their bonding site along [1 0] direction is observed. We study this phenomenon systematically and found that the diffusion probability shows a very sharp increase at the bias voltage of 250 mV, which corresponds to the excitation of CO stretch vibrational mode. In similar manner, ethylene molecule adsorbed on the same surface is also enhanced to hop to the neighboring sites by irradiating electrons that correspond to the excitation of the internal stretching modes. These clearly demonstrate that the vibrational mode excited by inelastically tunneled electrons opens a route to induce hopping of the adsorbed molecules on surfaces. In the case of CO on Pd(110), thermal diffusion of CO was previously studied. At 100 K, one-dimensional CO arrays are formed and attaching and detaching of CO molecules are observed. The motion is restricted on [1 0] direction. The estimated diffusion barrier for a CO molecule in an array is ~180 meV, but the value for an isolated molecule should be much smaller in energy. Here we propose a model that the diffusion of CO is induced by an excitation of high lying vibrational mode (C-O stretch mode) which is further coupled with T-mode and R-mode through anharmonic coupling to induce surface diffusion . @FootnoteText@ @footnote 1@J.R. Hahn, H.J. Lee, and W. Ho, Phys. Rev. Lett. 85 1914 (2000) and references there in.

10:20am **SS1-WeM7 Determination of Atomic Potential Energy for Pd Adatom Diffusion Across the W (111) Islands and Surfaces***,* ***T.-Y. Fu,*** National Taiwan Normal University, R.O.C., R. O. C.*; L.-C. Cheng,* National Taiwan Normal University, R.O.C.*; T.T. Tsong,* Academia Sinica, Taiwan, R.O.C.

Using field ion microscopy (FIM), we have probed the diffusion behavior of Pd adatoms on W (111) surfaces and in the vicinity of surface steps. From the behavior of an adatom approaching the step from the upper terrace, we find the step to be reflective to Pd adatoms. The extra reflective barrier is determined to be 0.64±0.03 eV. The behavior of adatoms approaching the step from the lower terraces has also been studied. The activation energy for the step-up motion of Pd atoms of W (111) steps is 1.84 eV. The potential energy difference toward and away from the W (111) pole exhibits a free energy anisotropy of 0.013 eV. These experimental results of atomic processes are related to the phenomenon of impurity induced pyramidal facet formation.

11:00am **SS1-WeM9 Surface Dynamics During Etching of GaAs(001)***,* ***S.W. Robey,*** National Institute of Standards and Technology

We present results from an experimental investigation of the surface dynamics controlling morphology during CH@sub 4@/H@sub 2@ plasma and wet etching of GaAs (001) surfaces. In the case of plasma etching, height-difference correlation functions (extracted from AFM data) indicate that morphology development is dominated by diffusion below ~ 100 nm, while desorption/etching effects dominate on larger length scales. The crossover between these two regimes is temperature dependent. Below 600 K, oscillatory structure in the height correlation function, associated with a "rippled" surface morphology, arises due to an instability in the etching dynamics. We attribute this instability to Ehrlich- Schwoebel step-edge barriers. The behavior of the height-difference correlation function and the time-dependent roughening is found to be in good agreement with studies of continuum models based on the Kuramoto-Sivashinsky (KS) equation. However, the Laplacian term in the KS equation has components arising from both the ES barrier and etching/desorption effects so that the effect of the ES barrier in producing the instability is weakened, compared to thin film growth examples. Using theoretical expressions for the kinetic coefficients in the KS equation, we find that the Ehrlich-Schwoebel barrier is ~ 0.05 eV in this system. We will also present initial results studying "facetting" during wet etching of GaAs (001). The initial formation of anisotropic "hillock" structures develops in time to form a hill-and-valley structure along the (110) direction, with faces close to [111]. The length scale coarsens in time and is dependent on the etchant composition. Comparisons with theoretical studies of kinetically controlled crystal growth and etching will be discussed.

11:20am **SS1-WeM10 Step Motion on the Cu(100)-(@sr@2x2@sr@2)R45°-O Surface**, *C.L.H. Devlin,* Air Force Research Lab, U.S.*; J.P. Landry,* University of California, Davis*; N.C. Bartelt,* Sandia National Laboratories*; **S. Chiang**,* University of California, Davis

Low energy electron microscopy (LEEM) was used to study the motion of single-atom-high steps on a Cu(100) surface covered with the (@sr@2x2@sr@2)R45°-O structure. Curved steps exhibited capillary wave motion, which was analyzed using Langevin Dynamics.@footnote 1@ From this analysis, the dominant mode of adatom diffusion (i.e., along steps or over terraces) was deduced. Parameters such as the step stiffness and kink activation energy were also discovered. @FootnoteText@ @footnote 1@ N.C. Bartelt and R.M. Tromp, Phys Rev B 54 (1996) 11731.

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