Wednesday Morning, October 4, 2000

Thin Films
Room 203 - Session TF-WeM

Modeling of Thin Film Growth

Moderator: L. Hultman, Linköping University, Sweden

8:20am **TF-WeM1 Hyperthermal Ion Enhanced Deposition of Materials**, ***J.W. Rabalais,*** University of Houston **INVITED**

The chemical and physical interactions of ions with surfaces in the energy range 5 eV to several keV will be described. Hyperthermal reactive ions impinging on surfaces provide a method for deposition/growth/synthesis of materials within a unique nonequilibrium UHV environment, giving rise to the technique of ion beam deposition (IBD). IBD allows independent control over parameters such as ion energy and type, ion fluence and dose, substrate temperature, and background gases. The depth of penetration/interaction of the impinging ions with the surface is determined by the ion kinetic energy. The excellent control over ion dose allows deposition of thin films, e.g. < 30 @Ao@, with sharp film-substrate interfaces. The UHV conditions in the sample chamber allow deposition onto atomically clean and well-ordered surfaces. In situ diagnostic techniques, such as reflection high energy electron diffraction (RHEED), x-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES), mass spectrometry, and a microbalance allow direction characterization of the deposited/reacted layers. Examples of the use of mass- and energy-selected beams for hyperthermal surface reactions, film growth, and shallow implantation will include: Si+ ion homoepitaxy, growth SiO2 and TiSi2 films on silicon, growth of Ti and TixAlyOz films on sapphire (a-Al2O3), controlling cationic diffusion coefficients in sapphire, and interactions of chlorotitanium ions TiClx+ with graphite and silicon surfaces.

9:00am **TF-WeM3 Thin-Film Growth on Polymer Surfaces through Polyatomic Ion Deposition: Molecular Dynamics Simulations**, ***Y. Ji,*** *S.B. Sinnott,* The University of Kentucky

Ion deposition on polymer surfaces is widely used to deposit polymer thin films or modify the mechanical properties of the polymer surface. In this work the reactions of polyatomic ions with a polystyrene surface are investigated through classical molecular dynamics simulations. The classical reactive empirical bond order potential is used.@footnote 1@ The particular ions of interest are CH@sub 3@@sup +@ and C@sub 3@H@sub 5@@sup +@ which are deposited over a range of energies from 20 to 100 eV. The chemical reactions that occur on impact are shown to depend heavily not only on the incident energy but also on the structure and size of the ion. Information about penetration depths and energy transfers are also obtained from the simulations. The results are compared to experimental data obtained for the growth of fluorocarbon thin films through the deposition of the comparable fluorocarbon species on polystyrene. There is generally good agreement between the experimental and computational results.@footnote 2@ The simulations also address the effect of incident angle on the results of ion deposition. The differences between the reactions that occur at normal incidence and at various angles are discussed. This work is supported by the National Science Foundation (CHE-9708049). @FootnoteText@ @footnote 1@.S.B. Sinnott, L. Qi, O.A. Shenderova, D.W. Brenner, in Chapter 1 of Volume IV of ADVANCES IN CLASSICAL TRAJECTORY METHODS, Molecular Dynamics of Clusters, Surfaces, Liquids, and Interfaces, Ed. W. Hase (JAI Press, Inc., Stamford, CT, 1999), pp. 1-26. @footnote 2@M.B.J. Wijesundara, L. Hanley, B. Ni and S.B. Sinnott, Proceedings of the National Academy of Science, USA 97 23-27 (2000).

9:20am **TF-WeM4 Molecular Dynamics Simulation of Ion Bombardment on Hydrogen-terminated Si(001)-(2X1) Surfaces**, ***K. Satake,*** Mitsubishi Heavy Industries, Ltd., Japan*; D.B. Graves,* University of California, Berkeley

In crystalline Si growth using low-temperature plasma enhanced chemical vapor deposition (PECVD), it is important to clarify the role of ions in the surface reactions. We present here the interaction between an H-terminated Si(001)-(2X1) surface and normal incident SiH@sub 3@ @super +@ and H@sub 2@ @super +@ ions as a function of the incident energy (10 eV, 20 eV, and 40 eV) using molecular dynamics (MD) simulations. SiH@sub 3@ @super +@ was observed to penetrate less than 3-4 Å at 10 eV and 20 eV, increasing to about 5 Å at 40 eV. H@sub 2@ @super +@ penetrated the surface only slightly at 10 eV, but the penetration depth increased rapidly with increasing energy. At 40 eV, H@sub 2@ @super +@ was observed to penetrate up to 20 Å, or even farther. Per trajectory, SiH@sub 3@ @super +@ was observed to displace about 4 Si atoms in the lattice, an average distance of about 2-3 Å, at 40 eV. H@sub 2@ @super +@, by contrast, displaced on average, only 0.7 Si atoms per trajectory, and the displacement distance was about 1.5 Å, at 40 eV. It is suspected that ion impact creates sites which react more readily with neutral species. The generation rate of dangling bonds (DB) at the surface due to H@sub 2@ @super +@ ion impact is about twice that of SiH@sub 3@ @super +@ ions for the energies studied. In the DB generation by H@sub 2@ @super +@ ions, the primary process is direct surface H atom sputtering. In addition, we also observed the DB generation with dihydride and monohydride formation by H insertion into the Si dimer and H exchange. In the case of SiH@sub 3@ @super +@ ions, the probability of DB generation by direct sputtering is almost the same as that of insertion; however, in addition, the near-surface crystallinity is disrupted in most of the trajectories. The H@sub 2@ @super +@ ion bombardment under 20 eV, by contrast, can enhance the surface reactivity by creating defects only in the top surface layer without damaging the crstallinity of the underlying silicon.

9:40am **TF-WeM5 Low Temperature Growth of 2D Pb Islands on Si(111)7x7 Surfaces**, ***C.S. Chang,*** Academia Sinica, Taiwan, ROC*; S.H. Chang,* National Tsing Hua University, Taiwan, ROC*; W.B. Su, C.M. Wei,* Academia Sinica, Taiwan, ROC*; L.J. Chen,* National Tsing Hua University, Taiwan, ROC*; TienT. Tsong,* Academia Sinica, Taiwan, ROC

Lead (Pb) is known to grow on Si(111) with the Stranski-Krastanov (SK) mode at room temperature. With the variable temperature scanning tunneling microscopy, we study the low temperature growth of Pb films on the Si(111)-7x7 surface from T ~40 K to 200 K. The islands are formed after the completion of the wetting layer and display peculiar properties that cannot be categorized into any of the conventional growth modes. Their tops are all very flat and even more surprisingly, they prefer to grow into some discrete thicknesses corresponding to 4, 7 and 9 atomic layers. Among them, that equivalent to seven atomic layers is especially dominant. While the stress in heteroepitaxy may be the only dominant factor for a thick film and hence causes the film to form into 3D islands, for a thin film some other effects may be in play to counterbalance the stress. One of such effects is the "quantum size confinement", which could reduce the system energy due to quantization of the confined electrons in the film. Preliminary ab initio calculations seem to support this theory.

10:00am **TF-WeM6 Modeling of Cluster Ion-Surface Interactions with Full Inclusion of Internal Degrees of Freedom**, ***K.J. Boyd,*** University of New Orleans*; A. Lapicki, S.L. Anderson,* University of Utah

Molecular dynamics simulations with embedded atom or tight binding moment approximation potentials are used to investigate the interactions of small cluster ions (N<50) with metal surfaces. The simulations are performed at constant target temperature, with the cluster initially thermostatted independently. This allows the internal vibrational and rotational degrees of freedom of the cluster to be treated properly. At room temperature, the vibrational energy content of a 50 atom cluster may be several eV, which is comporable to the translational energy of the cluster. The rotational energy at room temperature is much lower, but the effect of cluster rotations is to change the momentum of cluster atoms such that they impinge at non-normal incidence on the target. This non-normal momentum component may alter the dynamics of cluster deposition by changing the fragmentation and penetration behavior.

10:20am **TF-WeM7 Extension Velocities for Level Set Based Surface Profile Evolution**, ***D.F. Richards,*** *S. Sen, M.O. Bloomfield, T.S. Cale,* Rensselaer Polytechnic Institute

Level set based front-tracking methods represent an attractive alternative to more traditional node and segment based approaches to tracking interface motion. Level set methods avoid many topological difficulties which arise in node-moving schemes and are easily extended to three dimensions. However, level set methods also require knowledge of the speed function at every point in the solution domain. This is a somewhat troublesome requirement for profile evolution models since the interface speed may have no physical meaning at points that are not on the surface. The solution to this problem is to formulate extension velocities that in some way extrapolate speeds from the interface to other points in the solution domain. We compare several different methods for determining extension velocities and discuss the characteristics of node and segment approach that are helpful in calculating extension velocities.

10:40am **TF-WeM8 Models of Electrochemical Deposition of Copper Thin Films:The Effect of Leveling Agents**, *S. Soukane,* ***T.S. Cale****,* Rensselaer Polytechnic Institute

As device sizes decrease, the ability of electroplating to create conformal films in deep features make it very attractive. Especially beneficial in interconnect applications is the "leveling" effect of certain organic additives. With the use of these leveling agents, electroplating offers the possibility of a superfilling effect, leading to void-free structures. This effect is often attributed to the inhibition of plating along feature sidewalls. Much feature-scale modeling work has been focused on reproducing the effect of the additive during deposition. The inhibition has been assumed to be due to operation at a mass transport-limited rate that allows the leveling agent to be completely depleted in the region near the surface. This may be a good assumption if the agent is highly reactive and used in quantities on the order of hundreds of ppm. Its inhibiting effect is usually correlated to the expression of the current density by a factor that is a function of the leveling agent flux to the surface. This approach limits the opportunities to look for explanations via chemical mechanisms. We show that the leveling effect can be explained via a more detailed chemical mechanism involving adsorbed species. We present a feature-scale model coupling the potential and concentration fields via the current density at the feature surface, together with a chemical mechanism involving surface species. In this chemical mechanism, copper ions go through two successive irreversible reactions. The first step is a charge transfer reaction, leading to an adsorbed copper species on the surface. The second is much faster, consisting of the adsorbate reduction and insertion into the film. It is assumed that the leveling agent is completely transformed on the surface to new species that play the important roles in the inhibition effect. These proposed surface species can undergo slow desorption reactions or can be incorporated in the solid at a rate much slower than copper insertion.

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