Surface Science
Room 209 - Session SS2+NS+TF-MoM

Nucleation and Growth
Moderator: G.L. Kellogg, Sandia National Laboratories

8:40am **SS2+NS+TF-MoM2 Homoepitaxial Growth of Ni on Ni(110) : Surface with Anisotropic Diffusivity and Energy Barriers**, ***B.-Y. Choi,*** Seoul National University, Korea*; S.-J. Kahng,* University of Illinois at Urbana-Champaign*; J.-Y. Park, Y. Kuk,* Seoul National University, Korea

The homoepitaxial growth of Ni was studied on Ni(110) surface with scanning tunneling microscopy. The Ni(110) surface does not reveal surface reconstruction, but it has corrugated channels along the [1 -1 0] direction and the resultant surface diffusion anisotropy. Homoepitaxial islands grow with high aspect ratio, as large as 1:1000, due to i) the diffusion anisotropy and ii) the energy barrier from an [1 -1 0] side wall to an [001] side wall around the adatom islands. The aspect ratio of the islands decreases with increasing temperature. The competition between these two mechanism will be discussed. At the high coverage (@>=@10ML), the aspect ratio decreases substantially and the growth structure transforms to 3D islands without asymmetry. At these coverage, the surface roughness saturates. Although the microscopic origin is unclear, the phenomenon can be explained with a KPZ type equation with some modifications.

9:00am **SS2+NS+TF-MoM3 Thermodynamics of Thin Film Alloys: Experimental and Theoretical Study of Ag and Co on Ru(0001)**, ***G.E. Thayer,*** University of California, Davis*; A.K. Schmid, V. Ozolins, N.C. Bartelt,* Sandia National Laboratories*; S. Chiang,* University of California, Davis*; R.Q. Hwang,* Sandia National Laboratories

It has long been known that the structure of materials in thin film configurations can differ significantly from their bulk phase. This is particularly true of alloy films. It has recently been shown that strain induced by the lattice mismatch between substrate and film can lead to the formation of novel alloys that do not exist in the bulk. One prototypical example is the system of one monolayer Ag/Co films grown on Ru(0001). In the bulk, Ag and Co are immiscible. However, on the Ru surface alloy phases of distinct stoichiometries are formed. We have investigated the phase diagram of 1ML AgCo/Ru(0001) films using scanning tunneling microscopy (STM) and first principles calculations. For Ag rich films, segregation between a pure Ag phase containing dislocations and a pseudomorphically strained alloy of stoichiometry Co@sub 0.6@Ag@sub 0.4@ is found. The driving force for the phase segregation is the competition between two strain relief mechanisms: dislocation formation and alloying. In the Ag saturated Co@sub 0.6@Ag@sub 0.4@ alloy, atomic resolution STM images show that the alloy consists of a Co film containing disordered, elongated Ag droplets with an average size of 30 atoms separated by an average distance of 10 Co atoms. As the composition of Ag in the film is decreased, the Ag droplets become more uniform in size and decrease to an average minimum size of 10 atoms. Simultaneously, the distribution of the droplets becomes uniform and dilute. This behavior has been predicted using first principles, local density approximation (LDA) calculations. These calculations, together with atomically resolved STM images, have quantified configuration energies for various stoichiometries of this system. This investigation has led to a quantitative interpretation of the competition between the chemically repulsive interaction of Ag and Co (also seen in their bulk miscibility gap) and the strain fields in the thin film alloy that they form.

9:20am **SS2+NS+TF-MoM4 Theory of the Nucleation and Growth of Iron on GaAs**, ***S.C. Erwin,*** Naval Research Laboratory*; M. Scheffler,* Fritz Haber Institute, Germany

By growing ultrathin films of ferromagnetic metals on semiconductor substrates, it is possible to create a partially spin-polarized electrical current in the semiconductor. This phenomenon is the starting point for a wide variety of magnetoelectronic devices based on the "spin-valve" effect, whereby an externally applied magnetic field can switch the current on and off. Considerable experimental effort has focused on ultrathin films of Fe grown by MBE on GaAs, in part because their small lattice mismatch results in nearly epitaxial films. Although a number of experiments have contributed to a detailed description of the phenomenology of magnetism in these films, little is known about the microscopic physics of magnetism at an intimate metal-semiconductor interface. We use spin-polarized density-functional total-energy methods to investigate the nucleation and initial growth phases of Fe on GaAs(001), focusing on the roles played by diffusion, magnetism, and defect chemistry. Our findings include the following results: (1) magnetism develops in the very first monolayer, and is in fact enhanced by the presence of the interface; (2) surface diffusion is strongly suppressed in the submonolayer regime by the tendency of Fe adatoms to form very stable Fe-As bonds. Finally, we discuss the influence of the initial GaAs reconstruction on the structure and magnetic properties of the Fe film.

9:40am **SS2+NS+TF-MoM5 Nucleation and Growth in Metal-on-Metal Epitaxy - Complications beyond Simple Systems**, ***R.J. Behm,*** University of Ulm, Germany **INVITED**

The quantitative atomic scale understanding of a surface process, as a sequence of elementary steps, is one of the primary objectives in Surface Science. Molecular beam epitaxial growth (MBE) is one the first areas where extensive and systematic studies, both experimental and theoretical, have led to such kind of understanding, at least for simple processes such as nucleation and two-dimensional growth on inert, bare and non-reconstructed substrates.@footnote 1@ In this talk I will focus on complications which arise when these conditions are not fulfilled, predominantly on the effect of coadsorbed species on nucleation and growth processes. These coadsorbates, which are generally present, e.g., in the case of chemical vapor deposition (CVD), are shown to affect not only the nucleation behavior, but may lead also to the formation of new, (metastable) film structures. A second topic to be discussed involves nucleation and growth on 'instable' surfaces, where growth competes with exchange processes and surface alloy formation. On such systems and under certain conditions metal deposition was found to cause a severe restructuring of the substrate, leading to pit formation. Mechanistic ideas will be presented and discussed. @FootnoteText@@footnote 1@H. Brune, Surf. Sci. Rept. 31, 121 (1998).

10:20am **SS2+NS+TF-MoM7 Preferential Nucleation of Metal Nanoclusters on S(4x4)/W(111)**, ***Q. Wu,*** *W. Chen, T.E. Madey,* Rutgers, The State University of New Jersey

Interactions of several metals (Cu, Pt and Pd) with the highly ordered S(4x4)/W(111) surface have been studied by means of Auger electron spectroscopy (AES), low energy electron diffraction (LEED), and scanning tunneling microscopy (STM). The substrate is a sulfur-induced nanoscale reconstruction of W(111) with (4x4) periodicity, characterized by broad, planar terraces (~ 30 nm in width). We find that fractional monolayers of vapor-deposited Cu grow as 3D clusters on the S(4x4) surface over a wide coverage range. At low Cu coverages (@<=@ 0.1 ML), Cu nanoclusters are observed to nucleate preferentially at characteristic 3-fold hollow sites on the S(4x4) surface; there is a clear energetic preference for one type of site over others. The formed Cu nanoclusters are uniform in size (~ 0.7 nm) up to 0.25 ML, indicating self-limiting growth. As coverage increases, additional sites are populated and Cu clusters grow in size. On the other hand, Pt and Pd exhibit a different behavior, disordering the (4x4) reconstruction and adsorbing beneath the outer S-layer. STM data are supported by LEED and AES measurements. The data are interpreted in terms of relative surface free energy, relative reactivity, and the metal-W, metal-S, and S-W binding energies, as supported by our previous TPD data.

10:40am **SS2+NS+TF-MoM8 Ultra-thin Al Films Grown Epitaxially on CaF@sub 2@/Si(111)**, ***Y.V. Shusterman,*** *N.L. Yakovlev, L.J. Schowalter,* Rensselaer Polytechnic Institute

Electron scattering at metal boundaries becomes increasingly important as interconnect structures shrink further. To improve our understanding of this phenomenon, studies of electron transport through ultra-thin metal films are needed. In such experiments, it is desirable to have smooth, single crystal metal layers grown on an insulating substrate. For this reason, we are studying epitaxial growth of Al on CaF@sub 2@/Si(111), with metal thickness as low as several nanometers. The structures discussed in this work were grown by molecular beam epitaxy and investigated by reflection high-energy electron diffraction (RHEED), scanning tunneling microscopy (STM) and atomic force microscopy (AFM). Hydrogen-terminated Si(111) was used as a substrate. The CaF@sub 2@/Si interface was formed at 700°C, followed by fluoride overgrowth at temperatures below 200°C, which resulted in improved continuity of the subsequent Al layer. The roughness of the final CaF@sub 2@ surface was below 1nm, as measured by AFM. The Al films grew epitaxially, as revealed by RHEED patterns that only contained streaks. The spacing between the streaks from Al was about 4/3 times larger than that from CaF@sub 2@, in agreement with bulk lattice mismatch. The growth proceeded through formation of 3-dimentional islands that then coalesced as the thickness increased. Using an Al deposition rate above 1nm/s at room temperature, we were able to

obtain continuous films as thin as 10nm with roughness less then 2nm. The STM images of these films showed atomic steps, some of them originating at screw dislocations. The density of these dislocations was around 10@super 11@ cm@super -2@. The dependence of Al conductivity on film thickness will also be presented.

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