Wednesday Morning, November 6, 2002

Surface Science
Room: C-110 - Session SS+EL-WeM

Nucleation & Growth of Semiconductors
Moderator: B.S. Swartzentruber, Sandia National Laboratories

8:20am **SS+EL-WeM1 Nucleation and Epitaxial Growth of Gallium Nitride on Sapphire (0001) using Ion-beam-assisted Molecular Beam Epitaxy**, ***B. Cui***, *I.P. Steinke, P.I. Cohen*, University of Minnesota

Molecular beam epitaxy (MBE) is a far from equilibrium growth technique that relies purely on thermal energy to provide high quality thin films. At the relatively low temperatures used a key limitation is often the widely disparate adsorptive and diffusive properties of the film constituents. To provide additional control over the growth kinetics, we have used a low energy ion beam from a Kaufman source to impinge on the surface at low glancing angle of about 4 degrees. First experiments examined the nucleation and growth of GaN on the basal plane of sapphire. The sapphire substrates were pretreated in an ion flux and then annealed for cleaning. The sapphire was then nitrided at 1100K for about 10 min. Then GaN was nucleated by a sequence of adsorption and annealing steps. Finally, a very thin film of GaN was grown under conditions of excess Ga. Ammonia was the nitrogen source throughout. For comparison a GaN film was grown under identical procedures but using an ion beam. An Ar ion beam at 300 eV with a current of 20 micro A/cm2 was incident on the sample after a few of the initial nucleation steps were carried out. Atomic force micrographs of the resulting films showed films with a granular structure. The grains were nearly doubled in size. Small islands apparent in the normal growth were not present when the films were grown using the ion beam. The evolution of the island sizes is compared to a rate equation model of the ion-assisted growth. Partially supported by the National Science Foundation and the Office of Naval Research.

8:40am **SS+EL-WeM2 STM Characterization of Ge Nucleation on Ge(001)**, ***M. Li***, *E.I. Altman*, Yale University

The initial stage of Ge homoepitaxial growth has been studied using scanning tunneling microscopy (STM). When 0.12 ML of Ge was deposited on the Ge(001) surface at 310 K, <130>-oriented metastable clusters dominated the surface with very few epitaxial dimer rows oriented across the substrate dimer row. Increasing the Ge coverage to 0.18 ML led to an increase in the density of epitaxial dimer rows. Metastable dimers disappeared at the same Ge coverage but at a higher growth temperature of 420 K, which can be explained by the competing process of the transition from metastable dimers to stable epitaxial dimers against that of the coalescence of metastable dimers to form <130>-oriented metastable clusters. At the same temperature, a myriad of epitaxial structures including single buckled B dimers, single nonbuckled dimer rows with ends terminated by either B and D dimers or D dimers only; single buckled dimer rows; pairs of buckled dimer rows with local c(4x2) structures; pairs composed of one buckled and one nonbuckled dimer rows; as well as larger epitaxial islands were first observed. The observed islands as well as second-layer nucleation elongate preferably along 2x direction of the islands and substrate respectively, which can be explained by 1) the fast diffusion of ad-dimers along 1x direction (dimer row direction) of the islands and substrate; and 2) the strong capture probability of diffusing ad-dimers along 2x direction of the islands and substrate. Nonbuckled SA steps and nonbonded SB steps, which were claimed not to exist on stepped and singular Ge(001) surfaces, were populated on single dimer rows. The interactions between various steps of epitaxial structures and neighboring dimers are also discussed.

9:00am **SS+EL-WeM3 High Resolution Large Area STM Analysis of Nucleationless Island Formation in SiGe/Si(100)**, ***P. Zahl***, *P.W. Sutter, J.S. Palmer, E.A. Sutter*, Colorado School of Mines

We present an STM analysis of quantum dot (QD) island self-assembly in lattice-mismatched heteroepitaxy. A primary objective of recent research on QD growth is the creation of long-range ordered arrays of QDs of uniform size, a major technological milestone that would pave the way for application of these nanostructures in electronic and optoelectronic devices. The formation of epitaxial QD islands is generally assumed to involve nucleation, a statistical process that would severely impede QD organization. Our recent observations by atomically resolved large area STM document the complete transition from initial surface roughening to the formation of faceted QDs in the heteroepitaxial SiGe/Si(100) system. QD self-assembly occurs in a coninuous process that avoids nucleation.[1,2] Combining growth with in-situ STM, we analyze the surface morphology evolution with increasing coverage. The key aspect of this analysis is the capability of our system to acquire very large STM scans (up to 400nm x 1000nm with 0.1nm resolution), with an unprecedented combination of image detail and statistics. The 2xn reconstruction and step meandering are analyzed at lower coverages, with the goal of identifying mechanisms that induce long-range order in the nucleationless islanding process. Statistical information is extracted using a SPA-LEED[3,4] like analysis of STM images in reciprocal space. At higher coverages the surface gets micro-rough and a transition to 3D growth of faceted, pyramid shaped QDs occurs. The arrangement and influence of the surrounding micro-rough area is analyzed in detail, depending on germanium concentration and growth conditions.

[1] P. Sutter and M.G. Lagally, Phys. Rev. Lett. 84, 4637 (2000)
[2] R.M. Tromp, F.M. Ross, and M.C. Reuter, Phys. Rev. Lett. 84, 4641 (2000)
[3] Spot Profile Analysing-LEED
[4] M. Horn-von Hoegen, Z. f. Kristallographie 214, 591, 727 (1999), I+II.

9:20am **SS+EL-WeM4 Scanning Probes and Transition States: Uncovering the Low-barrier Si ad-dimer Diffusion Mechanism on Si(001) by its Electric Field Dependence**, ***T.R. Mattsson***, *B.S. Swartzentruber*, Sandia National Laboratories, *R. Stumpf*, Motorola Labs, *P.J. Feibelman*, Sandia National Laboratories

Surface diffusion and reactions occur on a picosecond time scale, making direct observation of their atomic mechanisms difficult. Yet, understanding these processes is necessary to control the evolution of surfaces at the nanoscale. We show that the electric field dependence of barriers for surface diffusion and other surface processes can be used to discriminate between different proposed atomic mechanisms. Using density functional theory calculations, we show that "piecewise diffusion", the previously accepted atomic mechanism for ad-dimer diffusion on Si(001), where the ad-dimer partly splits during the transition, has the opposite field-dependence to what is observed. It therefore cannot be the dominant mass-transport mechanism. We describe an alternate process wherein the ad-dimer "walks" along the dimer row, combining rotational and translational motions. This process has a low barrier at zero electric field and a field dependence in agreement with measurements. This approach, comparing the measured and calculated effects of an electric field, is not limited to diffusion on semiconductors, but can also be used to study, e.g., dissociative adsorption barriers. Thus, the electric field in a scanning probe should not be considered a nuisance which is to be corrected for by extrapolating results to zero field, but instead a tool that helps us study states otherwise inaccessible. T.R.M. acknowledges support from the Motorola/SNL computational materials CRADA. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04- 94AL85000.

9:40am **SS+EL-WeM5 Simulations of Surface Diffusion on Amorphous Silicon**, ***A.S. Dalton***, *E.G. Seebauer*, University of Illinois

Surface diffusion over amorphous materials plays a governing role in an increasing variety of applications, including reflow of amorphous metals and oxides, and nanostructure formation for electronic memory devices. However, there exists little literature describing diffusion on amorphous surfaces. The structural and energetic heterogeneity of amorphous surfaces should lead to diffusivities that differ significantly from crystalline ones. Our recent experimental work has confirmed that that activation energy for surface-self diffusion on amorphous Si (a-Si) differs significantly from that for crystalline Si (c-Si), and that the activation energy is temperature dependent. Here we describe the results of molecular dynamics simulations to gain atomistic insights into these phenomena. Calculations using a modified Stillinger-Weber potential confirm marked differences between diffusion parameters on a-Si vs. c-Si, with lower activation energies for a-Si. Collective motions involving two or three atoms play a significant role, as do long hops over several atomic diameters. Both hopping motion and formation of mobile atoms can be described with distribution functions, which ultimately give rise to temperature-dependent Arrhenius parameters for diffusion.

10:00am **SS+EL-WeM6 Relaxation of a Single Silicon Mound during Silicon Deposition on the Si(111)(7x7)**, ***A. Ichimiya***, *Y. Tsutsui*, Nagoya University, Japan

Isolated single three dimensional (3D) silicon mounds on the Si(111)(7x7) surface between 700K and 800K have been produced using a tip of a scanning tunneling microscope (STM). Produced 3D mounds are like pyramids with certain facets for the both surfaces. Indices of main facets of the mounds on the Si(111) surface are {311} and small facets are {221}. Without silicon deposition, the pyramid begins to decompose just after the

deposition. During the decomposition of the mound, the facets of the pyramid transform into multi-bilayer steps. Finally the mound becomes a bilayer (2D) island with a truncated triangle shape. When silicon atoms are deposited on the surface with retracting the STM tip, the decay rate is reduced due to increasing chemical potential on the surface. For deposition of $5x10^{12}$ atoms at 700K, the mound is grown slowly just after the production. The height of the mound decreases and the top of the pyramid is truncated. The facets of {311} increase the area and the {221} facets are reduced. Then the pyramid becomes truncated pyramid with stable height of about 10 bilayers. Shapes of the bottom and the top layers are just triangles while these shapes become truncated triangles during decay of the mound without deposition. The difference between the shapes with and without deposition is due to the difference of the chemical potentials on the silicon surface. Therefore the {311} facets of the pyramid become dominant and the {221} facets disappear at growth mode of silicon on the Si(111). The behavior of the pyramid during deposition has been expected that the shape changes into two dimensional island, and the {221} facets remain, because silicon mounds tend to two dimensional island during growth on silicon surfaces. It is noted that the present result is different from expectation from the results of the decay process of the pyramid on the Si(111).

10:20am **SS+EL-WeM7 Morphology of Crystal Growth on Vicinal Surfaces: MBE and H-assisted MBE Growth on Laser-textured Ge(001)**, *A. Raviswaran*, ***D.G. Cahill***, University of Illinois

We delineate the growth conditions of temperature, substrate vicinality, and concentration of surface adsorbates that produce rough and smooth crystal growth of Ge by molecular beam epitaxy. Ge(001) substrates are modified by laser texturing to produce a large range of vicinalities $0<\theta<10°$ within a 5 μm diameter laser-dimple. We then deposit Ge on these modified substrates over a wide range of growth temperatures $150<T<450°C$, with and without an atomic hydrogen flux of 10^{13} cm^{-2} s^{-1}, and characterize the morphologies by atomic-force microscopy. Hydrogen flux suppresses the growth-mound instability at low vicinality and reduces the epitaxial critical thickness at large vicinality. Highly-elongated mounds continue to dominate the morphology to surprisingly high growth temperatures; at even higher temperatures, the morphology of vicinal surfaces is dominated by step-bunching instabilities and the formation of low angle facets. Hydrogen adsorbates continue to play a role in the growth morphology at $T=450°C$ when the steady-state hydrogen coverage is only a few percent.

10:40am **SS+EL-WeM8 Characterization of Si(100) Homoepitaxy Grown in the STM at Low Temperatures**, ***H. Grube***, *G.W. Brown*, *M.E. Hawley*, Los Alamos National Laboratory

We explore the growth of low-temperature bulk-like Si(100) homoepitaxy with regard to microscopic surface roughness and defects. We characterize films grown at different temperatures up to 500K in-situ by means of an effusion cell added to our UHV-STM. The development of novel architectures for future generation computers calls for high-quality homoepitaxial Si(100) grown at low temperature.[1] Even though Si(100) can be grown crystalline up to a limited thickness,[2] the microstructure reveals significant small-scale surface roughness[3] and defects specific to low-temperature growth.[4] Both can be detrimental to fabrication and operation of small-scale electronic devices.

[1] B. Kane, Nature 393, 133 (1998)
[2] DJ Eaglesham, J. Appl. Phys., 77, 3597 (1995)
[3] RJ Hamers et al., J. Vac. Sci. Technol. A 8, 195 (1990)
[4] MJ Bronikowski et al., Phys. Rev. B, 48, 12 361 (1993) .

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