Wednesday Afternoon, October 27, 1999

Surface Science Division Room 606 - Session SS1+EM-WeA

Semiconductor Surface Science

Moderator: C.T. Campbell, University of Washington

2:00pm SS1+EM-WeA1 Electronic Transport Properties of Silicon Surfaces@footnote 1@, K. Yoo, University of Tennessee; A.P. Baddorf, Oak Ridge National Laboratory; H.H. Weitering, University of Tennessee

Most of our information about surface electronic properties has come from spectroscopic measurements and first principles electronic structure calculations. Direct measurements of transport properties of ultrathin films have revealed interesting physical properties, including quantum size effects. However, to correctly measure the surface or thin film conductivity, the conduction path through the bulk or substrate must be eliminated. We attempt to accomplish this by using crystalline silicon of "silicon on insulator"(SOI) material. Using STM, we have recently shown that 40 nm-thick Si(100) layers on SOI can be prepared with a comparable degree of structural perfection as the surfaces of bulk Si.@footnote 2@ For these SOI films, we also observed that at room temperature, LEED spots drift and gradually disappear during prolonged exposure to the electron beam, indicating that the ultrathin Si top layer is fully depleted of mobile carriers, i.e. non-conducting. This leaves surface states as the only conduction channel. We have measured the surface conductivity of the Si(100)2x1 reconstruction on SOI as a function of temperature and Si film thickness during exposure to molecular oxygen using a four-point probe technique in ultrahigh vacuum. The oxygen induced conductivity changes strongly depend on the Si film thickness (@DELTA@@sigma@=-1.75x10@super -5@(@ohm@@super -1@) for 40 nm and (@DELTA@@sigma@=-9.219x10@super -6@(@ohm@@super -1@) for 90 nm thick films at room temperature. Differences are also observed in the temperature dependence, with possibly significant surface contributions to total sheet resistance at low temperature. These results indicate a correlation between transport properties and surface states, which will be discussed. @FootnoteText@ @footnote 1@ Work supported by National Science Foundation(DMR-9705246). @footnote 2@ K. C. Lin et al, Appl. Phys. Lett. 72, 2313(1998).@footnote *@ Managed by Lockheed Martin Energy Research Corp.

2:20pm SS1+EM-WeA2 Reinterpretation of the Scanning Tunneling Microscopy Images of Si(100) (2x1) Dimers-Observation on a Defect Free Surface, K. Hata, S. Yasuda, H. Shigekawa, University of Tsukuba, Japan

In this presentation, we demonstrate that STM images of dimers of Si (100) taken with usual tunneling conditions are seriously characterized by tunneling from surface resonances and bulk states. In some cases, tunneling from these states overwhelm tunneling from the surface states which STM is generally believed to observe. The key point was the success to fabricate an almost defect-free Si(100) clean surface (defect density ~0.1%), making observations at a very low bias possible (0.5V). STM images of the dimers at 80K and room temperature taken at such low biases showed several new features. (1) In the empty states, when the surface bias is above ~1.4V, regions between the dimers are observed. (2) At 80K, a bright row similar to that observed at room temperature is obtained. though a bright and dark (2x1) unit align alternatively along the dimer row direction. The brighter units observed at the high bias corresponds to the location of the upper atom. (3) In the filled states, each atoms of the dimers at room temperature when the surface bias is lower than ~-1V. Every time when the bias is increased, the STM images of the dimers would gradually revert to the usual bean-type image of dimers at ~-1V. High resolution CITS measurements and first principle calculations also showed consistent results. We revisit and refine the interpretation of the STM images of the dimers, insisting that tunneling from surface resonances and bulk states are very important. The new interpretation brings results of many experimental and theoretical researches into an unanimous agreement.

2:40pm SS1+EM-WeA3 STM-Study of the Absorption of Molecular Oxygen on GaAs(100), *P. Kruse, J.G. McLean, A.C. Kummel,* University of California, San Diego

There is currently a strong interest in making GaAs-oxide interfaces with very low defect densities to enable the use of GaAs-based FET technology. The interaction of oxygen with the GaAs surface plays an important role in this process. In this study, high-resolution scanning tunneling microscopy (STM) was used to image the chemisorption sites of molecular oxygen on

the three most common reconstructions of the GaAs(100) surface, c(2x8), 6x6 and c(8x2) . All studies were performed at room temperature. The sticking probability was greatest on the surfaces with As-As dimer bonds. Even though the molecular oxygen prefers to initially react with the empty dangling bonds of the Ga atoms, after dissociation the oxygen atoms seek to form bridge bonds between an electron rich As atom from an As-As dimer and a second atom, either As or Ga. These dimerized As atoms do not exist in the c(8x2) reconstruction, hence the greater inertness of that surface. This is in contrast to the reaction of these surfaces with halogens which only need to form one bond per halogen atom and equally attack all reconstructions.

3:00pm SS1+EM-WeA4 Chaotic-like Wavefunction Beating in Thin Silver Films with a Quasiperiodic Superstructure, *C.-S. Jiang*, *H. Yu*, University of Texas, Austin; *Ph. Ebert*, Forschungszentrum J@um u@lich, Germany; *X.-D. Wang*, *R. Diener*, *Q. Niu*, *C.K. Shih*, University of Texas, Austin

It has been shown that atomically-flat Ag films can be grown on GaAs(110) substrates. These surfaces with (111) orientation exhibit, in addition, a onedimensional quasi-periodic superstructure. Taking such surfaces as a model system, we investigated the effect of quasi-periodic scattering potential on the electronic structure by using spatially resolved scanning tunneling spectroscopy. Quantum well states due to the z-confinement of the 2-D thin film are clearly observed as a function of thickness. In addition, we have observed very intriguing chaotic interference patterns The observation of chaotic interference pattern is found to arise from the quasiperiodic superstructure acting as scattering potential for the 2-D electronic system. Theoretical calculations of the electronic states of quasiperiodic structure are currently underway.

3:20pm SS1+EM-WeA5 3C-SiC(100) c(4x2) Surface and Sub-Surface Probed by Core Level Photoemission Spectroscopy Using Synchrotron Radiation and by Scanning Tunneling Microscopy, V. Derycke, H. Enriquez, P. Fonteneau, V.Yu. Aristov, P.G. Soukiassian, Commissariat à l'Energie Atomique and Université de Paris-Sud/Orsay, France; G. Le Lay, CRMC2 -CNRS and Université de Provence, France; C. Grupp, A. Taleb-Ibrahimi, LURE, Université de Paris-Sud/Orsay, France

We investigate the 3C-SiC(100) c(4x2) reconstruction surface and subsurface regions by Si 2p core level photoemission spectroscopy using synchrotron radiation at various photon energies and by atom resolved scanning tunneling microscopy (STM). The latter experiments are performed by tunneling into the empty and filled electronic states which allows to clearly identify both up- and down dimers (AUDD) [1] of the c(4x2) surface reconstruction. Contrary to earlier core level studies, we identify two surface shifted components at the Si 2p core level having the same intensity. These two Si 2p spectral surface features are clearly related to the up- and down-dimers (AUDD) of the c(4x2) surface reconstruction.@footnote 1@ In addition, two sub-surface shifted components are also found which shows that the sub-surface region is also significantly affected by stress far away from the outer surface, indicating the long range influence of the latter. The results also confirm that the c(4x2) reconstruction is terminated by one Si monolayer as already well established by various quantitative experimental investigations.@footnote 2@ These novel core level photoemission using synchrotron radiation and STM results further support the AUDD model of the 3C-SiC(100) c(4x2) surface reconstruction.@footnote 1@ However, they are clearly inconsistent with predictions of a "missing row asymmetric dimers" model (MRAD) recently proposed on the basis of ab initio pseudopotential calculations and STM image simulations.@footnote 3@ @FootnoteText@ @footnote 1@P. Soukiassian, F. Semond, L. Douillard, A. Mayne, G. Dujardin, L. Pizzagalli and C. Joachim, Phys. Rev. Lett. 78, 907 (1997). @footnote 2@see e.g. V.M. Bermudez, Phys. Stat. Sol. (b) 202, 447 (1997); and references therein. @footnote 3@3-W. Lu, P. Krüger and J. Pollmann, Phys. Rev. Lett. 81, 2292 (1998).

3:40pm SS1+EM-WeA6 Mechanistic Studies of SiO@sub 2@ Deposition from TEOS / Ozone, L.D. Flores, C. Tindall, J.E. Crowell, University of California, San Diego

The low temperature deposition of SiO@sub 2@ from the reaction of tetraethoxysilane (TEOS) and ozone has been studied in-situ at atmospheric pressures. The studies were performed in a prototypical atmospheric pressure chemical vapor deposition (APCVD) reactor utilizing a commercial injector / vent assembly. The gas phase reactions were followed during deposition at 400°C using gas-phase transmission FTIR spectroscopy. Evolution of gas phase products during TEOS / O@sub 3@ reactions were compared and quite distinct from those observed during reaction of TEOS / O@sub 2@. The primary products produced upon

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ozonolysis of TEOS are acetic acid, formic acid, formaldehyde, carbon monoxide, carbon dioxide, and water. Mechanistic details of the deposition process were aided by model reaction studies performed in a gas cell using transmission FTIR spectroscopy. The model studies involved reaction of ozone with observed and potential deposition byproducts, such as acetaldehyde. The spectroscopic observations will be discussed with an emphasis on reaction mechanisms and the reactive pathways leading to the production of deposition precursors, and the influence of additives and byproducts on the morphological nature of SiO@sub 2@ film growth.

4:00pm **SS1+EM-WeA7** Microcalorimetric Heats of Adsorption of Metals on Metal Oxide and Si(100) Surfaces, *D.E. Starr*, University of Washington; *D.J. Bald*, Intel Corporation; *J.E. Musgrove*, *J.T. Ranney*, *J.H. Larsen*, *C.T. Campbell*, University of Washington

Single crystal adsorption microcalorimetry has been proven to be a powerful method to study the heats of adsorption of gaseous atoms or molecules onto single crystal surfaces. Recently, a microcalorimeter has been built which possesses the capability to measure heats of adsorption of metal atoms onto single crystal surfaces as a function of coverage. A sensitive pyroelectric polymer is used to detect the heat released due to the adsorption of pulses of gaseous metal atoms, each containing ~2% of a monolayer, onto the surface. The microcalorimeter has been employed to study the energetics of film growth from the initial stages of deposition through the multilayer regime for metal on metal and metal on metal oxide systems. For the metal on oxide systems, an initial heat of adsorption which is much lower than the heat of sublimation of the metal is observed. This provides detailed insight into the thermodynamic driving force for the metal overlayer to form three dimensional islands. Auger electron spectroscopy was used to verify the growth morphology. In addition, the extension of this technique to study the heats of adsorption of metals onto silicon substrates allows the study of many systems important to metalsemiconductor contact technology. In order to accurately quantify the heats of adsorption, the metals sticking probability on the surface must be known. These have also been measured and will be discussed. In addition. via a thermodynamic cycle the adhesion energy of the metal to the substrate is obtained from the measured microcalorimetric heats of adsorption.

4:20pm SS1+EM-WeA8 Nucleation and Growth of Hemispherical Grained Silicon, D. Llera-Rodriguez, E.G. Seebauer, University of Illinois, Urbana

Hemispherical grained silicon (HSG) is a material beginning to find widespread use for electrodes in DRAM applications. HSG is formed by the chemical vapor deposition of amorphous Si, followed by a CVD "seeding" step under slightly different growth conditions to form nuclei for surface crystallization. Subsequent rapid thermal annealing to above 600°C induces the nuclei to grow into 100-nm hemispheres via surface diffusion, yielding an electrode with high surface area that increases the capacitance of the resulting device. In addition to the practical applications, however, HSG formation provides useful insights into the fundamental mechanisms of nucleation and growth in a two-dimensional amorphous-to-crystalline phase transition. For example, we can rationalize our experimental results for nucleation density in terms of a rate-equation-based nucleation theory. Furthermore, through a series of growth studies we show that subsequent growth of the initial nuclei can be well-described by a two-dimensional continuum model based on adatom-vacancy pair formation on the amorphous surface, together with diffusion of the atoms toward the growing hemispheres. The activation energy of 2.5 eV describing growth represents the sum of energies for adatom diffusion and surface vacancy formation on the amorphous surface. Somewhat surprisingly, this value for amorphous Si matches that measured by separate experiments for crystalline Si.

4:40pm SS1+EM-WeA9 Characterization by STM of Interface between Silicon and Silicon Dioxide Layers Fabricated by Highly Concentrated Ozone, H. Itoh, A. Kurokawa, K. Nakamura, S. Ichimura, Electrotechnical Laboratory, Japan

We will show that the silicon dioxide film fabricated by ozone exposure@footnote 1,2@ has smooth and flat interface keeping the original step and terrace feature. Hydrogen-terminated Si(100) wafer was used as a substrate. Flat surface was prepared by additional growth of epitaxial Si layers (thickness; 120 nm) on Si substrate, and atomic hydrogen was adsorbed on the surface for passivation. STM images showed that the prepared surface was atomically flat with wide terraces which is larger than 100nm. A high-concentration ozone generator was used to form ultra thin silicon dioxide film on the surface. The output from ozone generator was the mixture gas of ozone(30 vol%) and oxygen. The substrate was exposed

to the gas at room temperature for half an hour to form silicon dioxide film. The thickness of the oxide film formed by the exposure was estimated to be 1 nm, which was analyzed from intensity of XPS Si-2p peaks. After the oxidation, the silicon dioxide fill ! m was carefully removed by rinsing in HF solution to observe the interface structure. Slow etching rate in dilute HF solution(0.1%) was chosen to avoid uneven etching and the thickness was monitored every several minutes by XPS peaks to avoid overetching. The sample was inserted into ultra high vacuum(UHV) chamber and surface and interface was observed by scanning tunneling microscopy. STM images were obtained on the etched surface with monoatomic height resolution. Large terraces and few steps were observed in the STM images and surface roughness is estimated to be below 0.15 nm (rms.). This indicates that the silicon dioxide film was grown keeping the original step and terrace feature. The result suggests that Si was oxidized homogeneously and supports that the film was grown layer-by-layer mode. @FootnoteText@ @footnote 1@ A.Kurokawa et.al., Mater. Res. Symp. Proc.Vol. 513, p38, 1998, @footnote 2@ A.Kurokawa et.al., Mater. Res. Soc. Symp. Proc., 1999, in press

5:00pm SS1+EM-WeA10 Significant Effects of Arsenic Ion Implantation on Si Selective Epitaxy by Ultra-High Vacuum Chemical Vapor Deposition, *T. Furukawa*, *T. Nakahata, S. Maruno, Y. Tokuda, S. Satoh*, Mitsubishi Electric Corporation, Japan

Great attention has been paid on Si selective epitaxial growth for an application into ultra large scale integration. For the practical application, however, surface conditions of a Si substrate, which is affected by preceding process steps such as plasma etching and ion implantation, may have a great influence on growth behaviors. In this work, we have investigated the effect of low energy arsenic ion implantation on the Si selective epitaxy by use of ultra-high vacuum chemical vapor deposition. The substrates were prepared through conventional n-channel MOSFET fabrication sequence. In the arsenic ion implantation, dosage was varied from 0 to 4x10@super 15@cm@super -2@, while acceleration energy was fixed to be 10 keV. Before the Si growth, the wafers were cleaned by chemical wet etching, whereas chemical oxide was removed by diluted HF solution. The epitaxy was performed at nominal temperature of 600°C with a pure Si@sub 2@H@sub 6@ source gas. For a non-implanted wafer, island-like growth occurs. With sufficient dosage of arsenic ions, however, an epitaxial Si layer with excellent surface morphology was successfully grown. X-ray photoelectron spectroscopy measurements reveal that a thin SiO@sub x@ layer is formed below the substrate surface by a preceding plasma etching process. The growth mode change is interpreted in terms of reduction of the SiO@sub x@ layer by means of an additional sputtering effect of the ion implantation.

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