Tuesday Morning, November 1, 2005

Electronic Materials and Processing
Room 310 - Session EM1-TuM

Defects, Interfaces, and Surface Passivation in Electronic Materials

Moderator: L.J. Brillson, The Ohio State University

8:20am **EM1-TuM1 The Role of Defects at Nanoscale Semiconductor Interfaces**, ***Y.M. Strzhemechny***, *H.L. Mosbacker, M.J. Hetzer, M. Gao, B.D. White,* The Ohio State University*; D.C. Look, D.C. Reynolds, C.W. Litton,* Wright-Patterson AFB*; M.A. Contreras, A. Zunger,* National Renewable Energy Laboratory*; L.J. Brillson,* The Ohio State University **INVITED**

Current understanding and control of semiconductor contacts increasingly require measurements sensitive to defects and chemical changes at nanoscale interfaces. We offer examples illustrating dramatic macroscopic effects occurring in semiconductor systems as a result of nanoscale interface phenomena. In some cases, there is an interplay of several competing defect-driven mechanisms. Elucidating them and finding the leading ones requires careful experimental approach. For single-crystalline ZnO, we study the role of near-surface defects on the formation of Au Schottky contacts. Among factors degrading rectifying characteristics of such contacts one should consider the following. High concentrations of shallow donors in the surface and subsurface regions lead to barrier thinning, resulting in increased tunneling. Alternatively, the presence of deep defects near contact interface promotes tunneling by defect-assisted hopping. Nanoscale electronic and chemical studies show that independent reduction of both shallow donors and deep defects significantly improves rectifying performance of the Au/ZnO contacts. We find that processing of ZnO with remote O and H plasma allows for controllable tailoring of chemical and physical properties of the surface. By the same token, nanoscale compositional and electrostatic variations between grain boundaries and grain interiors in thin polycrystalline films of Cu(In,Ga)Se@sub 2@, absorber layers in record-setting solar cells, show how nanoscale arrangement of near-surface stoichiometric defects may improve the overall photovoltaic efficiency. Confirming theory, we find a 50% reduction in Cu composition from grain interior to boundary and a p-type potential barrier that acts to reduce majority carrier hole recombination. These and related examples emphasize the practical significance of nanoscale chemical and electronic features at electronic material interfaces.

9:00am **EM1-TuM3 Interstitial Oxygen Related Defects and Current Leakage in UMOSFET on Epi/As++ Structure**, ***Q. Wang***, *M. Daggubati, H. Paravi,* Fairchild Semiconductor*; R. Yu, X. Zhang,* Lawrence Berkeley National Laboratory

Interstitial oxygen (O@sub i@) related defects and current leakage in UMOSFET on Epi/As++ structure has been investigated. The devices fabricated on heavily arsenic doped wafer with poly-silicon backside exhibited an increased yield loss in reverse current leakage with increasing O@sub i@ concentration in the wafer. For the wafers with the same O@sub i@ content, the leakage yield loss increases with decreasing device geometry. This leakage yield loss was attributed to the O@sub i@ related defects in active region (well junction). Transmission electron microscopy (TEM) study revealed, in the well junction region, the existence of extrinsic stacking faults and half-hexagonal dislocation punch-through defects, characteristic of oxygen precipitation. Defects created by the heavy body boron implantation seem to enhance O@sub i@ precipitation in the active region. In addition, the O@sub i@ is also found to diffuse to the interface of the poly-silicon layer and bulk silicon and precipitate out. This precipitation may consume the poly layer and reduce the gettering effect of poly silicon, which also leads to an O@sub i@ dependent current leakage. Similar experiments carried out with damaged backside wafers showed that current leakage yield loss was independent of O@sub i@ in the wafer and was low in general. The detailed TEM work indicated that the O@sub i@ did precipitate out in the bulk close to the back surface. The O@sub i@ precipitates may result in an intrinsic gettering and thus improve the current leakage yield. This comparative study between poly-silicon and damaged back-surfaces indicates that for heavily arsenic doped silicon wafers, intrinsic gettering is much better than extrinsic gettering due to the facts discussed above.

9:20am **EM1-TuM4 Control of Defect Concentrations in Silicon through Surface Chemistry**, ***R. Vaidyanathan***, *K. Dev, R.D. Braatz, E.G. Seebauer,* University of Illinois at Urbana-Champaign

Point defects govern many aspects of the behavior of crystalline solids, especially for semiconductors. We show through self-diffusion measurements that defect concentrations deep in the semiconductor bulk can be varied controllably over several orders of magnitude through submonolayer-level adsorption at the surface. For example, less than 0.01 monolayer of nitrogen adsorbed on silicon (100) that is undersaturated in defects lowers their concentration and inhibits diffusion, with the effects extending at least 0.5 µm into the bulk. The measurements have been made using a new method for determining key diffusion parameters via the short-time decay of an initial step concentration profile in an isotopic heterostructure. This method takes advantage of the relative ease with which step concentration profiles can be fabricated by thin film deposition, and in the limit of very short times provides particularly simple analytical means for obtaining parameters connected to diffusion length and defect formation. The adsorption phenomena discovered here open the possibility of precise defect engineering for numerous applications.

9:40am **EM1-TuM5 The Role of Etching in Film Growth during Wet Chemical Oxidation of H:Si(100)**, ***K.T. Queeney***, *J.W. Clemens, S.K. Green, C.A. Shea,* Smith College

Exposure of hydrogen-terminated Si(100) to aqueous solutions is an integral part of most wafer cleaning processes in microelectronics manufacturing. The quality of the thin oxide films formed (either intentionally or unintentionally) during this processing can have a profound effect on ultimate device performance. We have used transmission infrared spectroscopy to study this wet chemical oxidation of H:Si(100), allowing us to monitor both the evolution of SiH@sub x@ species and the growth of Si-O modes from the oxide film. While dissolved O@sub 2(aq)@ is the primary oxidizing species in H@sub 2@O, etching of the Si(100) surface by OH@super -@ species in the water plays an important role in oxidation. Sharpening of the Si-H bending modes in the earliest stages of oxidation suggests that this etching creates a more homogeneous surface, which is consistent with the high quality of the single layer SiO@sub x@ as judged by the evolution of Si-O optical phonons during oxidation. Studying the subsequent oxidation of surfaces first etched in deoxygenated water provides some temporal separation of the concomitant etching and oxidation processes and reveals that the relative reactivity of sites exposed by this etching is distinct from reactivity of analogous sites on extended Si surfaces, highlighting the importance of defect-driven chemistry during oxidation.

10:00am **EM1-TuM6 Experimental and Theoretical Studies of Various Oxides on the Ge(100)-2x1/4x2 Surface: Deposition of SiO and Oxidation by O@sub 2@ and NO**, ***T.J. Grassman***, *A.C. Kummel,* University of California, San Diego

To further the development of a germanium-based metal-oxide-semiconductor field effect transistor (MOSFET) a suitable gate-oxide material must be found which yields a high-quality, electrically-unpinned interface. For this, the semiconductor/oxide interface needs to be free of charge traps and other such interfacial defects that can cause Fermi-level pinning. Unfortunately, germanium's native oxide has been shown to be inadequate for the task of providing a clean, unpinned interface. We have investigated the bonding and electronic structures of various oxides on the Ge(100)-2x1/4x2 surface using scanning tunneling microscopy (STM), scanning tunneling spectroscopy (STS), and density function theory (DFT) modeling, including correction for the infamous DFT band gap problem. We will present atomically resolved images of the clean Ge(100) surface, the Ge(100) surface after oxidation with both O@sub 2@ and NO, the Ge(100) surface after deposition of SiO at various coverages, and the Ge(100) surface after nitridation with a neutral nitrogen plasma. Our STM and DFT studies show that SiO, unlike O@sub 2@ or NO, spontaneously forms an oxide bilayer by way of molecular SiO trimers, without displacing Ge atoms or oxidizing the surface. STS and DFT studies show this bilayer SiO absorption leaves the Fermi level unpinned. Such a bilayer formation makes SiO a strong candidate for use as a passivating buffer layer for further gate oxide growth. Conversely, NO and O@sub 2@ dosing causes Ge displacement and does not spontaneously form oxide or nitride bilayers.

10:20am **EM1-TuM7 Optimized Chemical Cleaning Method for Producing Device Quality Ge(100) Surfaces**, ***S. Sun,*** Stanford University; *Y. Sun, Z. Liu, D. Lee, S. Peterson, P. Pianetta,* Stanford Synchrotron Radiation Laboratory

Ge(100) surfaces treated by aqueous HF solutions with three different concentration (1:2, 1:5, and 1:25) have been systematically studied by synchrotron radiation photoemission spectroscopy (SR-PES) at Stanford Synchrotron Radiation Laboratory (SSRL). After HF treatment, the sample surface is hydrophobic and hydrogen terminated. HF solutions with higher concentration leave the Ge surfaces with less oxide, but relatively larger roughness. Hydrogen coverage also depends on the HF concentration. HF:H@sub 2@O (1:5) is a good choice, since it leads to a Ge(100) surface with approximately 0.9 monolayer hydrogen and less than 0.1 monolayer carbon and oxygen. The residual carbon and oxide come from the aqueous solutions. Solutions with higher concentrations of HF do not improve the surface cleanness. Additionally, a 10% HCl solution was also used to clean the Ge(100) surface. A hydrophilic and Cl terminated surface is achieved after HCl treatment. Relatively more residual carbon and oxide are left on the surface, which is due to the hydrophilic nature of treated surface. More details of the work will be discussed in the oral presentation.

10:40am **EM1-TuM8 XPS Study of Se-passivated Si(100)**, ***F.S. Aguirre-Tostado****, R.M. Wallace,* University of Texas at Dallas; *J. Zhu, G. Larrieu, E. Maldonado, W.P. Kirk, M. Tao,* University of Texas at Arlington

The presence of strained and dangling bonds on the atomically clean Si(100) surface leads to a metastable surface structure not suitable for the growth of high-k oxides. In the present work, we have examined the passivation of the Si(100) surface with one monolayer of selenium upon thermal annealing. Ex-situ analysis by x-ray photoelectron spectroscopy reveals that while Se-oxide formation is below the limit of detection, SiO@sub 2@ formation is observed. Assuming a 2D Se layer growth, we speculate that the formation of SiO@sub 2@ takes place at the atomic steps on the surface and at defect sites in the Se layer. It is also possible that there exists a cooperative inter-diffusion of Se and topmost Si atoms, leading to SiO@sub 2@ formation on top of the Se layer. From in-situ thermal annealing studies up to 425 °C, we find that adventitious C concentrations are below detectible limits above 100 °C while Se-Si and SiO@sub 2@ species surface concentrations remain unchanged. From photoelectron attenuation measurements, the SiO@sub 2@ thickness is around 8 Å. The mechanism of formation of the Se layer and SiO@sub 2@ will be discussed. This work is supported in part by the Texas Advanced Technology Program and SEMATECH.

11:00am **EM1-TuM9 Surface Passivation of Semiconductors**, ***D.R.T. Zahn,*** Chemnitz University of Technology, Germany **INVITED**

Considering GaAs(100) very often chalcogen atoms, i.e. sulphur and selenium, are employed for passivating its surface. Passivation can be achieved by exposing the surface to a beam of chalcogen atoms under ultra-high vacuum conditions or employing an ex situ wet chemical treatment followed by annealing in vacuum. We have studied both types of preparation using photoemission as well as Raman spectroscopies. Both techniques are capable of determining the change of band bending resulting from the passivation process. It is quite accepted that the chalcogen passivation induces a considerable reduction in band bending for n-type substrate material. However, the band bending is increased when p-type GaAs is used indicating that the density of surface states is changed but not removed from the band gap of the semiconductor. Core level photoemission data reveal that there are two distinct chalcogen atom environments on the passivated surface and that very similar surfaces are prepared independent on the preparation technique. The core level spectra provide very a very important input for DFT-LDA structure calculations which indicate that the reconstruction is likely to be different from the previously suggested chalcogen dimer terminated one. Moreover, we probe the passivated surfaces by addition of sub-monolayer coverages of organic molecules. The sharpening of core level spectra upon absorption of the molecules is indicative of some inhomogeneities in surface band bending being healed. Finally we address the influence of the passivation on electrical transport in metal/semiconductor structures.

Author Index

Bold page numbers indicate presenter

— A —
Aguirre-Tostado, F.S.: EM1-TuM8, **2**
— B —
Braatz, R.D.: EM1-TuM4, 1
Brillson, L.J.: EM1-TuM1, 1
— C —
Clemens, J.W.: EM1-TuM5, 1
Contreras, M.A.: EM1-TuM1, 1
— D —
Daggubati, M.: EM1-TuM3, 1
Dev, K.: EM1-TuM4, 1
— G —
Gao, M.: EM1-TuM1, 1
Grassman, T.J.: EM1-TuM6, **1**
Green, S.K.: EM1-TuM5, 1
— H —
Hetzer, M.J.: EM1-TuM1, 1
— K —
Kirk, W.P.: EM1-TuM8, 2
Kummel, A.C.: EM1-TuM6, 1
— L —
Larrieu, G.: EM1-TuM8, 2
Lee, D.: EM1-TuM7, 2
Litton, C.W.: EM1-TuM1, 1
Liu, Z.: EM1-TuM7, 2
Look, D.C.: EM1-TuM1, 1
— M —
Maldonado, E.: EM1-TuM8, 2
Mosbacker, H.L.: EM1-TuM1, 1
— P —
Paravi, H.: EM1-TuM3, 1
Peterson, S.: EM1-TuM7, 2
Pianetta, P.: EM1-TuM7, 2
— Q —
Queeney, K.T.: EM1-TuM5, **1**
— R —
Reynolds, D.C.: EM1-TuM1, 1
— S —
Seebauer, E.G.: EM1-TuM4, 1
Shea, C.A.: EM1-TuM5, 1
Strzhemechny, Y.M.: EM1-TuM1, **1**
Sun, S.: EM1-TuM7, **2**
Sun, Y.: EM1-TuM7, 2
— T —
Tao, M.: EM1-TuM8, 2
— V —
Vaidyanathan, R.: EM1-TuM4, **1**
— W —
Wallace, R.M.: EM1-TuM8, 2
Wang, Q.: EM1-TuM3, **1**
White, B.D.: EM1-TuM1, 1
— Y —
Yu, R.: EM1-TuM3, 1
— Z —
Zahn, D.R.T.: EM1-TuM9, **2**
Zhang, X.: EM1-TuM3, 1
Zhu, J.: EM1-TuM8, 2
Zunger, A.: EM1-TuM1, 1