Electronic Materials and Processing
Room 2003 - Session EM-MoA

Contacts, Interfaces and Defects in Semiconductors

Moderator: F. Ren, University of Florida

2:00pm **EM-MoA1 Metals are not Created Equal: Metal Barrier-layer Dependent Ohmic Performance of Ti/Al/Metal/Au Schemes on AlGaN/GaN Heterostructures**, ***F.M. Mohammed***, *L. Wang, I. Adesida,* University of Illinois at Urbana-Champaign

AlGaN/GaN HEMTs are useful for application in microwave power amplification. Low-resistance ohmic contacts are required for enhanced performance of these devices. To this end, Ti/Al/MetalAu schemes, where Metal layer is a high melting-point element such as Ni, Ti, Mo, etc. have been investigated. In such a design, Ti participates in interfacial reactions yielding TiN and rendering the contact/GaN interface n-type doped. Coupling it with metals of high conductivity, such as Al, can enable direct Ohmic contact formation. However, the propensity of Al to easily oxidize upon annealing poses major reliability challenges. To solve this problem a Metal/Au bilayer cap is deposited. The Metal layer is believed to act as a barrier against the outdiffusion of Al and the indiffusion of Au. However, microstructural characterizations of Ti/Al/Mo/Au and Ta/Al/Mo/Au indicate that the Mo layer is not effective as a diffusion barrier. Therefore, a critical assessment of the presumed role of the Metal-layer acting as a diffusion barrier is needed. Here, we present the study of Ohmic performance and surface morphology of Ti/Al/Metal/Au schemes, where Metal is Ti, Mo, Pt, Ir, Ni, Ta, or Nb, carried out to identify the role of the barrier layer on contact formation and reliability of the metallizations. A strong dependence of contact resistance and specific contact resistivity, as well as surface morphology, on the type of Metal layer used was found. SEM/EDS characterization has shown evidence for alloy segregation, Metal layer fragmentation, Al-Au solid solution formation, and possible Au and/or Al reaction with Metal layer. The observed variations in Ohmic performance and surface morphology did not correlate with the properties of elemental Metal-layers. Contrary to the generally accepted opinion of the layer acting as a mere diffusion barrier layer, results from the present study provide new insights on the active role this layer plays on the characteristics of metallizations.

2:20pm **EM-MoA2 Tailoring the Interfacial Reactions between Ti/Al/Mo/Au Ohmic Contacts and AlGaN/GaN by Si lAyers: An Investigation by Cross-Sectional TEM**, ***L. Wang***, *F.M. Mohammed, I. Adesida,* University of Illinois at Urbana-Champaign

The interfacial reactions activated during annealing between Ti-containing metallizations and GaN or AlGaN are believed to be the ohmic contact formation mechanism. During annealing, Ti extracts N from the nitride layers and forms Ti-nitrides, such as TiN, AlTi2N, etc, triggered by their low enthalpies of formation as compared to that of GaN or AlGaN. It is believed this reaction generates a highly n-type layer in GaN or AlGaN which facilitates carrier tunneling. It was widely observed that the resulting Ti-nitride layers are continuous. However, our observation of the Ti/Al/Mo/Au contacts on AlGaN/GaN indicated that TiN did not always form as a continuous layer. Discrete TiN islands were observed to grow preferentially along dislocations and penetrate through AlGaN. The TiN islands, having an electrical resistivity as low as 13 ï¼©-cm depending on N content being smaller than Ti, electrically link the metal layer with the 2DEG at the AlGaN/GaN interface and make direct transport of carriers possible. This mechanism is also observed in the contacts to GaAs-based devices. In this paper, we demonstrate, with the aid of analytical TEM, that the interfacial reaction of Ti/Al/Mo/Au contacts on AlGaN/GaN heterostructures could be tailored by adding Si layers. Of particular importance is the Si/Al ratio. At low Si/Al ratio [0.138 and 0.276 (atomic ratio)], discrete metal islands rich in Al and Au form along dislocations and penetrate through the AlGaN layer. At medium ratio of 0.415, no island formation along dislocation is observed, rather a continuous layer of AlN forms at the interface. In both low and medium Si/Al ratio cases, Si dissolves in the metal and no silicide is perceived. At high Si/Al ratio (0.829), silicides, such as TiSi and MoSi2, are observed to precipitate. The observed reaction pathways are discussed in light of the Al-Si phase diagram. Meanwhile, the effects of the reactions on ohmic characteristics of different contacts are also presented.

2:40pm **EM-MoA3 2006 AVS Gaede-Langmuir Award Lecture - Interface Bonding, Reactions and Defect Formation at Semiconductor Interfaces**, ***L.J. Brillson***[1], The Ohio State University **INVITED**

The formation of barriers to charge transfer at semiconductor interfaces has been a focus of considerable research, much of it led by AVS scientists, for over fifty years. While early work centered on the intrinsic physical properties of the semiconductor, ultrahigh vacuum surface studies revealed the importance of extrinsic, interface-specific effects in understanding the systematic behavior of these Schottky barriers. Without intervening adsorbate layers, chemical reactions and interdiffusion can occur, even near room temperature, which alter the interface region, introducing new phases, crystal defects, and localized electronic states. Surface science techniques display local atomic bonding that depends systematically on thermodynamics and a qualitative transition between reactive and unreactive interfaces. Indeed, atomic-scale interlayers that change such chemistry introduce macro-scale electronic effects. These effects increase in importance as electronic structures shrink to nanoscale dimensions and interfaces constitute much of the entire structure. Detecting these states at or near interfaces requires techniques orders of magnitude more sensitive than conventional surface science provides. Low energy, nanoscale depth-resolved cathodoluminescence spectroscopy (NDRCLS) yields this capability, revealing states at the surface as well as tens to hundreds of nanometers below. DRCLS studies show the importance not only of interface chemistry but also crystal defects. Defects both resident in the semiconductor as well as created by interface reaction and diffusion can impact Schottky barrier formation. GaN, AlGaN, SiC and ZnO - metal junctions provide representative examples of chemically-induced defects near interfaces. Indeed, such defects appear to play a role in limiting Schottky barrier heights for semiconductors in general. These systematics suggest new ways to predict and control Schottky barriers in the nanoscale regime.

3:20pm **EM-MoA5 Inhomogeneous Schottky Contacts on Silicon Carbide: Localized Fermi Level Pinning by Defects**, *D.J. Ewing,* Carnegie Mellon University*; Q. Wahab, M. Syväjärvi, R. Yakimova,* Linköping University, Sweden*; S. Tumakha, M. Gao, L.J. Brillson,* The Ohio State University*;* ***L.M. Porter***, Carnegie Mellon University

Schottky barrier inhomogeneities, apparent as a knee in the low-voltage (Log I)-V characteristics, were present in a significant percentage of 4H-SiC diodes prepared from a variety of methods, sources, and contact materials. More than 500 Ni, Pt, or Ti diodes were characterized by a variety of techniques. Both commercially-produced chemical vapor deposited (CVD) epilayers and noncommercially-produced CVD and sublimation epilayers were used. The combined results from current-voltage measurements and modeling, electron beam induced current (EBIC), and site-specific and depth-resolved cathodoluminescence were used to develop a model to describe the relationship between specific defect states and the inhomogeneous behavior. By modeling the inhomogeneities as two Schottky barriers in parallel, high and low Schottky barriers were calculated for the non-ideal diodes. The high-barrier (ideal) barrier-heights for Pt, Ni, and Ti increased with metal workfunction with a slope parameter of 0.44, whereas the low barriers were predominantly centered at one of three values: 0.6, 0.85, and 1.05 eV. The site-specific and depth-resolved CL measurements of non-ideal diodes also revealed three different emission peaks (at 2.2, 2.4, and/or 2.65 eV), with the 2.4 eV peak originating from stacking faults observed in EBIC images; these peaks are the complements of the low barrier height values. Based on the results, the low-barrier barrier-heights can be explained by localized Fermi level pinning by specific material defects within the SiC epilayers. This model will be presented in terms of the defect level positions in the bandgap and their correspondence with the low barriers.

3:40pm **EM-MoA6 Carbon Nanotube Based Transparent Contacts for Photovoltaics**, ***T.M. Barnes***, *J. van de Lagemaat, M. Contreras, G. Rumbles, S.E. Shaheen, T.J. Coutts,* National Renewable Energy Lab*; C.L. Weeks, I.A. Levitsky, J.A. Peltola, P.J. Glatkowski, D.A. Britz,* EIKOS, Inc

Transparent electrodes are an integral part of photovoltaic (PV) devices, and the transparent conducting oxide (TCO) films currently in use are not ideal for all PV applications. Nanostructured bundles of single wall carbon nanotubes (SWCNT) can be solution-deposited to form highly conductive and transparent thin films. The films consist of entangled bundles of SWCNTs with a large fraction of void space. The optoelectronic properties of the SWCNT films approach those of commonly used TCO films. Unlike

[1] **Gaede Langmuir Award Winner**

ZnO and other traditional TCOs, however, the SWCNT film has little absorption in the visible or near infrared. Furthermore, in stark contrast to other available TCO materials, the SWCNT films are essentially hole conductors due to the intrinsic p-type conductivity of the SWCNTs. In this paper, we demonstrate the utility of SWCNT-based transparent contacts on several different types of thin-film solar cells. First, they were successfully used to replace ZnO in high-efficiency CIGS devices. Second, the SWCNT coating was used to replace ITO and PEDOT:PSS in excitonic, bulk heterojunction devices, resulting in an exceptionally high efficiency for a device without indium or PEDOT:PSS. These coatings work well in excitonic devices because the large void fraction allows for interpenetration of the active polymer at the nanoscale. They are also highly amenable to use on flexible substrates. This abstract is subject to government rights.

4:00pm **EM-MoA7 Tuning the Schottky Barrier Height in Mg/Si Diodes***, **H. Nienhaus**, S. Glass,* University of Duisburg-Essen, Germany

Thin metal film Mg/p-Si(111) Schottky diodes have been successfully used for sensing of chemically induced electron-hole pairs.@footnote 1@ Controlled variation of the homogeneous Schottky barrier height allows to probe the energy distribution of hot charge carriers. Different types of Mg/p-Si diodes were prepared by thermal evaporation of thin Mg layers on H-passivated Si(111) surfaces at low temperatures followed by various annealing procedures. After deposition at 190 K, the current-voltage characteristics of the diodes are typical for interfaces with lateral inhomogeneity and high ideality factors. The homogeneous barrier height is measured as 0.8 eV. This value is much larger than expected from theory of metal-induced gap states. The deviation is explained by interface dipoles due to the monatomic hydrogen layer between Mg and Si. The hydrogen is removed by annealing the diodes to room temperature. This procedure leads to the formation of an intermediate Mg silicide layer and to a significant reduction of the barrier height. The annealed diodes exhibit excellent current-voltage properties. Applications of the diodes for chemical sensing (chemicurrents) and for internal photoemission are discussed. @FootnoteText@ @footnote 1@ S. Glass, H. Nienhaus, Phys. Rev. Lett. 93 (2004) 168302.

4:20pm **EM-MoA8 High-Resolution Depth Profiling of Implanted As and Sb in Si(001) with Excess Vacancy Concentration***, M. Dalponte, H. Boudinov,* Universidade Federal do Rio Grande do Sul, Brazil*; **L.V. Goncharova**, T. Feng, T. Gustafsson, E. Garfunkel,* Rutgers University

Medium energy ion scattering (MEIS) was used to investigate the near-surface defect distribution and As and Sb redistribution in silicon substrates with excess vacancy concentration and separation by implantation of oxygen (SIMOX) substrates, and also the effects of post-implantation annealing. As and Sb are the preferred n-type dopant for Si due to their small depth penetration during implantation and low diffusivity during annealing. Also, Sb requires a lower thermal budget to achieve the desired junction parameters, compared to As. A 150 nm deep vacancy-rich layer was formed by O@sub 2@@super +@ or N@sub 2@@super +@ implantation at 240keV, using a dose of 2.5x10@super 16@cm@super -2@ at 400°C. As and Sb were then implanted at 20keV to a dose of 5x10@super 14@ cm@super -2@ at room temperature. Dopant segregation to the SiO@sub 2@/Si interface and some dopant loss was observed in all samples. Several effects related to the nature of the defects present in the sample as well as to the pre-implantation species were observed after longer annealing. The amount of dopant loss appears to be correlated with the structure of the defects. The highest dopant losses were observed in the N and O pre-implanted samples, where the vacancies had point defect character. In Si (no excess vacancies) and SIMOX (vacancies in the form of stable complexes) the dopant loss was much lower than in the N and O samples. Effects due to the different chemical nature of pre-implanted species were also observed. The N pre-implanted samples had the lowest segregated Sb percentage and uniform dopant distribution. The nitrogen accumulation at the SiO@sub 2@/Si interface appears to reduce dopant losses, compared to the O pre-implanted samples with the same vacancy structure. CNPq, CAPES, NSF and SRC/Sematech are gratefully acknowledged for their financial support.

4:40pm **EM-MoA9 Mechanism of Initial Oxidation of Hydrogen and Halogen Passivated Ge Surfaces***, **S. Sun**,* Stanford University*; Y. Sun, Z. Liu, D. Lee, P. Pianetta,* Stanford Synchrotron Radiation Laboratory

In order to keep scaling down the CMOS, new semiconductor materials are needed. Germanium (Ge) is one of the good candidates, because of its high intrinsic low field carrier mobilities. Research shows that Ge surface can be cleaned by HX (X = F, Cl, Br, I) and passivated by hydrogen or halogen. However, our experimental results show that neither hydrogen nor halogen passivated surfaces are stable in the room air. To be more specific, oxide will grow on these passivated surfaces in the room air. In order to probe the mechanism of the initial surface oxidation, systematic study is performed by synchrotron radiation photoelectron spectroscopy (SR-PES) at Stanford Synchrotron Radiation Laboratory (SSRL). Experimental results for samples with different passivation (hydrogen and halogen) and under various oxidation conditions (dry oxygen, moisture, and mixture of oxygen and moisture) will be shown, respectively. Then, results for different sample orientations, i.e. (111), (100) and (110), will be compared. Finally, the oxidation mechanism will be discussed in detail.

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