Final Report for Department of Energy Grant DE-FG02-97ER45666 "Interface Diffusion and Deep Level Formation of SiC and Other Wide Gap Materials"

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This research effort focused on the nature of charge transfer and localized electronic structure at semiconductor interfaces, one of the most fundamental issues in the solid state. The basic charge exchange between two materials in general is directly connected with the systematic atomic bonding changes and redistribution that occurs at the nanoscale interface. Our program aimed to extend our understanding of the atomic-scale nature of electrostatic barrier formation, heterojunction band offsets, and the optical and electronic features of impurity confinement in a set of model materials systems, including nanometer-scale wide band gap semiconductor and insulator structures. This fundamentally new class of materials investigation utilized a powerful and unique combination of techniques that are revealing the atomic-scale movement, chemical bonding, and resultant charge transfer across well-defined model interfaces.

Our Department of Energy-supported research effort has aimed to extend our understanding of the localized states at atomic-scale electronic materials' interfaces, their impact on electronic barrier formation and the lineup of electronic band structures, especially for quantum confined structures. Atomic-scale bonding changes to control these states can dramatically improve performance of solar power generation, catalysis, and integrated optoelectronic environmental sensors. We have developed a powerful and unique combination of techniques to characterize both the chemical interactions and the associated electronic states on an atomic scale. We have used wide band gap materials such as GaN, SiC, and metal oxides as ideal test structures to address: the formation of extrinsic interface states by local chemical bonding and atomic interdiffusion, the nature of localized states at heterojunctions, and UHV surface atomic techniques to control the extrinsic electronic states produced at quantum-scale surfaces and interfaces. This work has resulted in 55 publications (45 since 2001) in refereed journals, 75 presentations at national or international conferences, including 28 invited talks. The results described here represent a subset of this work and are intended to highlight key advances.

GaN, SiC, ZnO and related compounds are important in a wide range of micro- and optoelectronic applications. Their epitaxial growth relies not only on the lattice match between epilayer and substrate but also their chemical stability. GaN epilayers are commonly grown on sapphire, and our studies of this interface have revealed multiple chemical processes that can dominate its electronic properties. For hydride vapor phase epitaxy (HVPE) grown GaN on Al₂O₃, our cross sectional CLS demonstrated that O diffusing hundreds of nm from Al₂O₃ into GaN is the cause of the well-known degenerate GaN doping. This work showed the detailed correspondence between the emission intensity of a new donor bound exciton detected by low temperature CLS and the spatial variation of O measured by SIMS depth profiling.[5,6] Besides such impurity doping, micro-AES mapping of the cross sectional GaN/ Al_2O_3 junction reveals both cross-diffusion and interfacial alloying. The SEM image and elemental distributions in fig.1 include not only O extending into GaN, but also extensive N diffusion into Al_2O_3 and Al into GaN. CLS features in fig. 2 show the transformation of 3.4 eV GaN emission in the bulk to a 3.53 eV intermediate AlGaN phase near the junction to 3.8 eV defects associated with Al-O-N complexes.[7] Cross sectional SIMS maps of this interface confirm these chemical redistributions, demonstrate Ga-O and AlGaN bonding in the GaN, Al-O-N bonding in the $A₁₂O₃$, and indicate O diffusion via grain boundaries. Consistent with interface thermodynamics, these results show that GaN heterojunction constituents can diffuse and react to form ternary

compounds and impurities with major changes in electronic properties. Nevertheless, similar interfaces intentionally grown with monolayer Zn diffusion barriers produce nm-abrupt junctions, highlighting the chemical and electronic importance of the initial interfacial layers.[8] Finally, the nanoscale imaging of multicomponent chemical interactions and their optical emissions provides a consistent "picture" relating heterojunction electronic properties to local chemical structures.

We have extended these microanalytical techniques to Schottky barrier formation of wide band gap semiconductors involving ternary alloys. Such alloys are now in state-of-the-art optoand microelectronic device structures due to their wide range of band gaps and heterojunction properties. Studies of the widely used Ni/AlGaN interface revealed a phenomenon not encountered over decades of interface studies of binary compounds, namely Schottky barriers driven by nanoscale changes in atomic composition and band gap. These experiments involved AlGaN grown epitaxially on GaN buffer layers, cleaned with three commonly used chemical processes, and prepared with diode arrays involving different chemical treatments on the same wafer. Schottky barriers were measured using internal photoemission spectroscopy (IPS), avoiding many experimental artifacts associated with current and capacitance voltage measurements.[2] These measurements demonstrated a pivotal role of surface oxide formation on ternary alloy barrier heights. IPS spectra showed two types of behavior, as illustrated in fig. 3. Diodes prepared without strong oxidation exhibited a normal $(Yield)^{1/2}$ functional dependence and a single barrier height φ_{b1} , as expected for uniform Schottky diodes. (Undulations are due to interference effects in the metal film.) Diode cleaning involving oxidation and oxide removal revealed *two* barriers due to different interface compositions. AES and SIMS show

that Al-O and Ga-O bonding form during cleaning with ~30% more Al-O bonds due to the stronger Alvs. Ga-O bond strength. Subsequent oxide removal effectively reduces the Al alloy composition in the AlGaN at the interface. SIMS depth profiles show that this altered alloy composition is only 5 nm thick, compared with the 25 nm overall AlGaN layer thickness. This well-defined interface composition change takes place even though the thermodynamic heat of reaction between metal and semiconductor [10] is relatively small. Instead, the much stronger metal-oxide bonding dominates the interface behavior by dissociating the first few nanometers of AlGaN.[11] The altered AlGaN alloy composition changes the Schottky barrier properties.

Figure 3. Representative IPS spectra showing single or dual Schottky barrier heights ϕ_{b1} and ϕ_{b2} .

LEEN measurements centered at depths [12] corresponding to the intimate Ni-AlGaN interface reveal a striking contrast between diodes with vs. without Al-O and Ga-O bonding at an intermediate stage. Figure 4 shows depth-resolved spectra obtained *through* the diodes' metal overlayer and at the intimate junction, all on the same wafer. Diodes with reduced Al content exhibited two near band edge (NBE) peaks separated by 0.2 eV and dominated by the lower energy peak. Diodes with unchanged composition exhibited only the one, higher energy peak. An IPS barrier height difference of 0.2 eV reflects this difference in band gap. Significantly, the

absolute 1.75 and 1.55 eV barrier heights agree with those expected for a Schottky work function model based on the Ni work function and electron affinities extrapolated from the two band gaps (based on unity bowing parameter).

In other words, both the absolute Schottky barriers and their difference follow the classical model. Alloy changes dominate any effect of trace impurities detected by SIMS at these interfaces. *These are the first definitive results that describe how contacts to ternary alloys can change atomic composition on a nanoscale and barrier heights on a macroscale. [11]* These findings depend critically on our ability to

detect both electronic and atomic composition changes in ultrathin layers buried below the free surface. In principle, they also suggest a new method to "engineer" a hetero- junction by altering

Figure 4. LEEN spectra of diodes with and without interface oxidation and removal on same wafer.

the composition over nanometer thicknesses to achieved graded interfaces.

We have extended our nanoscale interface techniques beyond III-V compounds to Column IV wide gap semiconductors and 4H-SiC in particular. 4H-SiC is the polytype of choice for the fabrication of SiC high power devices due largely to its high mobility and near isotropy of its mobility in different crystallographic directions. The 4H-SiC barrier heights extend over a

wide range yet exhibit only a sub- linear dependence on work function, indicative of intermediate densities of interface states. Such states are not measurable directly by currentvoltage, capacitance-voltage, or deep level transient spectroscopy, which cannot probe the first few nanometers at the intimate metal-semiconductor junction. We studied a representative set of metals on the Si face of 4H-SiC – Au, Ag, Ni, and Ti, known to span a 0.7 eV range of barrier height Φ_B with a Φ_B =0.7 Φ_M – 1.95 eV dependence on metal work function Φ_M and therefore a low but finite density of interface states.[13] Until now, the detection of such states could only be inferred from indirect transport and capacitance measurements. However, these techniques are unable to probe within nanometers of the metal-SiC interface. LEEN spectra tuned to the first few nanometers below the various metal overlayers reveal the presence of such states, their transition energies, and their spatial distribution as a function of metal and subsequent annealing, again *through* the metal. Figure 5 illustrates the change in LEEN spectra obtained for 4 nm Au deposited by UHV thermal evaporation on a 4H-SiC Si face, namely the appearance of a broad emission peak at $1.7 - 2$ eV. Similar coverage of Ag on this face produces nearly an identical result. These changes are detected only for excitation within the first 5-10 nm of the interface, decreasing into the SiC bulk. Surprisingly, UHV thermal annealing at 500-800 °C can reverse these changes. In contrast, 3 nm of a much more reactive metal such as Ti deposited on this surface produces no change at room temperature. Indeed, new features appear only after extended high temperature annealing, as shown in fig. 6. Similar features are observed for Ni, another reactive metal. The striking similarities between thermodynamically unreactive metals Au and Ag versus between the more reactive metals Ti and Ni demonstrate that metal-specific bonding is not a primary factor in forming these localized states. Rather, the pronounced Au and Ag interface changes occurring at room temperature and their reversal with annealing suggest

Figure 5. 4 nm Au on 4H-SiC vs. bare surface showing Au-induced states.

Figure 6. 3 nm Ti on 4H-SiC before and after 800 °C anneal showing Ti-induced states.

that point defects associated with metal-SiC interdiffusion are responsible. Indeed, dynamic SIMS profiles provide evidence of Au-Si interdiffusion with high temperature annealing, although only over ~ 15 nm. [14,15] This is further supported by similar observations of 1.7-2 eV and 2.85 eV emissions associated with partial dislocations and stacking faults, respectively, [16- 19] produced by electrical or thermal stress. In the case of dislocations, point defects are commonly localized in Cottrell atmospheres surrounding these extended defects. The energy levels within the band gap of these morphological features as well as those induced by the metals we have measured in fact nearly align with the Fermi level positions at the upper and lower limits of the range of reported Schottky barriers.[14,15] This level alignment with the Schottky barrier limits suggests their effect on the Fermi level stabilization. The high thermodynamic stability of SiC is consistent with the lack of any pronounced interface reaction for any of these metals. Thus metal-induced intermixing and thermally- induced redistribution of mobile defects rather than any metal-specific states are the likely origin of 4H-SiC interface states.

Among II-VI compound semiconductors, the wide gap semiconductor ZnO is expected to be a leading optoelectronic material because of its deep free exciton that limits thermal activation, thereby reducing thresholds for population inversion and power consumption. High efficiency emission from ZnO nanocrystals already confirm this feature. Schottky diodes to ZnO are commonly believed to follow a classical Schottky model, yet high barrier contacts to atomically clean ZnO have proved difficult to achieve due to high doping and tunneling associated with deep level defects, particularly those associated with a broad ~ 2.5 eV "green" luminescence (GL) peak. In turn, this mid-gap state is believed due either to oxygen vacancies V_O or zinc interstitials Zn_I .[20,21] Previously we showed that oxidation at elevated temperatures reduces or enhances this defect emission, depending on both the ZnO temperature and pressure, corresponding to O in- or out-diffusion, respectively. We have now demonstrated the ability to reduce these defects using remote plasma enhanced oxidation (RPEO). We developed a custom built chamber to isolate the O plasma and thereby control ZnO temperature independent of plasma power. Depth-resolved LEEN spectra in fig. 7a illustrate the decrease in GL luminescence relative to the ZnO NBE emission. The unchanged NBE indicates that no new donor or acceptor dopants are introduced and only GL defects are reduced.[22] Figure 7b shows the near-surface enhancement of this defect and its decrease after the RPEO treatment. Before oxidation, the GL exists throughout the crystal, but increases by nearly a factor of 3 within 50 nm of the free surface. After oxidation, the GL /NBE ratios decrease substantially within the outer 50 nm of ZnO. Au diodes deposited on the RPEO-treated surfaces showed an even more pronounced decrease in relative defect emission near the surface. These decreased defect densities are sufficient to alter the Schottky barrier characteristics significantly. Figure 7c

^{2.0} ^{2.2} ^{2.4} ^{2.6} ^{2.8} ^{3.0} ^{3.2} ^{3.4}
Fig. 7a. Surface-sensitive LEEN spectra before and after RPEO showing "green" defect reduction.

Fig. 7b. Reduction of "Green" defect vs. NBE intensity ratio. vs. depth pre- and post-RPEO.

rectifying contact after RPEO.⁵ Fig. 7c. I-V characteristics showing conversion of ohmic to

illustrates the dramatic change in I-V characteristics for the Au/ZnO(000ī) junction due to RPEO treatment. Before oxidation, the high density of defects within the ZnO depletion region permits tunneling via a high density of closely spaced defect gap states. Reduction of this density largely eliminates this current pathway, resulting in a Schottky barrier height of 0.45 eV. We anticipate even higher barrier heights with further defect reduction. This result has practical significance for real ZnO devices. From a fundamental point of view, this result is significant as well since *we can now affect Schottky barrier heights by modifying point defects inside a semiconductor crystal*. It is only with the nanoscale depth resolution of LEEN that this modification can be shown and distinguished from simple formation of a surface oxide. Also, LEEN spectra gauge the spatial extent as well as the overall reduction in defect concentration. In-house optical DLTS in collaboration with Prof. Steven Ringel (see Appendix B) will calibrate the defect concentrations measured by LEEN at excitation depths beyond the depletion width. In turn, this calibration will enable a quantitative analysis of the defects' influence on the Schottky barriers.

The ability to obtain spatially localized electronic and chemical information on a nanometer scale enables us to correlate defects with changes in crystal stoichiometry, thereby identifying specific atomic ratio changes with particular defect emissions. This can be particularly effective in polycrystalline materials where such composition/defect comparison can be performed on statistically significant numbers of interfaces within the same specimen. The chalcopyrite structure semiconductors, especially the $CuIn_xGa_{1-x}Se_2$ (CIGS) quaternary alloy system are attractive in this respect due to stoichiometry changes known to occur between grain interior (GI) and grain boundary (GB). CIGS is also important as a leading solar cell material, especially with Na introduced to the grain boundaries. We have now performed AES and CLS studies on CIGS provided by Dr. Miguel Contreras at the National Renewable Energy Laboratory (NREL). There is high interest to understand the relatively low GB recombination found for this polycrystalline material. Alternative models for this low recombination include: (1) passivation of dangling bonds or point defects near the GB,[23] (2) fluctuations in electrostatic potential due to random defects,[24], and formation of a potential barrier to majority carriers diffusing to the grain boundary as proposed by Persson and Zunger.[25] Understanding this phenomenon could lead intentional designs of optoelectronic device structures based on lower cost polycrystalline materials.[25] We are able to address the latter issue by directly measuring the potentials near the GB interface. This is possible by measuring the energy threshold for secondary electron emission with our high resolution energy analyzer versus distance from the GB. This secondary electron threshold (SET) technique has proved reliable for measuring work functions of metals as well as semiconductor surfaces [26] with spatial resolution determined by minority carrier diffusion length. Beam effects on the interface potentials are negligible for low current injection levels. In fact, both requirements are met when free carrier recombination is high, especially near surfaces and interfaces, the very regions of interest. CIGS layers on Mo on glass (solar cell geometry), can be cleaved in a UHV prechamber, then transferred directly into the UHV SEM (fig. 8a). Our initial AES, CLS, and SET studies of CIGS show strong chemical changes accompanied by p-type band bending at the GB

interfaces.[27] Figure 8b shows an AES line profile of Cu vs. In across several CIGS grains. For

function scan; (b) AES atomic composition variation across GB vs. GL; (c) SET measure of surface Figure 8. (a) SEM image of clean, cleaved CIGS surface including representative points for a work potential showing 0.35-0.45 eV decrease at GB, corresponding to p-type (downward) band bending.

these composition changes, we have measured for the first time the electric potential variations a bulk Cu/In composition of 0.99, the spectra show a 50% decrease at the GB. Corresponding to near the clean grain boundaries in UHV. Fig. 8c illustrates the change in threshold energy vs. position relative to two grain boundaries. With specimen grounded with the electron analyzer, the threshold energy gauges the semiconductor vacuum level relative to the common Fermi level, i.e., the work function. In turn, this work function varies with band bending. For clean surfaces, free of ambient adsorbates or defects that could produce additional band bending normal to the interface, the SET method yields work functions across the semiconductor depletion region and the interface. Fig. 8c displays decreasing work function equivalent to downward band bending of nearly half the CIGS band gap over several hundred nm on both sides of the interface. This band bending represents a barrier to majority carrier holes diffusing to the grain boundary, consistent with the barrier model for reduced recombination. Initial CLS measurements show little difference between GB and GI spectra, suggesting the presence of charge neutral sites at or near the interface. Previously, we found that compositional changes at surfaces of epitaxial CIGS on GaAs produces band gap variations and ~ 1 eV defect emissions consistent with a number of crystal defects.[28] However, defect energy calculations [29] show that formation energies of specific CuInSe₂ native defects depend strongly on stoichiometry and Fermi level position, and have characteristic transition energy levels in the band gap. Hence, the CIGS stoichiometry, Fermi level, and defect transition energy measured by AES, SET and CLS, respectively, can sort through the various defects predicted to be stable, *thereby offering a unique method to identify the physical nature of CIGS defects.*

Research supported by the Department of Energy since 2001 has yielded additional results on GaN, AlGaN, and related systems. These include: (1) the use of depth-resolved CLS and SIMS to identify the physical origin of deep levels in AlGaN with compositions extending across the entire alloy series.[30] This work identified both states due to concentration-dependent oxygen complexes [7] and carbon [31]. It also demonstrated that O changes from a shallow donor to a deep compensating center with increasing Al composition, thereby explaining the difficulty in doping $Al_xGa_{1-x}N$ for $x > 0.8.130$, 321; (2) the use of AES mapping at etched GaN surfaces to identify the physical nature of a microscopic process that suppresses current transport

through dislocation cores. This work identified a Ga oxide layer formed at the intersection of the dislocation with the surface.[33]; (3) the use of spatially-resolved CLS to describe the crystal quality of 500 nm diameter, micron length "whiskers" formed by photo-chemical etching around individual dislocations.[34] These whiskers exhibit remarkably strong NBE emission due in part to a reduction of defects that can be identified with stacking faults; (4) that AlGaN epilayers across the Al alloy series exhibit composition modulation[35] The ordering structure was unambiguously determined to be atomic-scale compositional ordering by high resolution elemental mapping, atomic resolution Z-contrast image and energy dispersed x-ray spectroscopy (EDS) line scanning in high spatial resolution scanning transmission electron microscopy (STEM) which showed clearly alternate stacking Al-N and Ga-N layers**.** The long range ordering was also detected directly using small-angle x-ray diffraction showing pronounced first order diffraction of the ordering. Significantly, the period of this modulation appears to change with alloy composition so that systematic variations across the AlGaN alloy series may well provide new insights into the possible driving forces of composition modulation in general.[36] In addition to the work described here, we have published or have submitted for publication a number of related studies involving surface and interface phenomena in wide band gap materials. These include: discovery of 4H-to-3C quantum-scale transitions in SiC under thermal stress;[16,17] correlation of interface diffusion and local states at InGaAs/InP heterojunctions with epitaxial growth transitions;[37] determination of oxidation effects on Mg-H complexing and dissociation in GaN;[38] and measurement of radiation damage in AlGaN/GaN.[39] All of these appear in the List of Publications Under Prior Department of Energy Support.

Publications Under Prior Department of Energy Support (45 since 2001)

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- 37. Y. M. Strzhemechny, J. Bae, L.J. Brillson, and D.C. Look, "Effect of Remote Hydrogen Plasma Treatment on ZnO Single Crystal Surfaces," Mat. Res. Soc. Proc. 744, M3.9.1-6 (2003).
- 38. S. T. Bradley, S. H. Goss, and L J. Brillson, "Deep Level Defects and Doping in High Al Mole Fraction AlGaN," J. Vac. Sci. Technol. 21 (6) 2558-2563 (2003).
- 39. P.Smith, S.T. Bradley, S.H.Goss, M. Hudait, Y. Lin, S.A. Ringel, and L.J. Brillson, "Chemical and Electronic Changes at InGaAs/InP Interfaces," J. Vac. Sci. Technol. B22, 554-559 (2004).
- 40. L.J. Brillson, S. Tumakha, R. Okojie, and P. Pirouz, "Electron-Excited Luminescence Spectroscopy of SiC Surfaces and Interfaces," J. Phys.- Condensed Matter 16, S1733-S1754 (2004).
- 41. L. J.Brillson, "Microcathodoluminescence Characterization of III-V Nitride Heterojunctions and Devices," Proc. Wide Band Gap Semiconductors for Photonic and Electronic Devices and Sensors III, eds. E.B. Stokes, R.C. Fitch, Jr., D.N. Buckley, P.C. Chang, D.W. Merfeld, and F. Ren (The Electrochemical Society, Pennington, NY, 2003) pp. 229-235.
- 42. Y. M. Strzhemechny, J. Nemergut, P.E. Smith, J. Bae, D.C. Look, and L.J. Brillson, "Remote Hydrogen Plasma Processing of ZnO Single Crystal Surfaces," J. Appl. Phys. 94, 4256-4262 (2003).
- 43. L.J. Brillson, S. Tumakha, R.S. Okojie, and P. Pirouz, "SiC Studied Via LEEN and Cathodoluminescence Spectroscopy," Mater. Sci. Forum 457-460, 543-548 (2004).
- 44. Y.M. Strzhemechny, H.L. Mosbacker, D.C. Look, D.C. Reynolds, C.W. Litton, N.Y.Garces, NC. Giles, L.E. Halliburton, S. Niki, and L.J. Brillson, "Remote Hydrogen Plasma Doping of Single Crystal ZnO," Appl. Phys. Lett. 84, 2545-2547 (2004).
- 45. S.T. Bradley, L.J. Brillson, J. Hwang, and W.J. Schaff, "Surface Cleaning and Annealing Effects on Ni/AlGaN Interface Atomic Composition and Schottky Barrier Height," Appl. Phys. Lett. 85, 1368-1370 (2004).
- 46. "Micro-Auger Electron Spectroscopy Studies of Chemical and Electronic Effects at GaN-Sapphire Interfaces," X.L. Sun, S.T. Bradley, G.H. Jessen, D.C. Look, R.J. Molnar, and L.J. Brillson, J. Vac. Sci. Technol. 22, 2284-2289 (2004).
- 47. X. Weng, R.S. Goldman, V. Rotberg, N. Bataiev, and L. J. Brillson, "Origin of Luminescence from Nitrogen Ion Implanted Epitaxial GaAs," Appl. Phys. Lett. 85, 2774- 2776 (2004).
- 48. L. J. Brillson, S.T. Bradley, S. H. Tumakha, S.H. Goss, X. L. Sun, R.S. Okojie, J. Hwang, and W.J. Schaff, "Local Electronic and Chemical Structure at GaN, AlGaN and SiC Heterointerfaces," Appl. Surf. Sci. 244, 257-263 (2005).
- 49. M. Hetzer, Y.M. Strzhemechny, L.J. Brillson, M.A. Contreras, and A. Zunger, "Direct Observation of Copper Depletion and Potential Changes at Copper Indium Gallium Diselenide Grain Boundaries," Appl. Phys. Lett. 86, 162105-7 (2005).
- 50. S.T. Bradley, S.H. Goss, J. Hwang, W.J. Schaff, and L.J. Brillson, "Pre-Metallization Processing Effects on Schottky Contacts to AlGaN/GaN Heterostructures," J. Appl. Phys. 97, 084502 (2005).
- 51. Y.M. Strzhemechny, H.L. Mosbacker, S.H. Goss, D.C. Look, D.C. Reynolds, C.W. Litton, N.Y. Garces, N.C. Giles, L.E. Halliburton, S. Niki, and L.J. Brillson, "Shallow Donor Generation in ZnO by Remote Hydrogen Plasma," J. Electron. Mater. 34, 399-403 (2005).
- 52. S. Tumakha, S.H. Goss, and L.J. Brillson, "Electronic Defect States at Annealed Metal/4H-SiC Interfaces," J. Vac. Sci. Technol. B23, 594-598 (2005).
- 53. P.E. Smith, S.H. Goss, M. Gao, M.K. Hudait, Y. Lin, S.A. Ringel, and L.J. Brillson, "Atomic Diffusion and Band Lineups at $In_{0.53}Ga_{0.47}As$ -on-InP Heterointerfaces," J. Vac. Sci. Technol. B23, 1832-1837 (2005).
- 54. H.L. Mosbacker, Y.M. Strzhemechny, B.D. White, P.E. Smith, D.C. Look, "Role of Near-Surface States in Ohmic-Schottky Conversion of Au Contacts to ZnO," D.C. Reynolds, C.W. Litton, and L.J. Brillson, Appl. Phys. Lett. 87, 012102-3 (2005).
- 55. S.P.Tumakha, D.J. Ewing, L.M. Porter, Q.Wahab, X.Ma, T.S. Sudharshan, and L.J. Brillson "Defect Driven Inhomogeneities in Ni/4H-SiC Schottky Barriers," Appl. Phys. Lett. 87, 242106-3 (2005).

Grant-Supported National or International Conference Presentations (75 total, 28 Invited)

1. "Atomic-Scale Control of Electronic and Chemical Structure of Heterojunctions," L. J. Brillson, Advancing Frontiers of Condensed Matter Science, Philadelphia, PA, October 15, 1997. **(Invited)**

- 2. "Low Energy Cathodoluminescence Spectroscopy of Etched 6H-SiC Surfaces," L.J.Brillson, American Vacuum Society National Symposium, San Jose, CA, October 21, 1997.
- 3. "Atomic Bonding and Electronic States at Buried Semiconductor Dielectric Interfaces," G. Lucovsky and L. J. Brillson, Department of Energy Free Electron Laser Workshop, Newport News, VA, January 14, 1998. **(Invited)**
- 4. "Changing Roles of Physicists in Industry," L.J.Brillson, American Physical Society March Meeting, Los Angeles CA, March 15, 1998. **(Invited Tutorial)**
- 5. "Models for Internship Programs," L.J.Brillson, American Physical Society March Meeting, APS Career and Professional Development Liaison Workshop, Los Angeles CA, March 15, 1998. **(Invited)**
- 6. "Cathodoluminescence Deep Level Spectroscopy of Etched and In-Situ Annealed 6H-SiC," A. P. Young, K. Aptowitz, and L. J. Brillson, Materials Research Society Spring Meeting, San Francisco, CA, April 14, 1998.
- 7. "Electronic Near-Surface Defect States Observed by Cathodoluminescence Spectroscopy in Mg-GaN Junctions," A. P. Young, J. Schäfer, L. J. Brillson, Y. Yang, G. J. Lapeyre, J. D. MacKenzie, and C. R. Abernathy, 40^{th} Electronic Materials Conference, Charlottesville, VA, June 24, 1998.
- 8. "Changing Roles of Researchers in Industry," L.J.Brillson, American Vacuum Society Michigan Chapter Meeting, Livonia, MI, October 27, 1998. **(Invited)**
- 9. "Near-Surface Variation of Gallium Nitride Cathodoluminescence with Annealing," T. M. Levin, J. Schäfer, A. P. Young, L. J. Brillson, J. D. MacKenzie, and C. R. Abernathy, American Vacuum National Symposium, Baltimore, MD, November 2, 1998.
- 10. "Depth-Resolved Cathodoluminescence Spectroscopy Studies of Defects Near GaN/InGaN/GaN Quantum Wells," L.J.Brillson, T.M.Levin, G. Jessen, and F.A.Ponce, Physics and Chemistry of Semiconductor Interfaces Conference, San Diego, CA, January 19, 1999 **(Invited)**
- 11. "Localized States at GaN Surfaces, Schottky Barriers, and Quantum Well Interfaces," L.J.Brillson, Fifth IUMRS International Conference on Advanced Materials, Beijing, Peoples Republic of China, June 17, 1999 **(Invited)**
- 12. "Near-Surface Cathodoluminescence Spectroscopy of Erbium Doped AlN, A.P.Young, S.H.Goss, L.J.Brillson, J.D.MacKenzie, C.R.Abernathy, Electronic Materials Conference, Santa Barbara, CA, July 2, 1999.
- 13. "Defect Formation Near GaN Surfaces and Interfaces", L.J.Brillson, T.M.Levin, G.H.Jessen, A.P.Young, F.A.Ponce, Y.Yang, and G.J.Lapeyre, 20th International Conference on Defects in Semiconductors (ICDS-20), Berkeley, CA July 26, 1999.
- 14. "Localized Electronic States Near GaN Surfaces and Interfaces," 1st GaN Electronic Device Workshop, Cornell University, Ithaca, NY, August 17, 1999. **(Invited)**
- 15. "Localized Electronic States Near GaN Surfaces and Interfaces," L.J.Brillson, 47th Annual Solid State Conference & Solid State Theory Symposium, Athens, OH, October 17, 1999. **(Invited)**
- 16. "Deep Level Electronic States of Clean GaN (0001) (1x1) Surfaces Prepared by In Decapping, A.P. Young, L.J.Brillson, and C.W.Tu, American Vacuum Society National Symposium, Seattle, WA, Oct. 26, 1999.
- 17. "Near Surface Chemical Dependence of Electronic States at Al-Doped TiO₂ (110) Ultrathin Films," S.H.Goss, L.J.Brillson, and S.A.Chambers, American Vacuum Society National Symposium, Seattle, WA, Oct. 28, 1999.
- 18. "The Effect of Nitrogen Ion Damage on the Optical and Electrical Properties of MBE GaN Grown on MOCVD GaN/Sapphire Templates," A.P.Young, L.J.Brillson, Y. Naoi, and C.W.Tu, Materials Research Society Fall Meeting, Boston, MA, Dec. 2, 1999.
- 19. "Cathodoluminescence Spectroscpy of Erbium Doped GaN Grown on Silicon by MBE and MOMBE," S. H.Goss, L.J.Brillson, J.D.MacKenzie, and C.R.Abernathy, Materials Research Society Fall Meeting, Boston, MA, Dec. 2, 1999.
- 20. "Depth-Resolved LEEN Spectroscopy Studies of Interface Defects in AlGaN/GaN HEMT Heterostructures," A.P.Young, L.J.Brillson, M.J.Murphy, W.J.Schaff, and L. Eastman, 27th Annual Physics and Chemistry of Semiconductor Interfaces Conference, Salt Lake City, Utah, Jan. 20, 2000.
- 21. "Influence of AlGaN Deep Levels on AlGaN/GaN 2DEG Carrier Confinement," S.T.Bradley, A.P.Young, L.J.Brillson, M.J. Murphy, W.J. Schaff, and L.F. Eastman, The Sixth Annual Wide Bandgap III-Nitride Workshop, Richmond, VA, March 13, 2000.
- 22. "Direct Observation of Bulk and Interface States in GaN on Sapphire Grown by Hydride Vapor Phase Epitaxy," S.H. Goss, A.P.Young, L.J.Brillson, D.C. Look, and R.J. Molnar, The Sixth Annual Wide Bandgap III-Nitride Workshop, Richmond, VA, March 13, 2000.
- 23. "Changing Roles of Researchers in Industry," American Physical Society Meeting, Minneapolis, MN, March 19, 2000 **(Invited Tutorial)**
- 24. "Role of Barrier and Buffer Layer Defect States in AlGaN/GaN 2DEG HEMT Structures," S.T.Bradley, A.P.Young, L.J. Brillson, M.J. Murphy, and W.J. Schaff, Electronic Materials Conference, Denver, CO, June 22, 2000.
- 25. "Low Energy Electron Excited Nano-luminescence Spectroscopy of GaN Surfaces and Interfaces," Tenth International Conference on Solid Films and Surfaces, L.J.Brillson, Princeton, NJ, July 10, 2000. **(Invited)**
- 26. "Growth-Dependent Electronic States and Strain in GaN Heterostructures," Polarization Effects on Semiconductors Workshop, Glacier National Park, MT, L.J.Brillson, August 28, 2000. **(Invited)**
- 27. "Analysis of Tunneling Magnetoresistance Structures by Low Energy Electron Nanoscale Luminescence Spectroscopy," S.H.Goss, S.S.K.Parkin, and L.J.Brillson, American Vacuum Society National Symposium, Boston, MA, October 5, 2000.
- 28. "Defects and Doping at GaN/Sapphire Interfaces," L.J.Brillson, International Specialist Meeting on Bulk Nitride Growth and Related Techniques, Foz do Iguaçú, Brazil, November 14, 2000. **(Invited)**
- 29. Direct Observation of Bulk and Interface States in GaN on Sapphire grown by Hydride Vapor Phase Epitaxy," S.H.Goss, L.J.Brillson, D.C.Look, and R.J.Molnar, Materials Research Society Meeting, Boston, MA, November 30, 2000.
- 30. "Low Energy Electron Excited Nanoscale Luminescence Spectroscopy of Defects at Buried Interfaces and Ultrathin Films," L.J.Brillson, Twenty-Eighth Physics and Chemistry of Semiconductor Interfaces (PSCI) Conference, Orlando, FL, January 9, 2001. **(Invited)**
- 31. "Depth-Resolved Low Energy Electron Excited Nanoscale Luminescence of ZnO Surfaces," J.Bae, Y. Strzhemechny, D.C. Look, and L.J. Brillson, American Physical Society Meeting, Seattle, WA, March 14, 2001.
- 32. "Low Energy Electron-Excited Nano-luminescence Studies of GaN and Related Materials," $8th$ International Conference on the Formation of Semiconductor Interfaces, Hokkaido, Japan, June10, 2001. **(Invited)**
- 33. "Point Defect Distributions and Interdiffusion at AlGaN/GaN HEMT Structures," S.T. Bradley, G.H. Jessen, L.J. Brillson, M.J. Murphy, W.J. Schaff, N. Ikeo, and Y. Sakai, Electronic Materials Conference, South Bend, IN, June 27, 2001.
- 34. *"*Electronic Defect States Observed by Cathodoluminescence Spectroscopy at GaN/Sapphire Interfaces," X. L. Sun, S. H. Goss, L. J. Brillson, D.C. Look, and R.J. Molnar, The 4th International Conference on Nitride Semiconductors, Denver, CO, July 16, 2001.
- 35. "Defects and Interface Chemistry at III-V Nitride and SiC Surfaces and Interfaces," L.J. Brillson, Workshop on Near-Surface Effects in Semiconductor Substrates, Kodiak Island, Alaska, August 5, 2001 **(Invited)**
- 36. "Metal-Induced States and Polytype Transformations at SiC Interfaces," S. Tumakha, L.J. Brillson, G.H. Jessen, R.S. Okojie, D. Lukco, IUVSTA 15th International Vacuum Congress, AVS $48th$ International Symposium, $11th$ International Conference on Solid Surfaces, San Francisco, CA, October 29, 2001.
- 37. "Nanoscale Phase Formation at $CuIn_{1-x}Ga_xSe₂ Surfaces," Y.M. Strzhemechny, P.E.$ Smith, S.T. Bradley, L.J. Brillson, D.X. Liao, A.A. Rockett, and K. Ramanathan, IUVSTA 15th International Vacuum Congress, AVS $48th$ International Symposium, $11th$ International Conference on Solid Surfaces, San Francisco, CA, October 30, 2001.
- 38. "Microcathodoluminescence Study of Zn-doped GaN on Al₂O₃ and Free-Standing GaN," X. L. Sun, S. H. Goss, L. J. Brillson, D.C. Look, and R.J. Molnar, Office of Naval Research Nitride Specialists Workshop, Boston, MA, Nov. 25, 2001.
- 39. "Study of the Optical Characteristics of Bi_2O_3 -doped ZnO Powder by Cathodoluminescence Microscopy," X.L. Sun, L. J. Brillson, and Y.-M. Chiang, Materials Research Society Meeting, Boston, MA, November 28, 2001.
- 40. "Polytype Transformation at SiC Surfaces and Interfaces," ONR Workshop on Extended Defects in Wide Gap Semiconductors: Electrical and Optical Effects, Belize,C.A., January 29, 2002. **(Invited)**
- 41. "Effect of Oxygen on Luminescence and Vibrational Spectra of Mg-Doped GaN," D.E. Walker, Jr., Y. Koide, B.D. White, L. J. Brillson, M. Murakami, S. Kamiyama, H. Amano, and I. Akasaki, American Physical Society Meeting, Indianapolis, IN, March 18- 22, 2002.
- 42. "Si Doping of High Al Mole Fraction $Al_xGa_{1-x}N$ Alloys with RF Plasma MBE," J. Hwang, W.J. Schaff, L.F. Eastman, S.T. Bradley, and L.J. Brillson, Electronic Materials Conference, Santa Barbara, CA, June 27, 2002.
- 43. "Doping and Deep Level Defects in High Al Content AlGaN," S.T. Bradley, P.E. Smith, L.J. Brillson, and W.J. Schaff, 4th Symposium on Non-Stoichiometric Compounds, Pacific Grove, CA, October 3, 2002.
- 44. "Low Energy Electron-Excited Nanoscale Luminescence Characterization of Proton Irradiated AlGaN/GaN Field-Effect Transistor Structures," American Physical Society Ohio Section Fall Meeting, Columbus, OH, October 18, 2002.
- 45. "Surface Photovoltage Spectroscopy and Transients of Single Crystal ZnO(0001)," T. Barrus, L.J.Brillson, D. C. Look, and N. Garces, American Physical Society Ohio Section Fall Meeting, Columbus, OH, October 18, 2002.
- 46. "Surface Photovoltage Spectroscopy and Transients of Single Crystal ZnO(0001)," T.T. Barrus, L. J. Brillson, and D. C. Look, Second International Workshop on ZnO, MRS Workshop, Dayton, OH, October 23, 2002.
- 47. "Remote Hydrogen Plasma Treatment of ZnO Single Crystals," Y. M. Strzhemechny, J. Bae, L.J. Brillson, and D.C. Look, Second International Workshop on ZnO, MRS Workshop, Dayton, OH, October 23, 2002.
- 48. "Interdiffusion, Alloying, and Defect Formation at GaN-Sapphire Interfaces, X.L. Sun, S.T. Bradley, G.H. Jessen, and L.J. Brillson, AVS 49th International Symposium, Denver, CO November 5, 2002.
- 49. "Effect of Remote Hydrogen Plasma Treatment on ZnO Single Crystal Surfaces," Y. M. Strzhemechny, J. Bae, L.J. Brillson, and D.C. Look, Materials Research Society Meeting, Boston, MA, December 3, 2002.
- 50. "Deep Level Defects and Doping in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ with High Al Mole Fraction," S. T. Bradley, S. H. Goss, and L. J. Brillson, 30th Conference on the Physics and Chemistry of Semiconductor Interfaces, Salt Lake City, UT, January 19, 2003.
- 51. "Thermal and Doping Dependence of 4H-SiC Polytype Transformations," L.J. Brillson, American Physical Society, Austin, TX, March 3, 2003. **(Invited)**
- 52. "Microcathodoluminescence and Secondary Ion Mass Spectroscopies of Defects in III-V Nitride Semiconductors and Heterojunctions," L.J.Brillson, ONR Workshop on Defect Characterization Techniques in Wide Gap Semiconductors, Maui, HI, March 16, 2003. **(Invited)**
- 53. "Microcathodoluminescence Characterization of III-V Nitride Heterojunctions and Devices," L.J. Brillson, Electrochemical Society Meeting, Paris, France, April 27, 2003. **(Invited)**
- 54. "Microcathodoluminescence Spectroscopy of Localized Electronic States at Photelectrochemically-Etched Whiskers," X.L. Sun, L.J. Brillson, T. Hossain, and I. Adesida, Electronic Materials Conference, Salt Lake City, UT, June 25, 2003.
- 55. "Interface Interdiffusion and Chemical Reaction in GaN/Sapphire and AlGaN/Sapphire Heterojunctions," X.L. Sun, S.H. Goss, L. J. Brillson, and D.C. Look, Electronic Materials Conference, Salt Lake City, UT, June 26, 2003.
- 56. "Process-Induced Defects at SiC Surfaces and Metal Interfaces," L.J. Brillson, ONR Workshop on Process-Induced Defects in Wide Gap Semiconductors, Rogue Valley, OR, July 19, 2003. **(Invited)**
- 57. "SiC Studied via LEEN and Cathodoluminescence Spectroscopy," L.J. Brillson, 10th International Conference on Silicon Carbide and Related Materials 2003, Lyon, France, Oct. 7, 2003. **(Invited)**
- 58. "Localized Defect States, Impurities, and Doping in $Al_xGa_{1-x}N$ Epilayers," S.T. Bradley, L.J.Brillson, S.H.Goss, D.C. Look and W.J. Schaff, 50th International AVS Symposium, Baltimore, MD, Nov. 3, 2003. **(Invited)**
- 59. "Atomic Bonding and Electronic Changes at InGaAs/InP Heterojunctions," P.Smith, S.T. Bradley, S.H.Goss, M. Hudait, Y. Lin, S.A. Ringel, and L.J. Brillson, 50th International AVS Symposium, Baltimore, MD, Nov. 3, 2003.
- 60. "Dependence of Schottky Barrier Height on Electronic and Chemical Properties of Ni/AlGaN Contacts," S.T. Bradley, L.J. Brillson, and W.J. Schaff, 2003 International Semiconductor Device Research Symposium, Dec. 12, 2003. **(Best Student Conference Paper)**
- 61. "Local Electronic and Chemical Structure at GaN, AlGaN and SiC Heterointerfaces," 12th International Conference on Solid Films and Surfaces (ICSFS-12), Hamamatsu, Japan, June 22, 2004. **(Invited)**
- 62. "Electronic Defect States at Annealed Metal/4H-SiC Interfaces," S.Tumakha, L.J. Brillson, and R.S. Okojie, 46th Electronic Materials Conference, Notre Dame, IN, June 23, 2004.
- 63. "Remote Hydrogen Plasma Doping of Single Crystal ZnO," Y.M. Strzhemechny, L.J. Brillson, and D.C. Look, 46th Electronic Materials Conference, Notre Dame, IN, June 23, 2004.
- 64. "Near Surface Defects and Schottky Barrier Formation at Au/ZnO(000ī) Interfaces," L.J. Brillson, H.L. Mosbacker, Y.M. Strzhemechny, P.E. Smith, B.D. White, D.C. Look, and D.C. Reynolds, Third International ZnO Workshop, Sendai, Japan, October 6, 2004. **(Invited)**
- 65. "Near Surface Defects and Schottky Barrier Formation at Au/ZnO(000ī) Interfaces," H.L. Mosbacker, Y.M. Strzhemechny, P.E. Smith, B.D. White, D.C. Look, and L.J. Brillson, AVS 51st International Symposium, Anaheim, CA, November 16, 2004.
- 66. "Interface and Defect States at Ultrathin $SiO₂/HiO₂/SiO₂/Si$ Junctions," M. Bataiev, S.P. Tumakha, Y.M. Strzhemechny, S.H. Goss, C.L.Hinkle, C.C. Fulton, G.Lucovsky, and L.J. Brillson, Physics and Chemistry of Semiconductor Interfaces Conference, Bozeman, MT, January 25, 2005.
- 67. "Atomic Diffusion and Band Lineups at InGaAs-InP Heterointerfaces," P.E. Smith, S.H. Goss, M.K. Hudait, Y. Lin, S.A. Ringel, and L.J. Brillson, Physics and Chemistry of Semiconductor Interfaces Conference, Bozeman, MT, January 26, 2005.
- 68. "Electronic and Chemical Structure at Micro-Interfaces of CuIn_{1-x}Ga_xSe₂ Grain Boundaries," M. Hetzer, Y.M. Strzhemechny, M. Gao, and L.J. Brillson, Physics and Chemistry of Semiconductor Interfaces Conference, Bozeman, MT, January 26, 2005.
- 69. "Nanoscale Deep Level Defect Correlation with Schottky Barriers in SiC-Metal Diodes," S.P. Tumakha, S.H. Goss, D.Ewing, L.M. Porter, X. Ma, T. Sudershan, Q.u.Wahab, and L.J. Brillson, Workshop on Compound Semiconductor Materials & Devices, Coconut Beach, FL, February 22, 2005. **(Invited)**
- 70. "Plasma Processing Control of ZnO Schottky Barriers," H.L. Mosbacker, Y.M. Strzhemechny, P.E. Smith, B.D. White, D.C. Look, and L.J. Brillson, Workshop on Compound Semiconductor Materials & Devices, Coconut Beach, FL, February 23, 2005. **(Invited)**
- 71. "Interface and Defect States at Ultrathin HfO_2-SiO_2-Si Junctions," M. Bataiev, S.P. Tumakha, Y.M. Strzhemechny, S.H. Goss, C.L. Hinkle, G. Lucovsky, and L.J. Brillson, Materials Research Society Meeting, San Francisco, CA, March 30, 2005.
- 72. "Electronic and Chemical Structure at Micro-Interfaces of $CuIn_{1-x}Ga_xSe₂ Grain$ Boundaries," M. Hetzer, Y.M. Strzhemechny, M. Gao, M.A. Contreras, A. Zunger, and L.J. Brillson, Materials Research Society Meeting, San Francisco, CA, March 31, 2005.
- 73. "Controlling Ohmic-to-Rectifying Conversion of Au-ZnO Interfaces and the Role of Near-Interface States," L.J. Brillson, Workshop on Materials and Devices Incorporating Functional Interfaces," Palm Springs, CA, April 13, 2005. **(Invited)**
- 74. "Spontaneous Atomic Ordering and Band Gap Narrowing in Epitaxial $Al_xGa_{1-x}N$," M. Gao, S.T. Bradley and L.J. Brillson, Electronic Materials Conference, Santa Barbara, CA, June 23, 2005.
- 75. "Schottky Barrier Formation at Non-Polar Au/GaN Epilayer Interfaces," D.E. Walker, L.J. Brillson, and W.J. Schaff, Electronic Materials Conference, Santa Barbara, CA, June 24, 2005.

Plus 48 invited university, Federal laboratory, and international institute lectures.

Graduate Students

Gregg Jessen, Ph.D. in Electrical Engineering, 12/13/02. Junjik Bae, M.S. in Physics, 6/13/02. Dennis Walker, Ph.D. in Electrical Engineering, 3/06.

Honors

- 1. American Physical Society Centennial Speaker (1998-99)
- 2. IEEE Fellow (2000)
- 3. Technical Achievement Recognition Award, IEEE Columbus Section (2000).
- 4. Ohio State University Lumley Research Award (2001)
- 5. Office of Naval Research Outstanding Speaker Award (2001)
- 6. Fellow, American Association for the Advancement of Science (2002)

Editorial / Program/Review Panel Responsibilities

- 1. Associate Editor, Journal of Electronic Materials (1992 present)
- 2. Program Committee, Electronic Materials Conference (1997-present)
- 3. Executive Committee, Electronic Materials Conference (2000-2002)
- 4. Advisory Board, International Conference on Atomically Controlled Surfaces, Interfaces, and Nanostructures (1998, 2000)
- 5. Senior Editor, Electronic Materials Reviews, Journal of Electronic Materials (2000)
- 6. NASA SBIR Phase II Review Panel (2002-present).

National Professional Service

- 1. Chair, American Physical Society Forum on Industrial & Applied Physics (1996-97)
- 2. Past Chair, American Physical Society Forum on Industrial & Applied Physics (1997-98)
- 3. Executive Committee, Electronic Materials and Processing Division, American Vacuum Society (1997-98)
- 4. Board of Trustees, American Vacuum Society (1999-2002)
- 5. Long Range Planning Committee, American Vacuum Society (1996-present)
- 6. Electronic Materials Committee The Minerals, Metals, and Materials Society (TMS) (2000-2002).