Synchrotron Radiation Spectroscopic Study of Surface and Bulk Electronic Structure of Wide Band Gap Semiconductors

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In this program, we use synchrotron-radiation based spectroscopies to measure the surface and bulk electronic structure of wide band gap semiconductors. Our goal is to understand how this structure effects the growth of thin films of wide band gap semiconductors, the growth of contact overlayers on the nitrides, and the chemical stability of the films and overlayers. These materials have numerous potential applications in optoelectronic and high temperature devices. Despite much study over the last decade, much remains unknown about their fundamental physical and chemical properties.

The results of two different experiments are reported here. In Figure 1 we report the first observation of resonant photoemission in GaN. Resonant photoemission is a phenomenon associated with the interaction of multiple decay channels for holes created via photoemission, and can be used to probe the degree of electron localization in solids. Analysis of this data is underway. In Figure 2 we report the first study of the interaction of atomic sulfur with clean GaN. The goal of this study is to explore the chemical passivation of GaN, whereby a S overlayer on GaN inhibits the formation of an oxide overlayer. The data in Figure 2 explore the S/GaN interface; oxygen exposure experiments are underway.

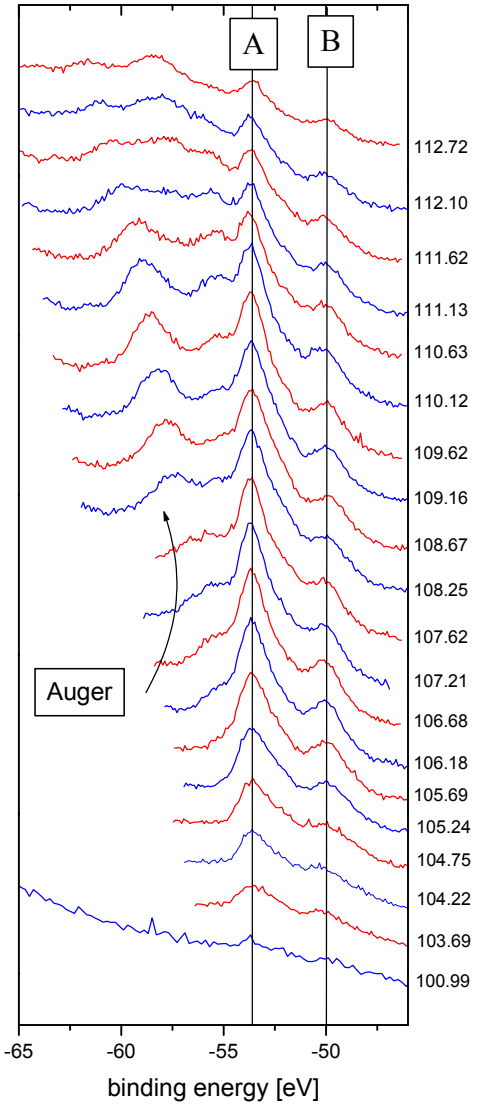

Figure 1: First observation of resonant photoemission effects in GaN. The figure shows a series of photoemission spectra taken from cleaved single crystal GaN as a function of excitation energy. Note the change in intensity of feature "A" as the incident photon energy is increased through the Ga *3p* absorption threshold. Features "A" and "B" are due to satellites of the main Ga 3*d* line related to the $3d^8$ multiplet. The dispersive features are $M_{2,3}$ $M_{4,5}$ $M_{4,5}$ Auger transitions. Features "A" and "B" are associated to the ^1G and ^1F terms of the $3d^8$ multiplet.

An important new class of semiconductor based on nitrogen compounds is the focus of intense scrutiny due to their numerous potential applications in lasers and other optical devices that operate in the blue/UV portion of the spectrum. These materials, know as wide band gap nitride semiconductors, also hold the promise of being used in electronic devices operating at much higher temperatures than conventional materials. While many simple devices have been fabricated from these materials, there remains an acute lack of knowledge about their fundamental electronic and chemical properties. It is of vital importance for the full commercial exploitation of these materials to understand their basic properties since, for example, the behavior of electrons near the nitride surface controls their chemical reactivity, their structural stability, and how other materials are bonded to them. The basic electronic properties of these materials will be studied using two probes: photoemission spectroscopy and x-ray emission spectroscopy. These probes involve the excitation of the electrons in the material by illumination with intense x-rays and measuring their response. This combination of spectroscopies will provide a comprehensive understanding of the electronic and chemical properties of these new important semiconductors. This program will also educate postdoctoral research associates, graduate and undergraduate students in the physics and chemistry of semiconductor materials, and the application of state of the art spectroscopic probes in their study.

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Educational Activities:
This program involves one undergraduate student (Sarah Bernardis), one graduate student (Leyla Colakerol) and one postdoctoral research associate (Dr. Lukasz Plucinski). *Note also that the PI has finished a two year appointment as the first Academic Director of the Center for Excellence in Teaching at Boston University. Furthermore, the PI was named the 2001 Massachusetts Professor of the Year by the Carnegie Foundation.*

Infrastructure Impact:
The PI used the present NSF award to leverage significant funds for scientific infrastructure enhancement. He was awarded $50,000 from the Defense University Research Instrumentation Program of the Army Research Office to purchase an Electron Cyclotron Resonance plasma source. This will be attached to our multi-technique spectrometer system based at the National Synchrotron Light Source, and will be used to clean GaN thin films. Our spectrometer system is fully operational and features both a high resolution angle resolved photoemission spectrometer (100 mm Scienta), and a high resolution soft x-ray emission spectrometer.

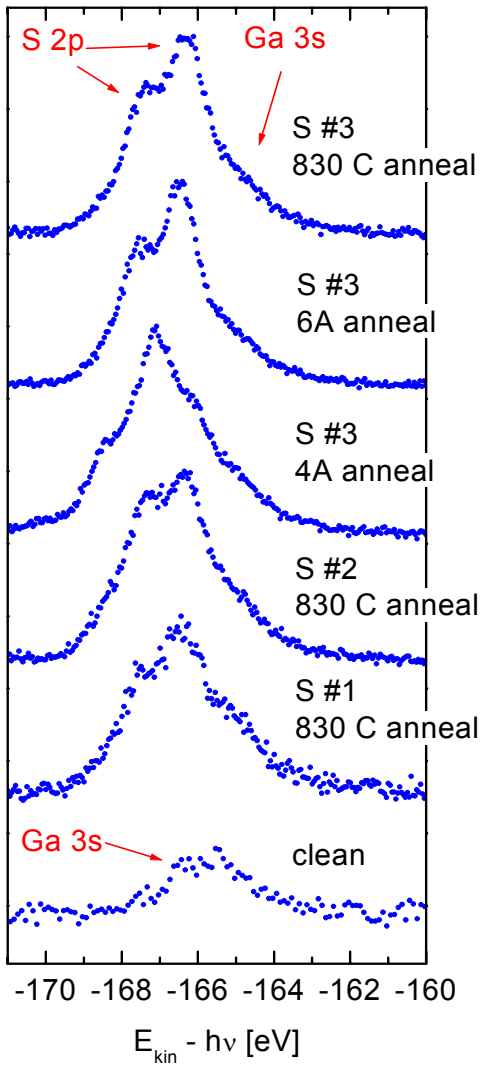

Figure 2:
High resolution soft x-ray core level photoemission from clean thin film GaN(0001) and GaN(0001) exposed to atomic sulfur in vacuum. S was deposited using an in-vacuum electrochemical source. Clear changes in the electronic structure of the S-GaN interface is observed as the surface is annealed to a variety of temperatures near the growth temperature for the GaN thin films. Ongoing experiments are probing the reaction of O_2 with such S-covered GaN surfaces