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Correlative Electron Energy-Loss Spectroscopy Bandgap Mapping and DFT Modeling in AlGaN Diodes

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The development of functional nanodevices demands the detailed understanding of structure-property-performance relationships on the nanoscale. Specifically, correlating electronic response with nanoscale chemical and structural features/interfaces is paramount to understanding macroscale properties and thus advancing associated semiconductor device technologies. These understandings - obtainable through high-resolution information - are vital for the development of semiconductor device design. While many electronic transitions are critical to ultimate device performance, the electronic bandgap is the property most used to design device behaviors. Nanoscale structural and chemical features have strong influence over the bandgap – and thus device performance – but can be challenging to track. This is especially true when searching for spatially resolved impacts of dopants which exist at low concentrations ranging from 10e16 to 10e20 cm^{-3}.

In this contribution, we analyze bandgap variations at critical p/n type interfaces in AlGaN power diodes through high energy-resolved, low-loss electron energy-loss spectroscopy (EELS) in the scanning transmission electron microscope (STEM). We study devices that have large differences in current leakage under reverse bias. Near the breakdown voltage of -900V, the high performing devices had leakage currents < 1 nA, while other devices had 20-200x greater leakage currents. For low-loss EELS, while using a square root function fit of $(E-E_b)^{0.5}$ - where E_b is the bandgap - to determine bandgap values in widegap materials is commonly accepted [1,2], we find that using the inflection point as described in ref [2] provides a more objective method of analyzing bandgap trends as it requires less user input. Bandgap mapping across the p/n type interfaces in AlGaN devices show an increase in the bandgap at interfaces in leaky devices and a decrease in the bandgap at interfaces in devices without current leakage as shown in Figures 1 and 2.

While we cannot say definitively if these bandstructure differences play a significant role in ultimate device performance, they may provide a means of indirectly measuring where the dopants in the device are. Normally energy dispersive x-ray spectroscopy (EDXS) or core-loss EELS in the TEM are used to track compositional variations in samples, but with concentrations < 1e19 cm^{-3}, there is not enough signal generated to determine where the dopants accumulate (if they do at all). Density functional theory (DFT) modeling of different interfaces in AlGaN materials - matching the ones used in this experiment - indicates that dopants accumulating at the interface leads to a decrease in the bandgap. Combining these DFT simulations with experimental low-loss EELS data provides insight into the behaviors of dopants in AlGaN power diodes and is applicable to electronic devices on a wider scale [3].

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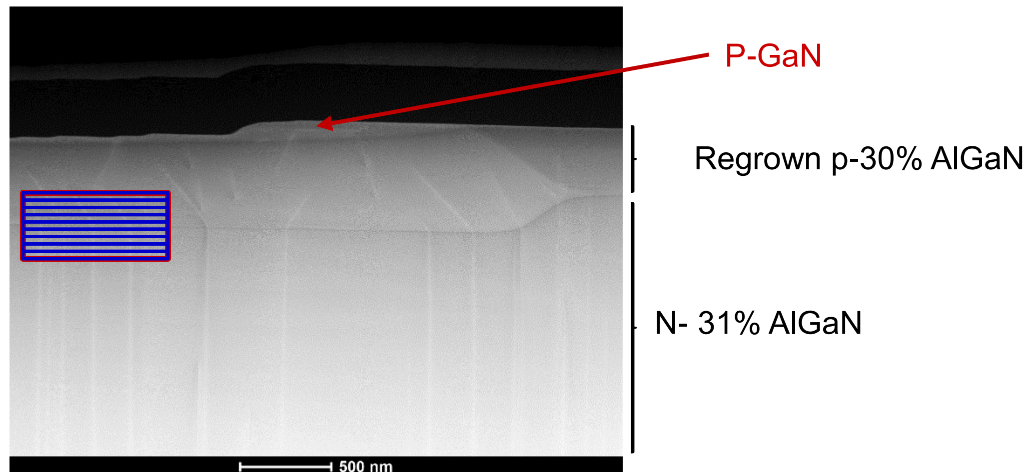

Figure 1. HAADF image of AlGaN device showing summed EELS regions analyzed

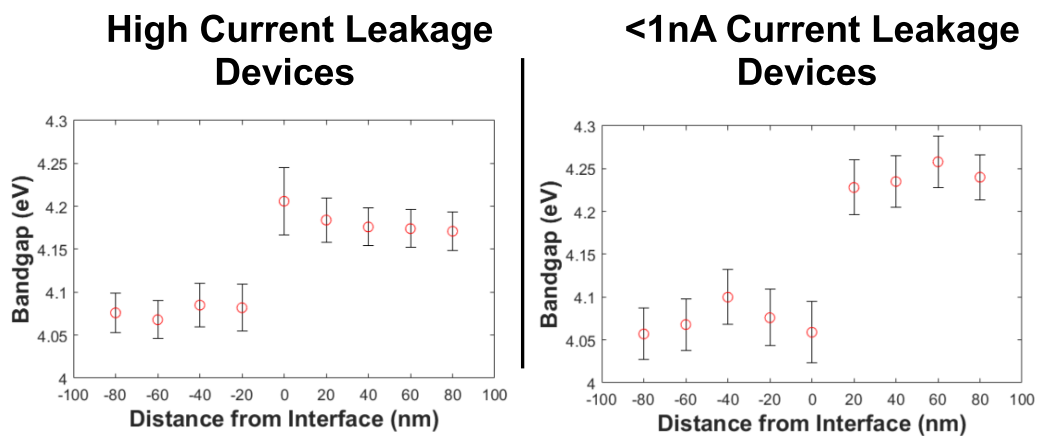

Figure 2. Bandgap variations across AlGaN p and n type interfaces in devices with (left) and without (right) current leakage.

References:

[1] B Rafferty and LM Brown, Phys. Rev. B **58** (1998), p. 10326.
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