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# Oxygen Segregation and Electronic Structure Changes at Dislocations in GaN

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Although oxygen is known to be an impurity present in GaN thin films, its origins and effects are still poorly understood, particularly in regard to its segregation to dislocation cores. The few studies that have been conducted on the presence of oxygen in GaN thin films have suggested that it may originate from being an impurity in the $NH_3$ precursor for metal organic chemical vapor deposition (MOCVD), from the remnant water vapor in molecular beam epitaxy (MBE) [1], or that oxygen from the $Al_2O_3$ substrate may diffuse into the GaN film from the disordered interfacial region [2]. However, since oxygen always seems to be present, perhaps the more important question is how it affects the optical and mechanical properties of the material. The focus of this research is therefore to identify the location of the oxygen impurities and understand the effect that they have on the material's properties.

The experimental analysis is performed here by a combination of atomic resolution Z-contrast imaging and electron energy loss spectroscopy (EELS) in the scanning transmission electron microscope (STEM) [3]. Figure 1a shows an image of a nanopipe, ~45nm in diameter, found in thin film GaN grown by metal organic chemical vapor deposition (MOCVD). Figure 1b shows the corresponding EEL spectra, with 5 different positions of the probe, starting at the edge and moving into the bulk (bottom to top in figure). Clearly, as the probe is moved in toward the edge of the nanopipe, the nitrogen signal in the EEL spectrum decreases while the oxygen signal increases. Finally, at the very edge of the nanopipe, there is no nitrogen signal left while the oxygen remains, indicating the formation of GaO lining the walls of the nanopipe. This result provides strong evidence that oxygen substitutes for nitrogen on the lattice sites, and not only specifically at the edge, but even further in towards the bulk of the sample, ~90Å [4]. The effects of oxygen segregation have been observed experimentally at two other types of screw dislocations (closed and filled) and the results from all three of these screw dislocations will be discussed.

In order to fully understand the structure-property relationships of this complex oxygen segregated system, theoretical simulations are required. For this analysis, we use first principles density functional theory (DFT) calculations using the pseudopotential total energy method [5]. The first step in calculating the density of states (DOS) using ab-initio methods is to simulate the bulk material to verify the input parameters, and to remember to take note of the energy resolution of the experimental spectrum so as to be able to compare experiment with theory properly. Figure 2 shows a plot of the initial DFT analyses with 0.4eV energy resolution as compared to an experimental spectrum with the same energy resolution. The DFT spectrum reproduces the fine structure from the experiment very well. Using these parameters, detailed first principles calculations investigating oxygen at open and closed screw dislocations are performed. These results will enable us to elucidate the effects of the oxygen segregation on the local electronic properties of the dislocation cores [6].

References

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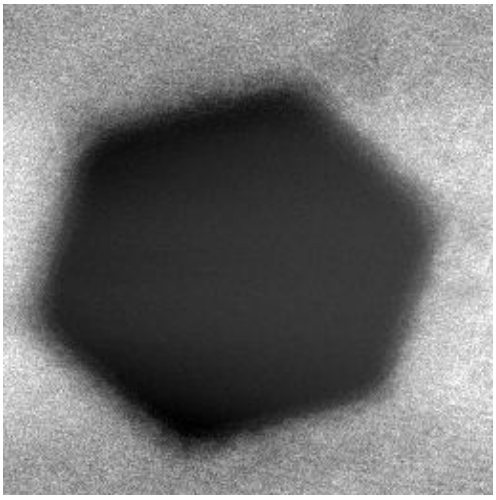

FIG. 1a. Z-contrast image of a nanopipe in GaN ~45 nm in diameter.

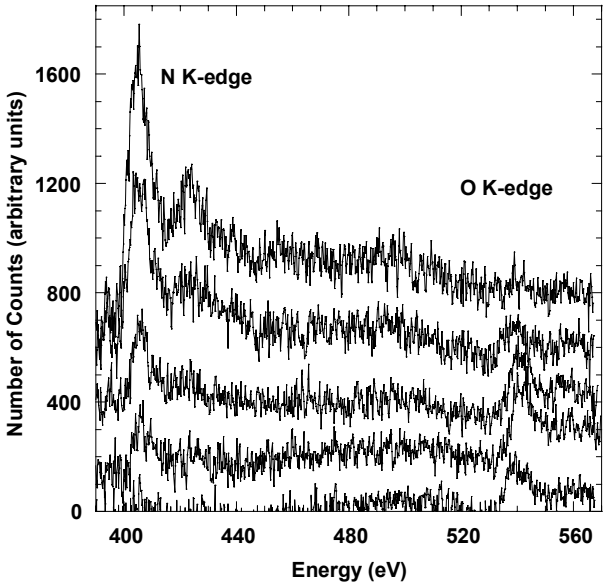


FIG. 1b. EEL spectra of the nitrogen and oxygen K-edges as the probe moves from the edge of the nanopipe into the bulk material.

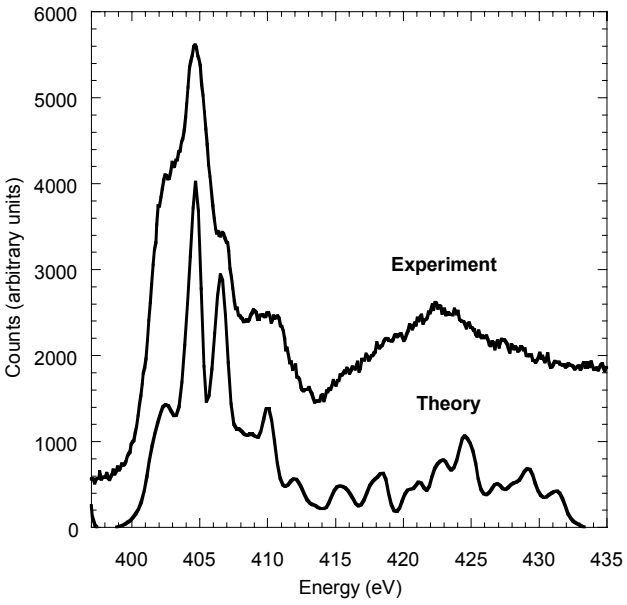


FIG. 2. DFT calculated DOS spectrum compared to an experimental spectrum, both with 0.4eV energy resolution.

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