Schottky barrier height dependence on polarity and doping density of GaN in epitaxially grown NbN/GaN structures

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Wurtzite GaN, with a non-centrosymmetric crystal structure, has been shown to have a polarity-dependent schottky barrier height with various metals [1, 2, 3]. The metal/Ga-polar (0 0 0 1) GaN diode shows a significantly larger barrier height than the metal/N-polar (0 0 0 $\bar{1}$) GaN diode for the same metal and same GaN doping density, N_d. In all of these studies, prior to the metal deposition by evaporation, the GaN samples were exposed to air. There is a strong evidence in the literature that the N-polar GaN is more reactive than the Ga-polar GaN [4]. Although these previous studies involved careful acid treatment to remove surface oxides prior to metal deposition, the observed difference in barrier heights can also be explained by enhanced oxygen contamination at the metal/N-polar GaN interface compared to the metal/Ga-polar GaN interface.

In our study, we use bulk GaN substrates with dislocation densities less than 10^4 /mm^2 to deposit epitaxial NbN on GaN using molecular beam epitaxy without breaking ultra-high vacuum to minimize the unintentional interface contamination. The as-grown NbN/GaN structures were studied by X-ray diffraction to confirm single crystal NbN and GaN layers with rocking curves around NbN (1 1 1) peak showing full width at half maximum of less than 70 arc-secs. Atomic force microscopy scans of these samples also show smooth surface roughnesses with root-mean square values of less than 2 nm. Secondary-ion mass spectrometry of NbN/GaN samples grown on both N-polar GaN and Ga-polar GaN together by co-loading revealed that the unintentional doping due to oxygen contamination of the epitaxially grown N-polar GaN is one order of magnitude higher ($\sim 4\times10^{17}$ /cm^3) than that of Ga-polar GaN ($\sim 2\times10^{16}$ /cm^3) similar to other reports in literature [4].

We observe a difference in Schottky barrier height of 0.41 eV for NbN/GaN junctions grown on Ga-polar and N-polar GaN with similar doping density of $N_d \sim 10^{18}$ /cm^3. The polarity dependence of Schottky barrier height was phenomenologically explained by Suemitsu et al., wherein they hypothesized a spread of polarization charges at the metal/GaN interface [2]. We extend this theory by including the doping density of GaN, which was previously neglected by Suemitsu et al. We then verify the doping density dependence, predicted by our model, on the Schottky barrier height of NbN/Ga-polar GaN diodes. By changing the doping density of Ga-polar GaN from $N_d \sim 10^{18}$ /cm^3 to $N_d \sim 10^{17}$ /cm^3, we observe that the Schottky barrier height of NbN/Ga-polar GaN increases by 0.12 eV.

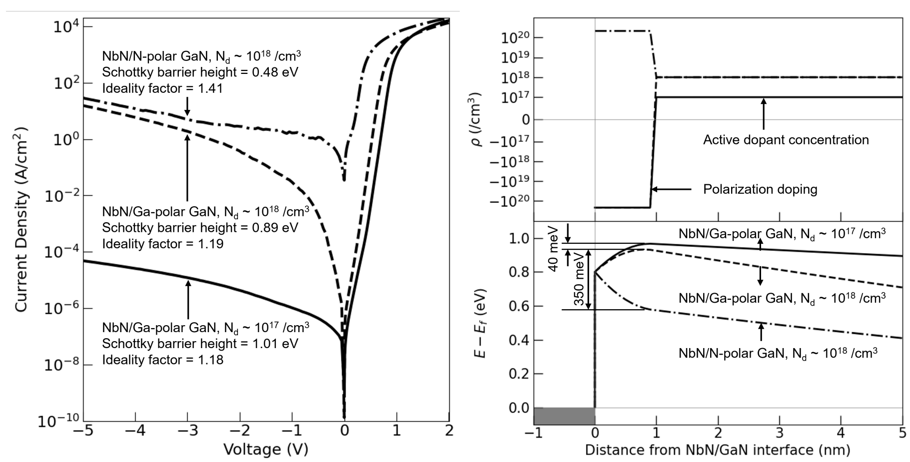

Fig. 1. (left) Current-voltage characteristics of NbN/GaN diodes. (right) Charge-conduction band diagrams of NbN/GaN diodes based on our model to explain the experimentally observed difference in Schottky barrier heights.

References

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