Abstract Submitted
for the CAL10 Meeting of
The American Physical Society

Oxidation of nitride surfaces and its effect on device performance[1]

MAOSHENG MIAO, LUKE GORDON, JUSTIN WEBER, CHRIS VAN DE WALLE, Materials Department, University of California Santa Barbara — Using computational methods based on density functional theory and Schrödinger-Poisson simulations, we investigate atomistic and electronic structures of oxidized GaN and AlN (0001) surfaces and their effects on the two-dimensional electron gas (2DEG) at AlGaN/GaN heterojunctions. Numerous structures with different oxide coverage and different stoichiometry are examined, and their stability is interpreted in terms of driving mechanisms such as the electron counting rule and oxide-stoichiometry matching. We discuss which structures are likely to form under a variety of oxidation conditions, and show that these structures explain the observed dependence of electron density on thickness and variations of surface barrier height. The surface donor states with distributed and finite density are implemented in Schrödinger-Poisson simulations of AlGaN/GaN high electron mobility transistors (HEMTs). The recent experimental observations of an increasing surface barrier height with increasing AlGaN thickness are fit very well by simulations including surface donor levels represented by a constant density of states (DOS) with a density on the order of 10^{13} $cm^{-2}eV^{-1}$. The highest occupied surface states are found to be around 1 eV below the conduction-band minimum, which is in good agreement with the first-principles results.

[1]Supported by ONR under award number N00014-08-1-0095, and made use of NSF-funded TeraGrid resources under grant No. DMR070072N.

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Date submitted: 26 Sep 2010 Electronic form version 1.4