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Atomic displacements in proton-irradiated AlGaN/GaN heterostructures YEVGENIY PUZYREV, 1, TANIA ROY, ENXIA ZHANG, RONALD SCHRIMPF, DANIEL FLEETWOOD, 2, SOKRATES PANTELIDES, 1, DEPARTMENT OF PHYSICS AND ASTRONOMY DEPARTMENT, VANDERBILT UNIVERSITY TEAM, DEPARTMENT OF ELECTRICAL ENGINEERING AND COMPUTER SCIENCE, VANDERBILT UNIVERSITY TEAM
— We report results of quantum molecular dynamics calculations of atomic recoils in AlGaN and GaN. The recoil energy required to create defects in a perfect AlGaN/GaN lattice is known to be over 40eV. However, drastic changes in atomic configuration occur when defect atom itself recoils with than 10eV. We show that both N antisite defects and N atoms near Ga vacancy require less than 10 eV to introduce N vacancies, divacancies and N interstitials. This phenomenon leads to additional donors that can account for a positive shift in threshold voltage, observed in our electrical measurements in AlGaN/GaN devices irradiated by 1.8 MeV protons.[1] In addition, divacancies and N vacancies have an electron transition level near the Fermi level in AlGaN which also provides explanation for the experimentally observed increase in 1/f noise after proton irradiation.[2]

[1]T. Roy, et. al., *IEEE Trans. Nucl, Sci.*, 2010. accepted
[2]T. Roy, et al, *Microelectron. Reliab.*, 2010, accepted.

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