Atomic displacements in proton-irradiated AlGaN/GaN heterostructures

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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 40 eV. However, drastic changes in atomic configuration occur when defect atom itself recoils with than 10 eV. 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.\(^2\)


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