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Effects of edge and screw dislocations on optical properties of Wurtzite GaN

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The wide bandgap and high temperature stability of GaN makes it a desirable material for applications such as blue light-emitting diodes, blue lasers, and high-power transistors. Despite these advantages, the large lattice mismatch in most epitaxial GaN leads to a high density of dislocations, on the order of $10^9 \text{cm}^{-2}$ for edge dislocations and $10^8 \text{cm}^{-2}$ for screw dislocations in WZ GaN. Edge dislocations are electron acceptors and take on a negative charge. Open-core screw dislocations are essentially voids, or nanopipes, in the material. The presence of these defects, plus the strain field associated with each dislocation type, change the density of states and reduce the PL intensity in typical epitaxial GaN device layers. In the present work, the effects of edge and screw dislocations in WZ GaN have been studied computationally as a function of dislocation density. Spectral properties are determined by solving a 6x6 multiband kp Hamiltonian in three-dimensions using a real-space finite element method. Results compare favorably to available experimental data.

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