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Probing the microstructure of the Si-N defect in GaAs[1] JOHN BUCKERIDGE, STEPHEN FAHY, Tyndall National Institute, Ireland and University College Cork, Ireland — The addition of N to Ga(In)As causes a dramatic decrease in the energy band gap. However Si doping of Ga(In)N_xAs_{1-x} after rapid thermal annealing results in a highly resistive material with an energy band gap governed by a net 'active' N roughly equal to the total N content minus the Si concentration. In order to understand this mutual passivation effect two defect complexes have been proposed: (a) Si and N substituting on adjacent Ga and As sites, and (b) Si and N atoms forming a split-interstitial defect on an As site. We present results of density functional theory (DFT) calculations on the full spectrum of localized vibrational mode of these defects, which can be used as experimental probes in determining the presence of either defect complex. We also present results of DFT calculations of the formation energies of the defects, confirming previous calculations [A. Janotti *et al.*, Phys. Rev. Lett. 100, 045505 (2008)]. We agree with their conclusions that the split-interstitial is the more likely configuration at the experimental annealing temperatures.

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