Probing the microstructure of the Si-N defect in GaAs\(^1\) JOHN
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versity 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\(_x\)As\(_{1-x}\) 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 \textit{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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