

Abstract Submitted
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Effect of indium on the localized vibrational mode of nitrogen in $\text{GaN}_x\text{As}_{1-x}$ ¹ A. M. TEWELDEBERHAN, Tyndall National Institute, Lee Maltings, Prospect Row, Cork, Ireland, STEPHEN FAHY, Department of Physics, University College Cork, Ireland — The effect of the substitution of nearest-neighbor gallium atoms by indium (In-N-Ga, In-N-In) on the frequency of the localized vibrational mode of substitutional nitrogen in the dilute nitride, $\text{GaN}_x\text{As}_{1-x}$, has been studied within first-principles density functional theory, using a supercell approach. The splitting of the highly localized triply-degenerate mode into singly- and doubly-degenerate modes is obtained and compared with available Raman and FTIR spectroscopy measurements. The results are in good agreement with the experimental values.

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