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High-resolution X-ray diffraction and Photoluminescence study of GaAsN epilayers

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Abstract
Incorporating nitrogen atoms into gallium arsenide (GaAs) significantly reduces the band gap, primarily due to a downward shift in the conduction band edge. This distinctive characteristic of gallium arsenide nitride (GaAsN) and other III-V-N alloys makes them promising candidates for various applications in semiconductor electronics, such as solar cells and telecommunication laser diodes based on GaAs.
In this study, GaAsN/GaAs layers were fabricated using metal-organic vapour phase epitaxy (MOVPE) on semi-insulating GaAs (100) substrates that were off-cut by 2° (±0.05) towards [100]. Before the growth of the GaAsN epilayer, a GaAs buffer layer with a thickness of 0.5 µm was deposited at a temperature of 600℃. GaAs1-xN$_x$ was grown using a novel combination of precursors: triethylgallium (TEGa), tertiary-butyl arsine (TBAs), and tertiary-butylhydrazine (TBHy), as sources for gallium (Ga), arsenic (As, and nitrogen (N), respectively. The structural and optical properties of GaAs1-xNx/GaAs were characterised through high-resolution X-ray diffraction (HRXRD) and photoluminescence (PL), performed over a temperature range of around 5–200 K.
HRXRD showed that the GaAsN and GaAs buffer layer peaks dominate for all samples. A noticeable shift to lower angles was seen for samples with higher nitrogen content, suggesting a significant lattice expansion due to increased nitrogen incorporation. PL of the GaAsN/GaAs epilayers reveals a reduction in peak emission energy as the nitrogen concentration increases. The redshift observed is approximately 18 meV and 240 meV for nitrogen contents of x=0.006 (Fig. 1) and x=0.012 (Fig. 2), respectively. These results show that the significant shift is attributed to the variation of the band gap with nitrogen incorporation and suggest that the band gap bowing parameter is not constant but varies depending on the nitrogen content of GaAs1-xNx. In addition, the PL spectral line (1.438 eV) shape indicates that the photogenerated carriers are trapped in localised states within the GaAsN matrix.

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