

Exciton localisation in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys

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Abstract:

The optical properties of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ epilayers with x ranging from 0.08 to 0.66 have been studied by photoluminescence (PL). The temperature dependent PL of the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ epilayers show a classical S-shape behaviour. This behaviour is attributed to exciton localisation due to compositional fluctuations in the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layers. The localisation energy is found to increase with Al composition, up to a value of 65 meV at the highest Al composition studied.

Introduction:

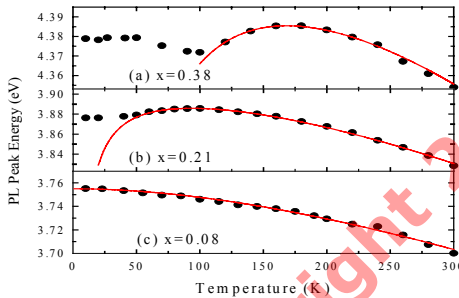
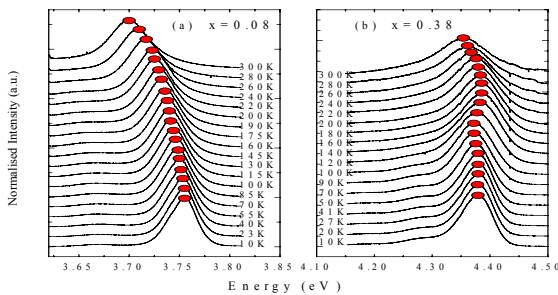
The $\text{Al}_x\text{Ga}_{1-x}\text{N}$ bandgap can be varied between 3.4 eV and 6.2 eV which makes $\text{Al}_x\text{Ga}_{1-x}\text{N}$ an ideal semiconductor material for ultraviolet (UV) applications (200 nm-400 nm) especially light emitting devices. However, due to lack of a lattice-matched substrate, a high dislocation density is observed in $\text{Al}_x\text{Ga}_{1-x}\text{N}$. These dislocations act as non-radiative recombination centres and greatly reduce the luminescence efficiency. Exciton localisation in nitride semiconductors may help to reduce the sensitivity of the optical efficiency to the dislocation density. High luminescence efficiency of InGaN based light emitting diodes is attributed to recombination of strongly localised excitons.[1] The excitons trapped in localised sites and are prevented from reaching dislocation centres and hence enhance luminescence efficiency.

S-shape Temperature Dependent PL:

The PL peak energy of our $\text{Al}_x\text{Ga}_{1-x}\text{N}$ epilayers shows a decrease-increase-decrease shift from 10 K to 300 K and looks like an S-shape.

This S-shape behaviour is a signature of exciton localisation. This exciton localisation behaviour observed in bulk $\text{Al}_x\text{Ga}_{1-x}\text{N}$ would suggest that there is some form of random alloy compositional fluctuation.

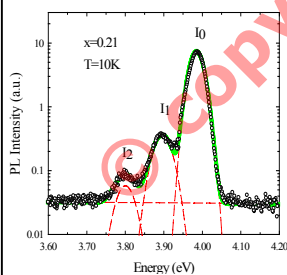
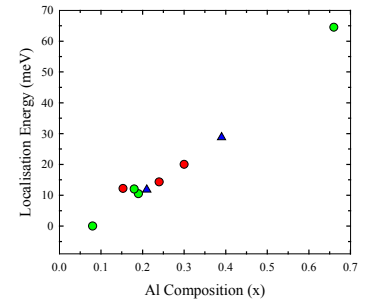
No S-shape behaviour is observed in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer with $x=0.08$. This would indicate that the Al content in this layer is too low to cause a compositional fluctuation that can affect the exciton luminescence.



The S-shape PL emission peak energy of our $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layers is modelled using a Varshni's expression based on band-tail model:

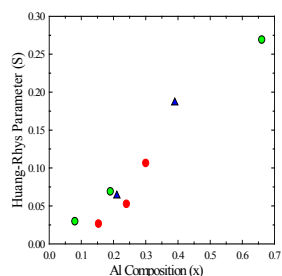
$$E(T) = E(0) - \alpha T^2 / (T + \beta) - \sigma^2 / (K_B T)$$

where $E(0)$ is bandgap energy of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ at 0 K. α and β are Varshni fitting parameters and σ is localisation energy of the exciton which indicates the degree of localisation. The localisation energy is found to increase with Al composition, x .



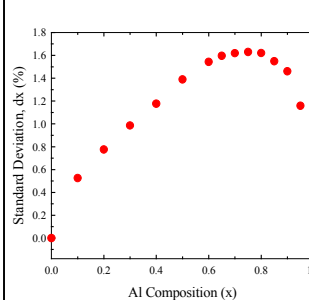
Electron-phonon coupling:

A series of LO phonon replicas in the lower energy side of main emission peak can be clearly observed from our $\text{Al}_x\text{Ga}_{1-x}\text{N}$ PL.



Huang-Rhys parameters show that exciton-phonon coupling strength increases with Al composition.

This indicates that degree of localisation increases with Al composition, agrees with S-shape PL results.



Simulations:

A simple simulation has been carried out to model the compositional fluctuations in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ based on a perfectly random alloy.

This simulation program computes the probability in finding Al atoms and Ga atoms within an exciton volume. The simulation results suggest that the degree of localisation in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ is the greatest at $x=0.75$.

Conclusion:

In summary, the exciton localisation in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ with x ranging from 0.08 to 0.66 has been studied. The localisation behaviour is due to compositional fluctuations in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloy. Our simulation based on a perfectly random alloy suggests that the degree of localisation in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ is the greatest at $x=0.75$.

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[1] S. Chichibu, K. Wada and S. Nakamura, Appl. Phys. Lett. 71, 2346 (1997)