

## Nano self-assembling in $\text{Al}_x\text{Ga}_{1-x}\text{N}_y\text{As}_{1-y}$ alloys

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The III-V alloys with an element having highly dissimilar properties are widely studied now due to their unique properties and device applications. The strong spatial correlation effects between the atoms leading to preferential formation of the Al-N bonds were experimentally established in the heavy N-doped  $\text{Al}_x\text{Ga}_{1-x}\text{N}_y\text{As}_{1-y}$  alloys. This preference in the bond formation should have a complicated nature. The bond transformation  $n\text{Al-As} + n\text{Ga-N} \rightarrow n\text{Al-N} + n\text{Ga-As}$  ( $1 \leq n \leq 4$ ) is carried through an exchange of the lattice sites between the cations or anions. The sum of the AlN and GaAs free energies is considerably smaller than the sum of the GaN and AlAs free energies. Thus, there is a thermodynamic preference of the simultaneous Al-N and Ga-As bonds formation. The lightly isoelectronically doped  $\text{Al}_x\text{Ga}_{1-x}\text{N}_y\text{As}_{1-y}$  ( $1 \times 10^{-8} < y < 1 \times 10^{-3}$ ) alloys are studied due to the impurity states standpoint. We predict the total self-assembling of the Ga (Al) impurity atoms around the As (N) impurity atoms in the AlN-enriched (GaAs-enriched) alloys. The cation impurity concentrations for the complete Ga (Al) tetrahedral surroundings of all As (N) atoms are estimated for the higher growth and lower annealing temperatures, respectively. The tetrahedral surroundings of the As (N) impurity atoms formed around the Ga (Al) impurity atoms in the AlN-enriched (GaAs-enriched) alloys are hardly probable due to the large elastic energy of such alloys.

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