# Band-gap "design" of semiconducting nitride alloys

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Band-gap tailoring, creation of semiconducting materials by alloying two binary compounds, AC and BC, to form a ternary alloy, $A_xB_{1-x}C$, is a widely used method to obtain band gap values which satisfy the requirements of specific applications such as production of light emitting diodes, solid state lasers, solar cells etc. operating in desired frequency ranges. Often a rather smooth and reproducible variation of the gap with composition *x* is found, and in some cases even a nearly linear *x* dependence has been observed. The III-nitrides AlN, GaN, and InN are materials of great importance for such "gap design" because their gaps span a wide energy range, 6.4 eV (AlN), 3.5 eV GaN down to 0.7 eV in InN, and the present work summarizes results [1,2] of theoretical calculations of the composition dependence of the gaps in ternary and quaternary semiconducting nitride alloys. The calculations are based on the density-functional theory, including approximations to obtain not only reliable ground state properties but also energies of excited states [3]. The calculated energy gaps, as well as their pressure coefficients, are compared to experimental data. The measured results as obtained from different research groups exhibit a strong scatter, exceeding the quoted error bars. From the calculations it is shown that the gaps in the III-nitride alloys depend sensitively on the geometrical arrangement of the cations in the lattice. Formation in In clusters produces a significant gap reduction, and with reasonable definition of "uniform" and "clustered" geometries it is possible essentially to span all available experimental data. This shows that for the alloys containing InN the gap values depend sensitively on the sample growth conditions. The anomalously large band gap bowing found in the In-containing nitrides can be related to specific properties of InN which do not follow [4] the trends observed in several other binaries (note, for example, its very small energy gap, 0.7 eV).

References

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