Large Band Gap Bowings and Anomalous Pressure Effects
in Nitride Alloys. Hypothesis about importance of short-range In-segregation

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Nitride alloys, (In,Al,Ga)N exhibit many anomalous features particularly strongly pronounced in InGaN and InAlN. The most disputed effects consist of localization of carriers and related In-segregation effects as well as large band gap bowings. A large spread of experimentally determined band gaps in theses alloys seems to be beyond the experimental error.

To examine the role of indium in nitride alloys we performed a comparison between In$_x$Ga$_{1-x}$N, In$_x$Al$_{1-x}$N, and the nitride alloy not containing indium, i.e., Ga$_x$Al$_{1-x}$N. Results of ab-initio calculations of the band gap, $E_g$, and its pressure coefficient, $dE_g/dp$, are examined together with experimental data available in the literature and obtained very recently. Effects of In-clustering (within the scale of 1-3 nm) are taken into account in the calculations. We found that:

i) the bowings of $E_g$ are extremely large for In-containing alloys (with uniform In-distribution among the cation sites) and evolution of the conduction band with In-content is responsible for these bowings. This tendency is more pronounced in the behaviour of $dE_g/dp$,

ii) clustered arrangements of In atoms lead to a decrease of $E_g$ and $dE_g/dp$ and to a strong enhancement of their bowings. These effects are related to the anomalous bowing of the valence band and its pressure counterpart, respectively. They originate from the increase of the valence band width due to hybridization of In ($p$ and $d$) states and uppermost N-derived valence states.

iii) the theoretical calculations of both $E_g$ and $dE_g/dp$ versus In-content are confirmed by large number of experimental data supplying results located essentially between the theoretical curves for uniform and clustered alloys. Thus, In-clustering is likely responsible for the large spread of experimental data for the dependence of $E_g$ and $dE_g/dp$ on chemical composition in the indium containing nitride semiconductors.