A Full-band Monte-Carlo Study of Carriers Transport in III-Nitrides Alloys

E. Bellotti*, S. Shishehchi*, and F. Bertazzi†
*ECE Department, Boston University, 8 Saint Mary's Street, 02215 Boston, MA
†DELEN and IEIIT-CNR, Politecnico di Torino, corso Duca degli Abruzzi 24, 10129 Torino, Italy
e-mail: bellotti@bu.edu

GaN and its compounds have made inroads into the application spaces normally dominated by both conventional III-V semiconductors and silicon. The availability of a rich family of ternary and quaternary alloys makes it possible to tailor these semiconductors to work as light emitters and detectors from the near infrared to the deep UV. Furthermore, the favorable high field transport properties make GaN and its ternary alloys materials of choice for a new generation of power devices that can enable the practical implementation of smart grids for energy distribution. In spite of these high expectations, significant problems exist, not only from the technological stand point but also due to the lack of understanding of the properties of this material system. In particular the knowledge of the high-field carrier transport coefficients, is sketchy at best. Consequently, understanding the carrier transport characteristics of $Al_xGa_{1-x}N$, $In_xAl_{1-x}N$, $In_xGa_{1-x}N$ alloys is one of the critical step needed to be able to design high voltage solid state switches, rectifiers, detectors and light emitters. The goal of this work is to present the results of a full band Monte Carlo (FBMC) investigation of the carrier transport and impact ionization processes in AlGaN, InGaN and AlInN alloys. Furthermore, we will elucidate the reasons that lead to a single carrier multiplication processes in some of these alloys.

Using a full-band Monte Carlo model we have computed[1] the carrier impact ionization coefficients in $Al_xGa_{1-x}N$ for seven alloy compositions between $x = 0$ (GaN) and $x = 1.0$ (AlN). We have found that holes dominates the impact ionization process for compositions below 50%, while electrons dominate for larger aluminum contents. The model also predicts that, due to the particular features of the $Al_xGa_{1-x}N$ valence band structure, holes impact ionization processes are effectively negligible for aluminum composition above 60%. Furthermore, we find that the electron-alloy scattering significantly reduces the electron ionization coefficients leading to the dominant behavior of holes in for an aluminum composition below 50%.

We have computed the electronic structure and developed a transport model for $In_{0.18}Al_{0.82}N$ that is lattice-matched to GaN[2]. Using this approach we have evaluated the electron and hole mobilities and drift velocities. We have found that the mobilities and drift velocity of both carriers are limited by the alloy scattering phenomenon. We have found that the hole impact ionization process is suppressed for this alloy composition. This is due to the particular features of the $In_{0.18}Al_{0.82}N$ valence band structure. Furthermore, we find that the electron-alloy scattering significantly reduces the electron ionization coefficients both for transport along the Γ-A and Γ-M direction.

ACKNOWLEDGMENT

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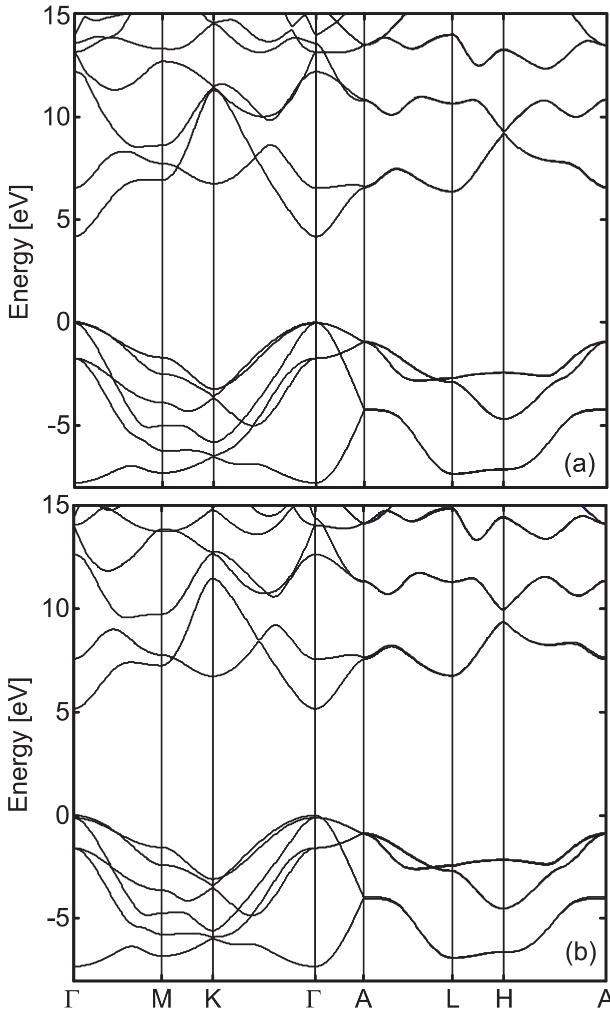

Fig. 1. Calculated electronic structure of (a) $Al_{0.4}Ga_{0.6}N$ and (b) $Al_{0.8}Ga_{0.2}N$

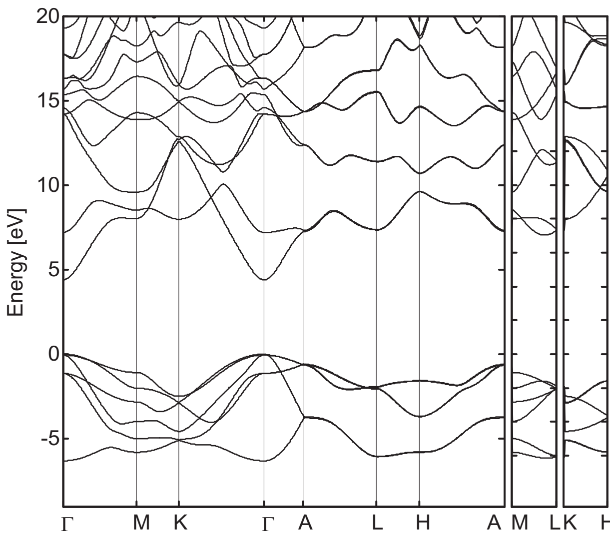

Fig. 2. Calculated electronic structure of $In_{0.18}Al_{0.82}N$

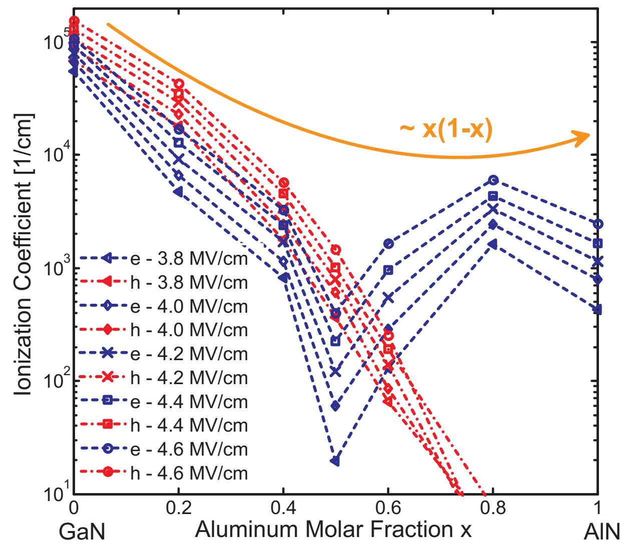

Fig. 3. Calculated electron (dashed lines, blue in color) and hole (dash-dot lines, red in color) impact ionization coefficients as a function of the aluminum molar fraction for five electric field strengths: 3.8 MV/cm (left triangles), 4.0 MV/cm (diamonds), 4.2 MV/cm (crosses), 4.4 MV/cm (squares) and 4.6 MV/cm (circles), including the alloy scattering.

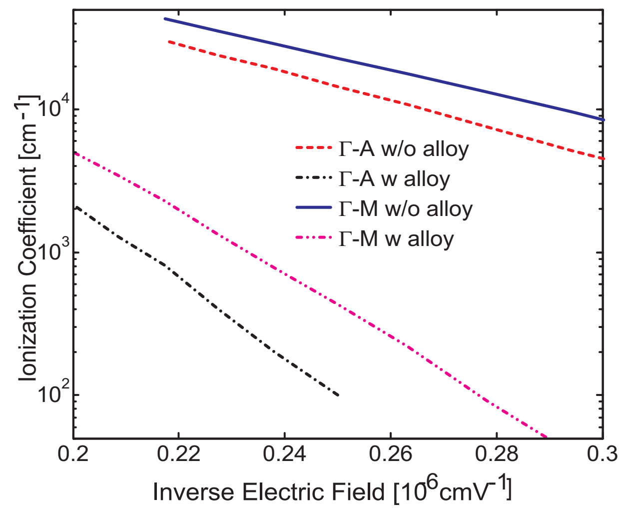

Fig. 4. Calculated electrons impact ionization coefficienst for $In_{0.18}Al_{0.82}N$ as a function of the crystallographic direction and the strength of the alloy scattering.