Comparative analysis of zinc-blende and wurtzite GaN for full-band polar optical phonon scattering and negative differential conductivity

C. Bulutay, B. K. Ridley, and N. A. Zakhleniuk

Citation: Appl. Phys. Lett. 77, 2707 (2000); doi: 10.1063/1.1320020
View online: http://dx.doi.org/10.1063/1.1320020
View Table of Contents: http://apl.aip.org/resource/1/APPLAB/v77/i17
Published by the American Institute of Physics.

Related Articles
Impact ionization and carrier multiplication in graphene
Hot-carrier trap-limited transport in switching chalcogenides
Transport characteristics of graphene-metal interfaces
High field carrier transport in graphene: Insights from fast current transient
Nonpolar resistive switching in Mn-doped BiFeO3 thin films by chemical solution deposition

Additional information on Appl. Phys. Lett.
Journal Homepage: http://apl.aip.org/
Journal Information: http://apl.aip.org/about/about_the_journal
Top downloads: http://apl.aip.org/features/most_downloaded
Information for Authors: http://apl.aip.org/authors

ADVERTISEMENT
Comparative analysis of zinc-blende and wurtzite GaN for full-band polar optical phonon scattering and negative differential conductivity

C. Bulutay\textsuperscript{a)} and B. K. Ridley

Department of Electronic Systems Engineering, University of Essex, Colchester CO4 3SQ, United Kingdom

N. A. Zakhleniuk

Caswell Technology, Marconi Caswell, Towcester, Northants, NN12 8EQ, United Kingdom

(Received 26 May 2000; accepted for publication 1 September 2000)

For high-power electronics applications, GaN is a promising semiconductor. Under high electric fields, electrons can reach very high energies where polar optical phonon (POP) emission is the dominant scattering mechanism. So, we undertake a full-band analysis of POP scattering of conduction-band electrons based on an empirical pseudopotential band structure. To uncover the directional variations, we compute POP emission rates along high-symmetry directions for the zinc-blende (ZB) crystal phase of GaN. We also compare the results with those of the wurtzite phase. In general, the POP scattering rates in the zinc-blende phase are lower than the wurtzite phase. Our analysis also reveals appreciable directional dependence, with the $1-L$ direction of ZB GaN being least vulnerable to POP scattering, characterized by a scattering time of 11 fs. For both crystal phases, we consider the negative differential conductivity possibilities driven by the negative effective mass part of the band structure. According to our estimation, for the ZB phase the onset of this effect requires fields above $\sim 1$ MV/cm. © 2000 American Institute of Physics.

\textsuperscript{a)}Author to whom correspondence should be addressed; present address: Department of Physics, Bilkent University, 06533 Ankara, Turkey; electronic-mail: bulutay@fen.bilkent.edu.tr

\begin{equation}
W_m(k) = \frac{2\pi}{\hbar} \frac{V}{(2\pi)^3} \sum_{m'} \int_{\text{1st BZ}} d^3k' \Delta_{m,m'}(k',k) \times |C_{\text{POP}}(q)|^2 \delta(E_{m'}(k') - E_m(k) + \hbar\omega_{\text{LO}}),
\end{equation}

where the emitted phonon wave vector is $q = -k' + k$ mapped to first BZ, the primed indices represent final-state electron labels over which a summation/integration is performed, $V$ is the total crystal volume, $E_m(k)$ is the band energy of the electron, and $\hbar\omega_{\text{LO}}$ is the longitudinal-optical (LO) phonon energy assumed to be dispersionless. The cubic POP coupling constant is given by $|C_{\text{POP}}(q)|^2 = 2\pi e^2 \hbar \omega_{\text{LO}} (\epsilon_\infty^{-1} - \epsilon_0^{-1})/(V q^2)$, where $\epsilon_0$ and $\epsilon_\infty$ are the static and high-frequency dielectric constants. The cell-periodic overlap parameter is given by $\Delta_{m,m'}(k',k) = |(1/\Omega) \int_\Omega u_{m}^*(r) u_{m'}(r) d^3r|^2$, where $u_{m}(r)$ is the cell-periodic part of the Bloch wave function and $\Omega$ is the volume of the primitive cell. This overlap parameter is vital to account for the restrictions brought by the symmetries of the participating wave functions to the scattering probabilities. For the parameters of GaN, up to room temperature the thermal phonon occupation remains negligible, hence, Eq. (1) actually governs the overall scattering rate up to room temperature.

We compute the scattering rate in two alternative ways: \textsuperscript{3} by direct integration over two spatial variables using the delta function or by means of the Lehmann–Taut BZ integration technique.\textsuperscript{5} In the former, we prefer to work in spherical coordinates and enclose the truncated-octahedron-shaped first Brillouin zone (BZ) by a sphere of radius $\sqrt{5}/2$ $(2\pi a)$, where $a$ is the lattice constant. The regions of the sphere that lie outside the first BZ are discarded by introducing a unit step function into the integrand. We em-

\[2707\]
ploy the linear tetrahedron interpolation\textsuperscript{5} of band energies and store the CB energies by sampling the irreducible wedge of the BZ by 16114 data points, giving more emphasis to the vicinity of the \textit{G} point. For the cell-periodic Bloch overlap parameter $D_m$, we use a less dense sampling of the irreducible wedge by 1604 final-state data points for each initial electron state under consideration.

To be consistent with our previous WZ GaN analysis,\textsuperscript{3} we use the following data for the cubic GaN phonons:

\[ \hbar \omega_{\text{LO}} = 92.12 \text{meV}, \ \epsilon_0 = 9.28, \ \text{and} \ \epsilon_{\text{e}} = 5.29. \]

Aiming for a directional assessment, we start from the CB minimum at the \textit{G} point, and trace the POP scattering rate of CB electrons along high-symmetry lines: \textit{G}–\textit{X}, \textit{G}–\textit{K}, and \textit{G}–\textit{L} directions, respectively; see the inset in Fig. 1. The effect of setting the cell-periodic overlap parameter to unity is indicated by the dashed lines in Fig. 1 for each direction; note the resultant overestimation in the scattering rates away from the CB edge. The results indicate that the \textit{G}–\textit{X} (\textit{G}–\textit{L}) direction has the highest (lowest) scattering rate. This directional dependence can be attributed to the CB satellite valley being located at the \textit{X} point, which is the major scattering destination at high energies, providing high density of final states. As the \textit{G}–\textit{L} direction is further away from the \textit{X} valley, it requires relatively larger phonon-wave vectors, which leads to less electron–phonon coupling. Furthermore, the lowest CB along the \textit{G}–\textit{L} direction\textsuperscript{4} does not enable an intravalley POP emission to the \textit{L} point, which is the key factor behind the low scattering rate.

The \textit{G}–\textit{L} directions of ZB GaN are related to the \textit{G}–\textit{A} and \textit{G}–\textit{U} directions of WZ GaN.\textsuperscript{6} We further note that in

\[ \hbar \omega_{\text{LO}} = 92.12 \text{meV}, \ \epsilon_0 = 9.28, \ \text{and} \ \epsilon_{\text{e}} = 5.29. \]

Aiming for a directional assessment, we start from the CB minimum at the \textit{G} point, and trace the POP scattering rate of CB electrons along high-symmetry lines: \textit{G}–\textit{X}, \textit{G}–\textit{K}, and \textit{G}–\textit{L} directions, respectively; see the inset in Fig. 1. The effect of setting the cell-periodic overlap parameter to unity is indicated by the dashed lines in Fig. 1 for each direction; note the resultant overestimation in the scattering rates away from the CB edge. The results indicate that the \textit{G}–\textit{X} (\textit{G}–\textit{L}) direction has the highest (lowest) scattering rate. This directional dependence can be attributed to the CB satellite valley being located at the \textit{X} point, which is the major scattering destination at high energies, providing high density of final states. As the \textit{G}–\textit{L} direction is further away from the \textit{X} valley, it requires relatively larger phonon-wave vectors, which leads to less electron–phonon coupling. Furthermore, the lowest CB along the \textit{G}–\textit{L} direction\textsuperscript{4} does not enable an intravalley POP emission to the \textit{L} point, which is the key factor behind the low scattering rate.

The \textit{G}–\textit{L} directions of ZB GaN are related to the \textit{G}–\textit{A} and \textit{G}–\textit{U} directions of WZ GaN.\textsuperscript{6} We further note that in
WZ GaN, there exists a BZ folding along the $c$ axis of the crystal, therefore, for the $\Gamma - A$ (WZ) direction both the lowest CB and its folded extension need to be considered. In general terms, the ZB phase has a smaller POP scattering rate than the WZ phase, which is essentially due to the lower density of states in the former. The quantitative comparison of the density of states for these two phases around the energies relevant to our work is given in Fig. 2. However, the lower density of states in ZB GaN is shown to have one order of magnitude greater sensitivity of the onset field to angular variations. Recently Monte Carlo investigations along this line did not encounter any drastic change up to fields $\sim 0.5$ MV/cm with respect to a variation of the energy of the $X$ valley, which further contradicts this previous prediction.

In summary, to aid the high-field characterization of GaN, we present a full-band POP scattering analysis of CB electrons, comparing the ZB and WZ crystal phases. In general, the scattering rates in the ZB phase are lower than the WZ phase due to the lower density of states in the former. This suggests a possibility to have enhanced high-field mobility in ZB GaN in comparison with WZ GaN. High-field transport along the $\Gamma - L$ direction of ZB GaN characterized by a scattering time of 11 fs has the lowest scattering rate, as the POP emission to the $L$ point is energetically not possible. The observation of NDC driven by the negative effective mass part of the band structure is predicted beyond a field of roughly 1 MV/cm for the ZB phase, and 2.3 MV/cm for the WZ phase.

This work is supported by ONR (Contract No. N00014-99-1-0014) and EPSRC (Contract No. GR/L/56725).

8. K. F. Brennan (private communication).