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The Influence of Phonon Emission on Electron Transport in Hexagonal and Cubic Gallium Nitride

R. Brazis and R. Raguotis

Semiconductor Physics Institute, A. Goštauto 11, 01108 Vilnius, Lithuania

Electron transport characteristics of GaN crystals in high electric fields are shown to be essentially influenced by different optical phonon modes inherent to the hexagonal and cubic phases of these compound crystals. Additional optical phonon modes (≈ 26 meV) competing with the higher-energy ones (≈ 92 meV) in hexagonal GaN, together with the low-lying satellite valley (Γ_3), dramatically reduce the drift mobility of electrons in comparison with conventional models. Presented Monte Carlo data are in excellent agreement with the time-of-flight experiment. The cubic GaN crystal phase with its satellite electron energy valleys shifted well above the main (Γ_1) valley is chosen as a convenient medium for elucidating the role of high-energy longitudinal optical phonon accumulation. A simple efficient one-particle Monte Carlo method is proposed for an account of excess phonons. Phonon heating is shown to bring about the moderate additional reduction of the drift mobility and an increase in mean electron energy.

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1. Effects of additional phonons in wurtzite GaN

Experimental data on the existence of a low-lying satellite valley Γ_3 [1] and additional low-energy LO phonons (≈ 26 meV) [2], as well as on the drift velocity of electrons [3] have been recently published raising doubts about the validity of the up-to-now reported Monte Carlo (MC) data [4] on electron transport in GaN. A revised model has been proposed [5] and proved to be in excellent agreement with experimental drift velocity data [3]. In this paper we compare MC and experimental data on electron mobility obtained at room temperature (Fig. 1). The low-energy longitudinal optical (LO) phonons alone reduce electron mobility at low fields but they are not efficient enough to take higher electron energy. Electrons transfer to the upper valley and their mobility is subject to further decrease (Fig. 1, curve 2) because velocity randomization during intense inter--valley exchange is dominating at high electric fields. In the absence of lower--energy LO phonons (Fig. 1, curve 3) electron mobility at low fields remains high

because the higher-energy phonons alone ($\approx$ 92 meV) do not prevent electrons from acceleration. Intense inter-valley exchange starts again in higher electric fields. Conventional models do not account for additional phonons and assuming the satellite valleys to be well above the main valley give the mobility much higher than the experimental one (Fig. 1, curve 4).

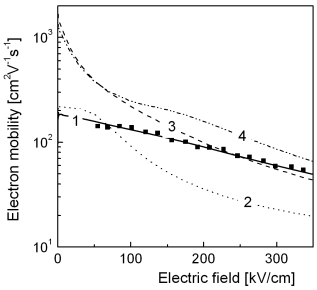

Fig. 1. Electron drift mobility in hexagonal GaN at 300 K calculated from experimental data [3] (dots) compared with the Monte Carlo data: 1 — the GaN parameter set [5] including the $\Gamma_1-\Gamma_3$ valley separation of 400 meV, the inter-valley phonon energy of 80 meV, the main LO-phonon energy of 92.7 meV, and additional LO-phonon energy 26 meV; 2 — the upper-energy LO-phonons (92.7 meV) excluded; 3 — the lower-energy LO-phonons (26 meV) excluded; 4 — conventional (actually cubic) data set [4].

At room temperature, LO phonons are emitted and absorbed at a very high rate therefore the LO phonon accumulation is not very important. One can expect, however, that the balance of LO phonon emission and absorption will be strongly perturbed by electrons accelerated in electric field at low lattice temperatures. We check next the influence of hot LO phonons on electron transport characteristics on the less complicated cubic GaN.

2. Effects of excess phonons in cubic GaN

Phonon generation in n-type cubic GaN crystals is studied at $T = 15$ K where the equilibrium LO-phonon number is negligible. In the presence of electric field the LO-phonon band population is subject to significant increase that in turn gives rise to the competing process of LO-phonon absorption. We divide momentum space into cubic cells of the volume $\Delta q^3 = \Delta q_x \Delta q_y \Delta q_z$ and count phonons entering and leaving a cell in the process of MC simulation. The LO phonon number $N_{\boldsymbol{q}}$ in a cell centered at the phonon momentum $\boldsymbol{q}$ is

$$N_{\boldsymbol{q}} = (\lambda_{\rm em} - \lambda_{\rm ab}) \frac{8\pi^3}{\Delta q^3} n_{\rm e} \tau_{\rm ph} + N_0. \tag{1}$$

Here $\lambda_{\rm em}$ and $\lambda_{\rm ab}$ are phonon emission and absorption rates in the cell, $\tau_{\rm ph}$ is the phonon lifetime, $n_{\rm e}$ is the electron density, and N_0 is the initial phonon number

in the cell. It is attractive to use the new phonon number as the initial for the second modeling step. It turns out, however, that this simplest scheme does not lead to the phonon number convergence. Seeking to obtain true phonons numbers we employed new algorithm:

(I) We start from equilibrium phonon distribution. Let t be the motion time of a probing electron. Let us observe the electron motion in time $\Delta t = t/n$, where n is the number of planned iterations. After the first observation we recalculate phonon emission and absorption rates as $\lambda_1 = N_1/t$, where N_1 is the number of emitted (absorbed) LO phonons in the cell, and repeat the procedure n times, in order to correct phonon emission (absorption) rates. Let us note that the probing electron moves scattered by the perturbed phonon number $N_{\boldsymbol{q}}$.

(II) With the obtained phonon distribution $N_{\boldsymbol{q}}$, the calculations are repeated K times in the same way as in the (I) scheme. Now the final emission (absorption) rates are $\lambda_{\mathrm{em,ab}} = N_{\mathrm{em,ab}}/Kt$. The desired final accuracy is achieved by selecting proper n and K values. The final state of the probing electron after each scattering on phonons has been determined by the MC method proposed in Ref. [6]. LO phonon lifetime was taken to be $\tau_{\mathrm{ph}} = 2$ ps, the ionized impurity and electron densities were taken to be $N_{\mathrm{imp}} = n_{\mathrm{e}} = 10^{17}$ cm^{-3}.

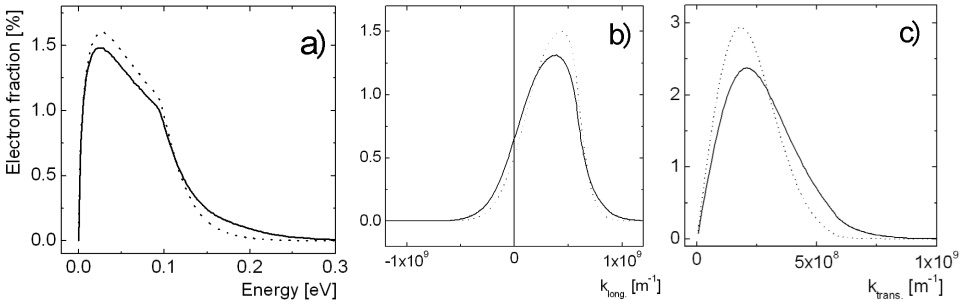

Fig. 2. The distribution of electron fraction over energy (a) and wave vectors (b, c) in cubic GaN at $T = 15$ K and $E = 30$ kV/cm; dashed lines: no LO-phonon accumulation; solid lines: excess LO phonons accounted.

Hot phonons tend to broaden electron distribution over the energy and wave vectors (Fig. 2). As is seen in Fig. 3, the most remarkable result of phonon accumulation is the immense increase in the LO phonon absorption rate. It becomes nearly equal to the rate of LO-phonon emission calculated without an account for the phonon accumulation. Nevertheless, LO-phonon emission rate increases as well. It remains $\approx$ twice higher than the rate of LO-phonon absorption.

Electron drift velocity reduces by $\approx 10\%$ and their mean energy increases over 20% at higher fields under influence of excess LO phonons (Fig. 3).

We conclude that the additional phonon modes and close satellite valleys are crucial for electron transport in hexagonal GaN crystal [5]. Phonon accumu-

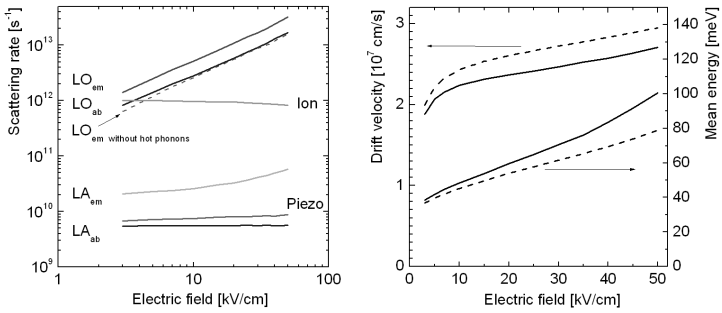

Fig. 3. Electron scattering rate, drift velocity and mean energy as function of electric field in cubic GaN at $T = 15$ K accounting (–) and neglecting (- - - -) hot phonons.

lation is another interesting point becoming exceedingly important at low lattice temperatures. Besides of the electron transport, the phonon accumulation and their transport is of great interest although the lifetime of phonons is not yet well known. The one-particle method of phonon counting proposed in this work is proved to be convenient and efficient even at high rates of phonon emission.

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