Electron drift velocity in high electric fields in zincblende, wurtzite and rocksalt GaN

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Abstract. The influence of GaN crystal symmetry (zincblende, wurtzite, and rocksalt) on the drift velocity of electrons in high electric fields is studied employing Monte Carlo method. The highest drift velocity as well as the most pronounced negative differential mobility is predicted in the zincblende phase. Wurtzite-phase crystals turn out to be inferior in these respects due to the complications of electron and phonon dispersion brought by the lowering symmetry. Experimental data on wurtzite phase reported by Wraback et al. are in excellent agreement with the data of modelling taking into account intense (low-energy phonon-mediated) scattering of electrons between the lowest- and the closely-located upper gamma-valleys. Barker et al. revealed experimentally the velocity-field dependence in cubic GaN to be higher than that in wurtzite phase, however, the experimental drift velocity turned out to be lower than the theoretical one. This might be the signature of coexisting different phases in experimental samples. The rocksalt GaN (still expecting experimental verification) is predicted to manifest the lowest drift velocity of electrons and no negative differential mobility, as a result of the fast exchange of electrons between the lowest-energy X-valleys preventing electron runaway to the upper gamma-valley.

1. Introduction

Gallium nitride crystals are in the focus of recent material science and technology seeking for applications in high-power electronics and ultrafast photonics. Remarkable differences in the electron and phonon dispersion in zincblende (ZB), wurtzite (WZ) and rocksalt (RS) phases present a challenge for the research of kinetic characteristics of these phases. Experimental data on electron drift velocity in high electric field have been reported for the WZ and ZB phases, leaving the RS phase unexplored. Monte Carlo (MC) modelling has been presented primarily without a detailed discrimination of parameters for the WZ and ZB phases, leaving the RS phase unexplored again. In the presented paper the results of MC simulation are reported for the three phases of GaN crystals, and compared with the available experimental data.

2. Model and parameters

Calculations have been performed with standard MC code [1] using the set of parameters given in Table 1. The set is tentative, as many of the GaN electronic parameters are not yet well established. ZB GaN parameters have been selected seeking to obtain better coincidence of the calculated drift velocity with the available experimental data.

The set of WZ parameters has been selected in our previous work [2]. The parameters for RS phase were determined from the electron and phonon dispersion branches [3, 4]. Other parameters for RS were taken by the analogy with ZB and WZ phases. The RS GaN has indirect band gap with the lowest conduction-band valley in the X point. The highest valleys lie quite atop. They do not manifest in the kinetic phenomena in the treated electric field range.
Non-elastic optical and acoustic scattering mechanisms were taken into account [1]. Impurity and piezo-acoustic scattering were employed in accordance with Ref. 5. Impurity scattering has been treated using the third-body exclusion method [5], which encompasses well-known Brooks-Herring and Conwell-Weisskopf approximations. Lattice temperature was equal to \( T = 300 \, \text{K} \).

### Table 1. GaN parameters

|                          | ZB          | WZ\textsuperscript{26} | RS\textsuperscript{1,4} |
|--------------------------|-------------|-------------------------|-------------------------|
| Valley separation, eV    | 0.8\textsuperscript{(\Gamma-X)} | 0.4 (\Gamma_1-\Gamma_3) | 2 (X-\Gamma)           |
|                          | 2.2\textsuperscript{(\Gamma-L)} | 2.1 (\Gamma_7-LM)       | 4 (X-L)                 |
| Electron effective mass  | 0.193\textsuperscript{(\Gamma)} | 0.2 (\Gamma_1)          | 0.47 (X)                |
|                          | 0.4\textsuperscript{(X)}       | 0.22 (\Gamma_3)         | 0.4 (\Gamma)           |
|                          | 0.6\textsuperscript{(L)}       | 0.6 (LM)                | 1 (L)                   |
| Nonparabolicity coefficient, eV\textsuperscript{-1} | 0.21\textsuperscript{(\Gamma)} | 0.183 (\Gamma_1)        | 0 (X)                   |
|                          | 0.065\textsuperscript{(X)}     | 0.065 (\Gamma_3)        | 0 (\Gamma)             |
|                          | 0.029\textsuperscript{(L)}     | 0.029 (LM)              | 0 (L)                   |
| Polar optical phonon energy, meV | 92\textsuperscript{8,10}     | 92 and 26               | 77                      |
| Equivalent-valley phonon energy, meV |            |                         |                         |
| Non-equivalent intervalley phonon energy, meV | 65.84\textsuperscript{11}  | 2                       | 19 (X\textsubscript{ij}) |
| Acoustic deformation potential, eV | 12\textsuperscript{9}       | 8.3                     | 7.2                     |
| Intervalle coupling constant, 10\textsuperscript{6}eV/cm | 1.2           | 1                       | 1                       |
| Mass density, g/cm\textsuperscript{3} | 6.1\textsuperscript{10}       | 6.15                    | 7.83                    |
| Sound velocity, km/s     | 4.57\textsuperscript{10}      | 5.94                    | 6.15                    |
| Piezoelectric const., C/m\textsuperscript{2} | 0.5\textsuperscript{12}       | 0.375                   | 0.375                   |
| Static dielectric const. | 10.4\textsuperscript{13}      | 9.95                    | 57                      |
| Optic dielectric const.  | 5.47\textsuperscript{13}      | 5.35                    | 7                       |

### 3. Results

The results obtained by the MC simulation are presented in Figure 1 (lines) together with the available experimental data. The MC results in the case of ZB phase are plotted for compensated semiconductor with electron concentration equal to \( n_e = 1\times10^{17} \, \text{cm}^{-3} \) and impurity density \( N_i = 1\times10^{18} \, \text{cm}^{-3} \). The calculated drift velocity for ZB case gives somewhat larger values than measured ones. The calculated mobility of electrons in the low-field limit (~ 50 V/cm) in ZB case is about 500 cm\(^2\)/Vs. This value is nearly two times larger than experimental one [14]. The authors [14] performed full-band MC simulation and obtained good coincidence with experimental results up to the fields of 120 kV/cm. However, at higher fields their MC values of the drift velocity rolled over too soon.

MC calculations for WZ phase GaN were performed using wurtzite model proposed in Ref. [2]; this model is suggested accounting for the inelastic scattering of electrons on the additional low-energy phonon modes (~26 meV), and the satellite valley location close (400 meV) to the conduction band bottom allowing for the fast (acoustic-phonon mediated) exchange of electrons between both the gamma-valleys. The impurity and electron densities were taken equal to 1\times10^{17}. As it is seen, the good agreement is obtained with the time of flight experiment [15].
Rocksalt GaN characteristics are quite different from those of ZB and WZ phases. The lowest valley is at X point and the next nearest Γ valley is located at ~ 2 eV higher. Therefore, the highest-valley electron population does not exceed 0.1%. The main scattering mechanism is polar optical one. The scattering intensity on deformation optical vibrations is about one order of magnitude smaller. The calculated mobility at low fields is of the order of 200 cm²/Vs.

4. Conclusions
The Monte Carlo simulation of electron drift velocity has been performed for zincblende, wurtzite and rocksalt phase of GaN crystals at $T = 300$ K. Using the updated parameters (Tab.1), and including impurity compensation, we obtain significantly lower electron drift velocity and low-field mobility in ZB phase, as compared to our previous work [2b]. However, the velocity is seen to remain higher than experimental one (Fig. 1). This may be due to the still non-precisely determined ZB electronic parameters, or due to the presence of inclusions of the other phases that could reduce the spatially-average electron mobility in the experimental samples. The possibility of an admixture of ZB and WZ phases has been actually mentioned in [14]; RS phase inclusions seem to be feasible, as well. We leave the topic for separate investigation.

The strong point for WZ GaN applications is the availability of versatile technology. As the WZ phase grows most easily, it is likely to be relatively free of other phase inclusions, allowing for quite adequate MC modelling of electron drift velocity. The weak point of this phase is its relatively low peak drift velocity of electrons.

Modelling of electron transport in the RS phase is performed to our best knowledge for the first time. The rocksalt GaN reveals the lowest drift velocity of electrons and no negative differential mobility.

Figure 1. Drift velocity versus electric field in three phases of GaN crystal. Close triangles – experiment [14], closed squares – experiment [15]. Lines – present MC.
This is due to the fast exchange of electrons between the lowest-energy X-valleys preventing electron runaway to the high-located upper gamma-valley. Such a remarkable difference in the behaviour of electrons in ZB, WZ and RS phases presents a challenge for further experimental and theoretical research aiming at manufacturing heterostructures comprising of chemically identical but different-symmetry compounds.

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