Comparison of Steady State Electron Transport Properties in Binary Nitride Materials Using Three Valley Monte Carlo Model

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Abstract

An ensemble Monte Carlo simulation is used to compare high field electron transport in bulk GaN, AlN and InN. For all materials we found that electron velocity overshoot only occurs when the electric field is increased to a value above a certain critical field .This critical field is strongly dependent on the material parameters. For example about 0.74×10^{7} Vm^{-1} for the case of InN, 2.79×10^{7} Vm^{-1} for AlN and 1.74×10^{7} Vm^{-1} for GaN. At higher electric fields the drift velocity decreases eventually saturating at around 2.03×10^{5} ms^{-1} for both GaN and AlN and 1.8×10^{5} ms^{-1} for InN.

Keywords

Ensemble Monte Carlo; Overshoot; Critical Field; Drift Velocity

Introduction

In recent years, III-Nitride semiconductors including compounds such as GaN, AlN, InN and their alloys, have been used variously in optoelectronic devices like light emitting diods (LEDs), laser diods (LDs) and field effect transistors, because of having unique properties such as wide band gap in a range of about 0.7-6.2 eV limit from IR to UV

electromagnetic spectrum. In addition to optical properties, III-Nitride semiconductors have been used differently in high frequency electronic devices like high electron mobility transistors (HEMTs), applied devices at high temperature, chemical room and power devices and thermo sensors, because of having good chemical resistance and suitable performance at high temperature. They can be used for making ceramics with high melting point and fire-bricks. They can also apply in anti-abrasion coatings, shaping and cutting appliances, because they are very hard [1-3].

Different numerical methods can be used for calculating properties of electron transport in semiconductors and parts which of made them such as relaxation-time approximation, iterative method to solve the Boltzmann equation and Matthiessen's rule [4].

In this article, we study electron transport in wurtzite GaN, AlN, and InN under high electric field application. Initially, we employ Monte Carlo simulations to study electron transport in the III–nitride semiconductors.

Material and Method

In this work, a three valley model for the conduction band is employed. Non-parabolicity is considered in all valleys. The scattering mechanisms are ionized impurity, polar optical phonon, piezoelectric and acoustic deformation potential. Elastic ionized impurity scattering is described using the screened Coulomb potential of the Brooks-Herring model. In each simulation, the motion of 3000 electrons is considered, and the initial electron distribution is set according to equilibrium Fermi–Dirac statistics. Throughout this study, we focus on the wurtzite phases of GaN, AlN and InN, as these are the stable phases under ambient conditions. The material parameters used for these simulations are tabulated in table 1 and 2.

Table 1. Material parameter selections for wurtzite GaN, InN, and AlN [5-6]

	GaN	AlN	InN
Mass density (g/cm^3)	6.15	3.23	6.81
Sound velocity (m/s)	6560	9060	6240
Acoustic deformation potential	8.3	9.5	7.1
Static dielectric constant	9.5	8.5	15.3
High frequency dielectric constant	5.35	4.77	8.4
Effective mass (Γ valley)	0.2	0.31	0.11
Direct energy gap (eV)	3.5	6.2	2

Table 2. Valley parameter selections for wurtzite GaN, InN and AlN [5-6]

	GaN	AlN	InN
m^*_Γ	0.2	0.31	0.11
m^*_U	0.4	0.39	0.4
m^*_K	0.3	0.54	0.3
α_Γ	0.189	0.32	0.419
α_U	0.065	0.5	0.065
α_K	0.7	0.03	0.7
Γ - U	2	0.61	1.9
Γ - K	3.1	0.67	2.63

Degeneracy effects are expected to be negligible over almost all of the temperature and electron concentration ranges of interest here and, hence, are not considered in the calculation. Electron particles in the ensemble Monte Carlo simulation occupy non-parabolic ellipsoidal valleys in reciprocal space, and obey Boltzmann statistics. Herring-Vogt transformations are used to map carrier momenta into spherical valleys when particles are drifted or scattered. The electric field equations are solved self-consistently with the electron transport using a finite difference method and the device grid potentials are updated at each ensemble drift timestep (1 femtosecond).

Results

The bulk group III-Nitride velocity-field characteristics, predicted by our model are shown in Fig 1. For all cases, the temperature is 300 K and the donor concentration is 10^{23} m^{-3}. We see that each compound exhibits a peak in its velocity-field characteristic. The peak drift velocity for InN is around 4.15×10^5 ms^{-1}, while those for GaN and AlN are about 3.08×10^5 ms^{-1} and 2.17×10^5 ms^{-1}, respectively. At higher electric fields the drift velocity decreases, eventually saturating at around 2.03×10^5 ms^{-1} for both GaN and AlN and 1.8×10^5 ms^{-1} for InN [7-8].

The threshold fiels are 1.74×10^7 Vm^{-1} and 2.79×10^7 Vm^{-1} for GaN and AlN, respectively. For InN the peak drift velocity occurs at a significantly lower electric field at about 0.74×10^7 Vm^{-1}. It shoud also be noted that the drift velocity of InN is substantially greater than that of GaN for low electric fields. The behavior of InN can be explained in terms of the energy band structure. In particular, the electron effective mass within the central valley

is different (0.11 m_0 in InN versus 0.2 m_0 and 0.31 m_0 in GaN and AlN, respectively). It is seen that the drift velocity of electron is decreased when the effective mass is increased.

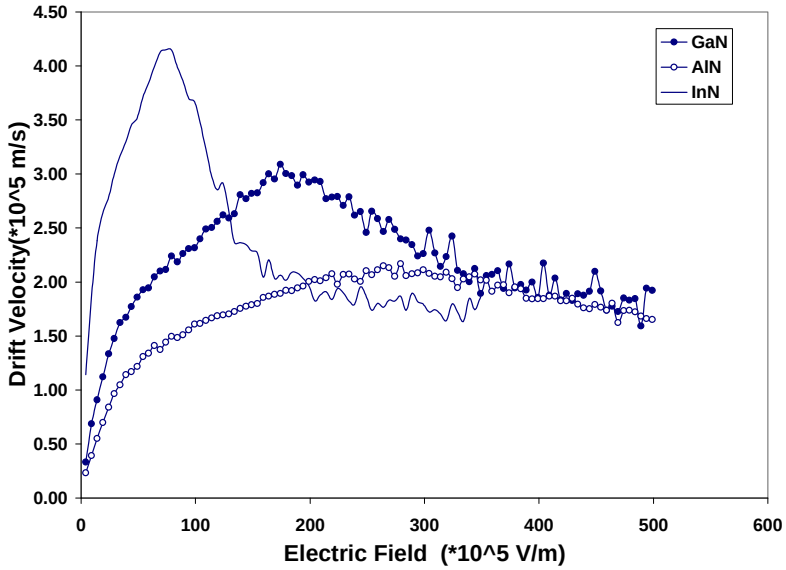

Figure 1. Calculated electron steady-state drift velocity in bulk InN, GaN and AlN as a function of applied electric field. The donor concentration is set to 10^{23} m^{-3} and temperature to 300 K.

The valley occupancies for Γ, U and K are illustrated in figure 2 and show that the inclusion of the satellite valleys in the simulation is important. Significant intervalley scattering into the satellite valleys occurs for fields above the threshold field for each material. This is important because electrons which are near a valley minimum have small kinetic energies and are therefore strongly scattered. It is apparent that intervalley transfer is substantially larger in InN over the range of applied electric fields shown, due to the combined effect of a lower Γ effective mass, lower valley separation energy, and slightly lowers phonon scattering rate within the Γ valley.

In the figure we can also see that the behaviour of AlN is different from other semiconductors, because of having small energy gap between the Γ valley and the other valleys and large effective mass of Γ valley. At the field corresponding to the peak velocity in AlN, we find occupancies of 8% and 2% for the U and K valleys, respectively.

In figure 3, we plot the Γ valley occupancies in each material as a function of Electric field at various temperatures. The total scattering rate of electrons increases, when the temperature increases and energy of electrons decreases due to collisions. Therefore, the number of

electrons increases in central valley and decreases in Adjacent valleys.

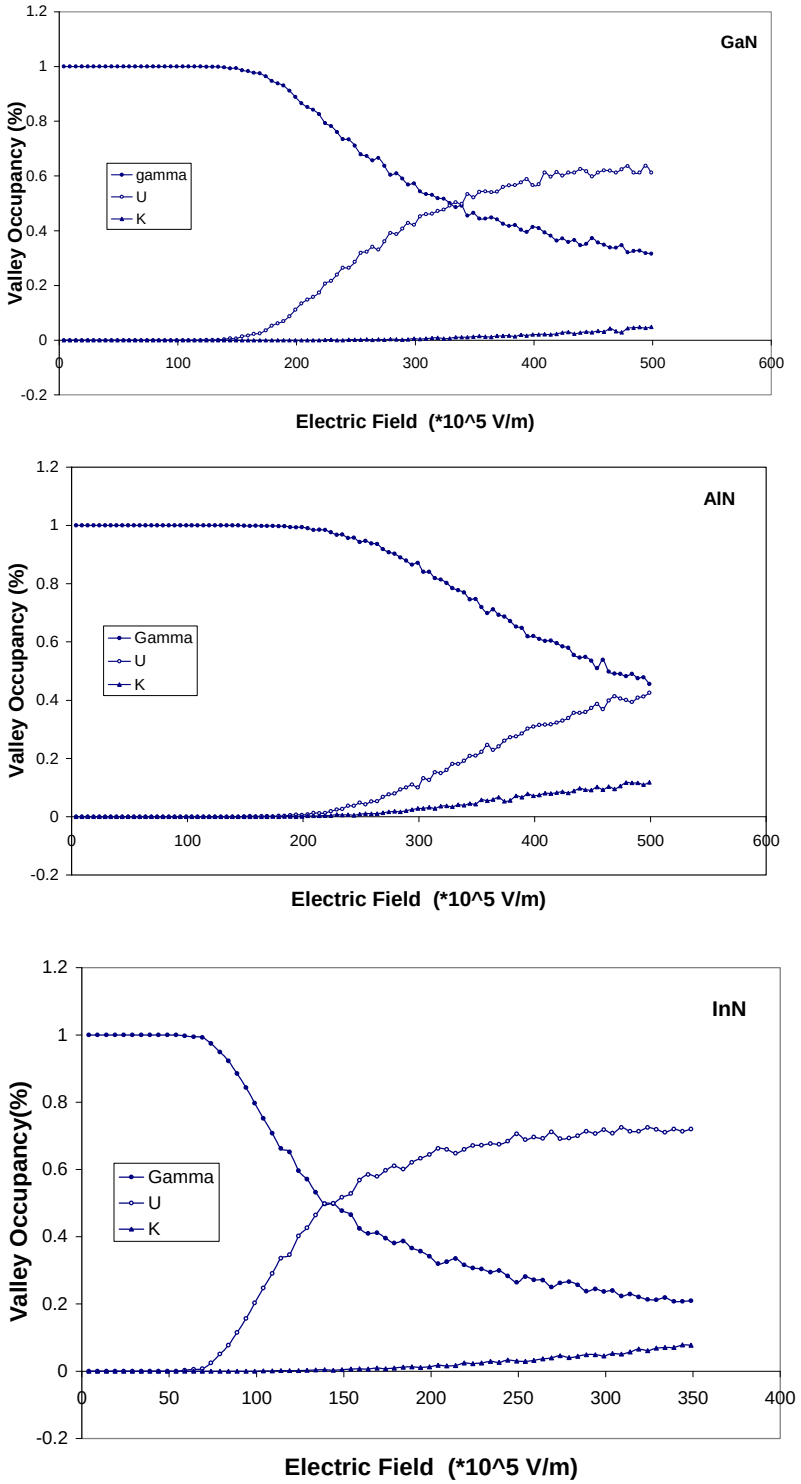

Figure 2. Comparison of the valley occupancies as a function of electric field in bulk wurtzite GaN, AlN and InN structures at 300 K

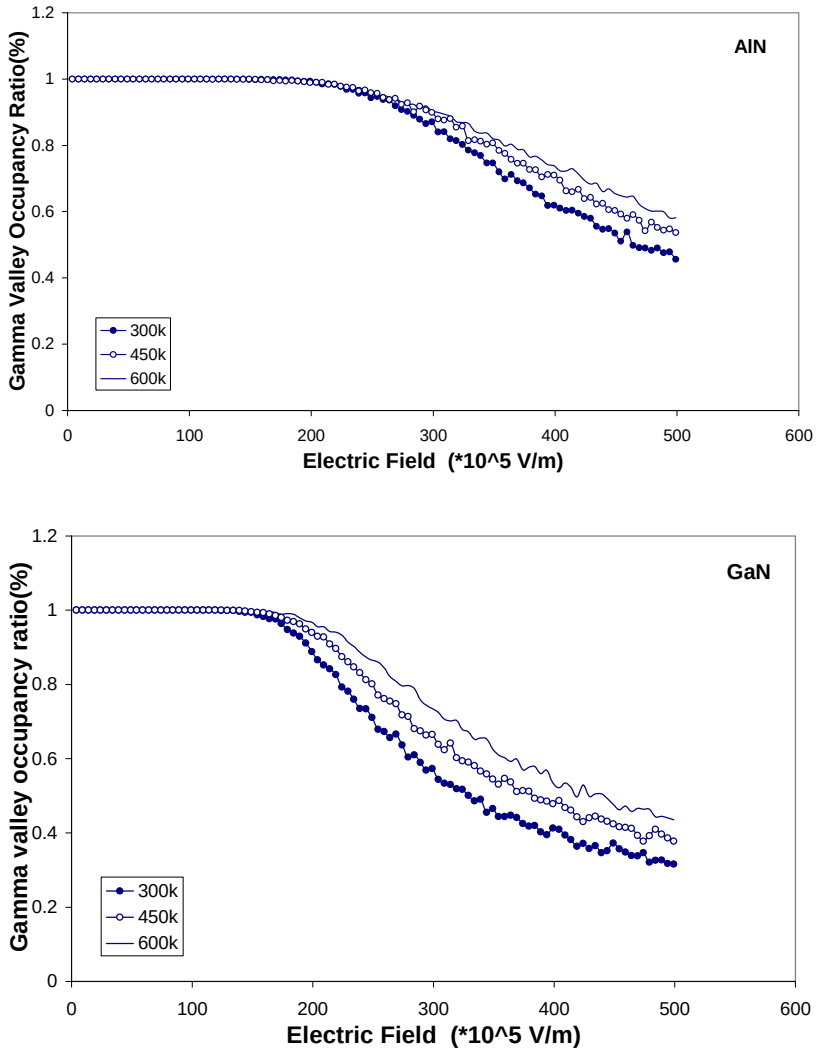

Figure 3. The Γ valley occupancies in wurtzite AlN and GaN at 300, 450 and 600 K

In figure 4, we have plotted the drift velocity in each material as a function of Electric field at various temperatures. With increasing temperature, we can see a decrease in drift velocity at electric fields lower than threshold field, because of increasing intravalley scattering rate (scattering due to the acoustic phonon, ionized impurity, piezoelectric). The decrease in velocity at higher fields is due to increased intervalley scatterings. It is clear that increasing temperature, there are decreasing in the peak of drift velocity and shifting to higher electric field.

For InN the peak drift velocity occurs at a significantly lower electric field which is in good agreement with the results of Turner et al. [4] who used a five-valley model, and of Arabshahi [2] who used a three-valley model. It should also be noted that the drift velocity of InN is substantially greater than that of GaN for low electric fields. The behavior of InN can be

explained in terms of the energy band structure.

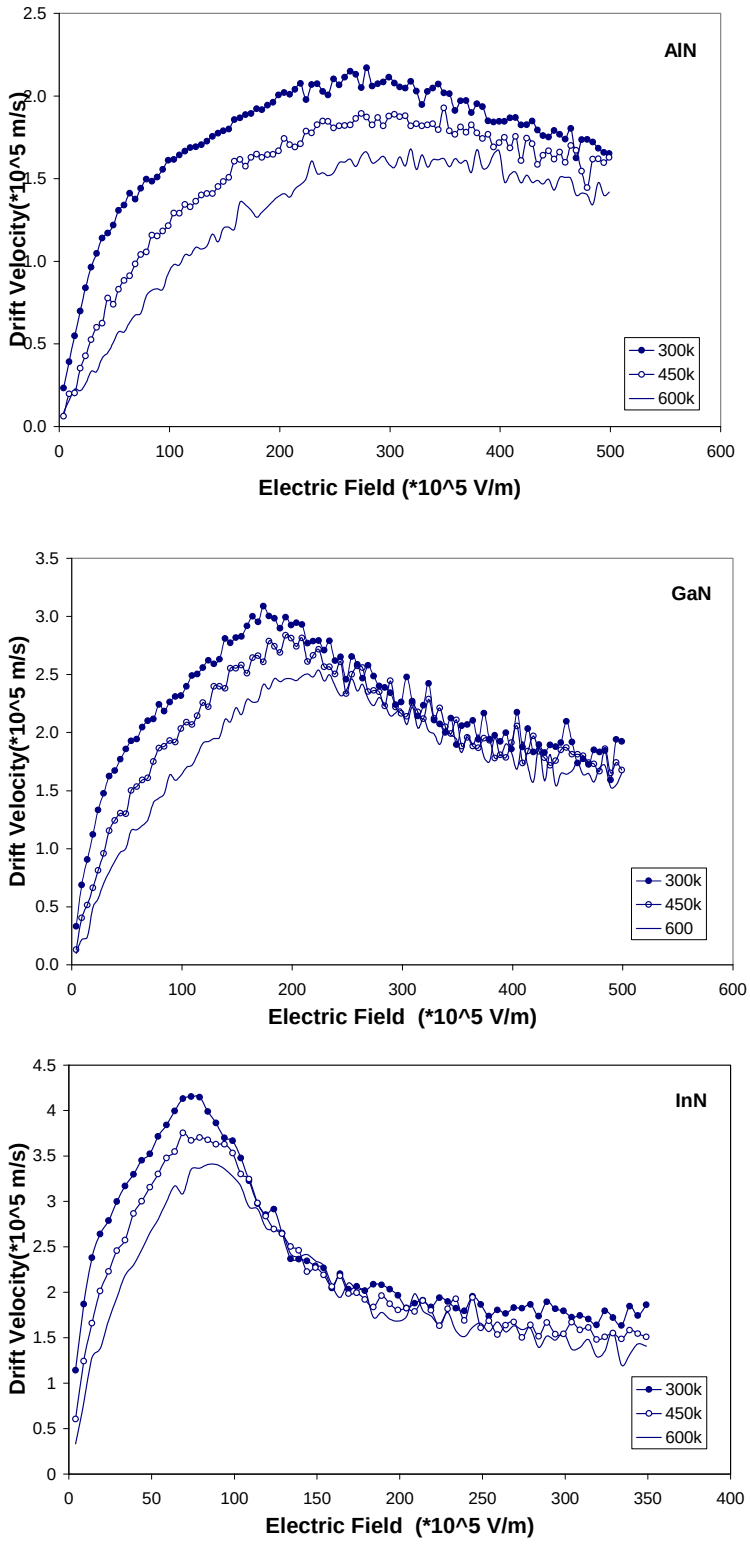

Figure 4. The drift velocity in wurtzite GaN, AlN and InN as a function of electric field at 300, 450 and 600 K

Conclusions

The computed steady-state and transient electron transport in wurtzite GaN, AlN and InN show that InN has superior electron transport properties. Using valley models to describe the electronic band structure, calculated velocity-field characteristics show that the intervalley transitions in high electric fields play an important role in these materials.

We have shown that steady-state drift velocity in GaN is greater than others. So, it suggested for making the high frequency electronic devices.

The peak of drift velocity in InN is 4.15×10^5 ms^{-1} at high electric fields at room temperature. So, it has good electronic properties and this material is suggested for making the electronic and optoelectronic devices.

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