Monte Carlo Calculation of Gallium Nitride

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Abstract

We present the results of an ensemble Monte Carlo simulation of electron velocity in gallium nitride (GaN). Our calculation shows that intervalley electron transfer plays a dominant role in GaN at high electric field leading to a strongly inverted electron distribution and to a large negative differential conductance. The calculated values of the electron mobility are much higher than measured values which suggests that most GaN samples are highly compensated.

1. Introduction.

Recently, GaN has recently attracted considerable interest because of potential device applications for blue-light emitting diodes and lasers. The breakdown field in this wide band gap(about 3.5eV) material is quite large [1]. Hence , one can apply high electric fields leading to hot electron effects, in particular to the intervalley transfer (Ridley-Watkins-Hilsum-Gunn effect). These hot electron phenomena are studied in this paper using Monte Carlo simulations.

Our Ensemble Monte Carlo simulation takes into account polar optical phonon, piezoelectric potential, deformation potential and ionized impurity potential scattering in a non-parabolic band. We used the same material parameters as in [2]. Since GaN becomes degenerate at approximately $n=2x10^{18}$ cm^{-3}, we accounted for degeneracy in the screening length formula . We also accounted for the Pauli exclusion principle for the central valley of the conduction band, using the rejection technique, described reported in [6]. We assumed a 1.5 eV separation of the satellite valleys from the central valley minimum [3][4], and used the same value for the intervalley coupling coefficient as for GaAs (D = $1x10^9$ eV/cm). The electron effective mass in upper valleys was taken to be equal to the free electron mass. We simulated 1000-10000 particles and for 15-30 psec, depending upon electric fields.

2. Electron energy.

First, following Littlejohn et al. [2], we performed the Monte Carlo simulations for electrons in GaN at 300 K taking into account only the central valley at 300K. The results show that, in high electric fields, the electron distribution spreads widely in the energy space, with average electron energies reaching a few electron volts in the electric fields on the order of 200 kV/cm (see Figs. 1 and

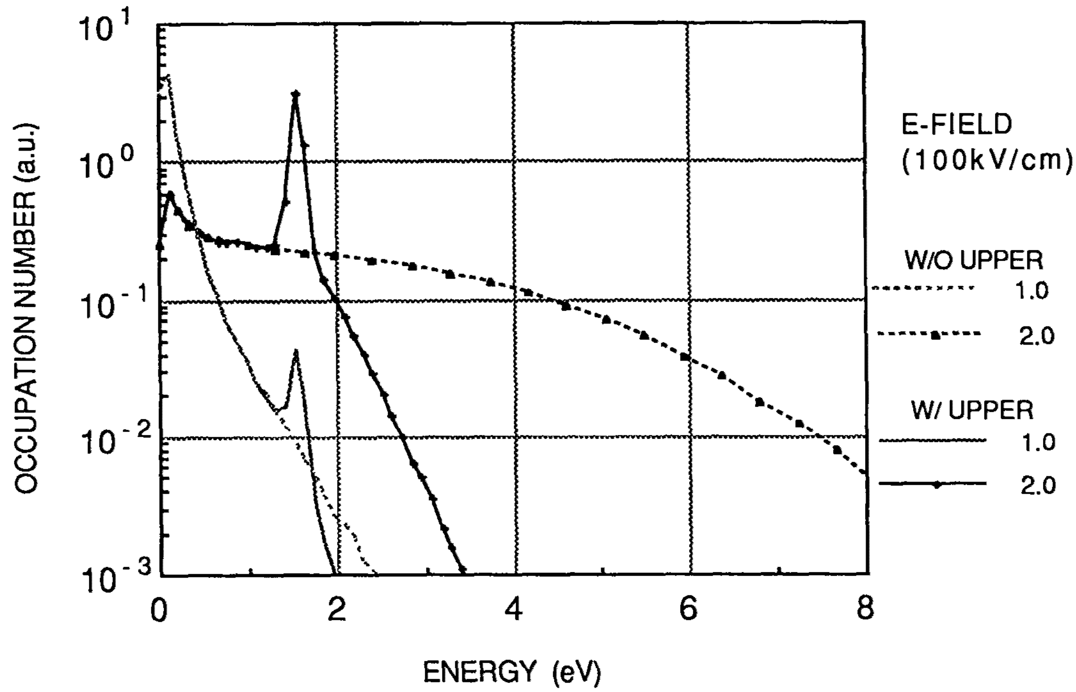

Fig.1 Electron occupation numbers in GaN at 300K for two electric fields.

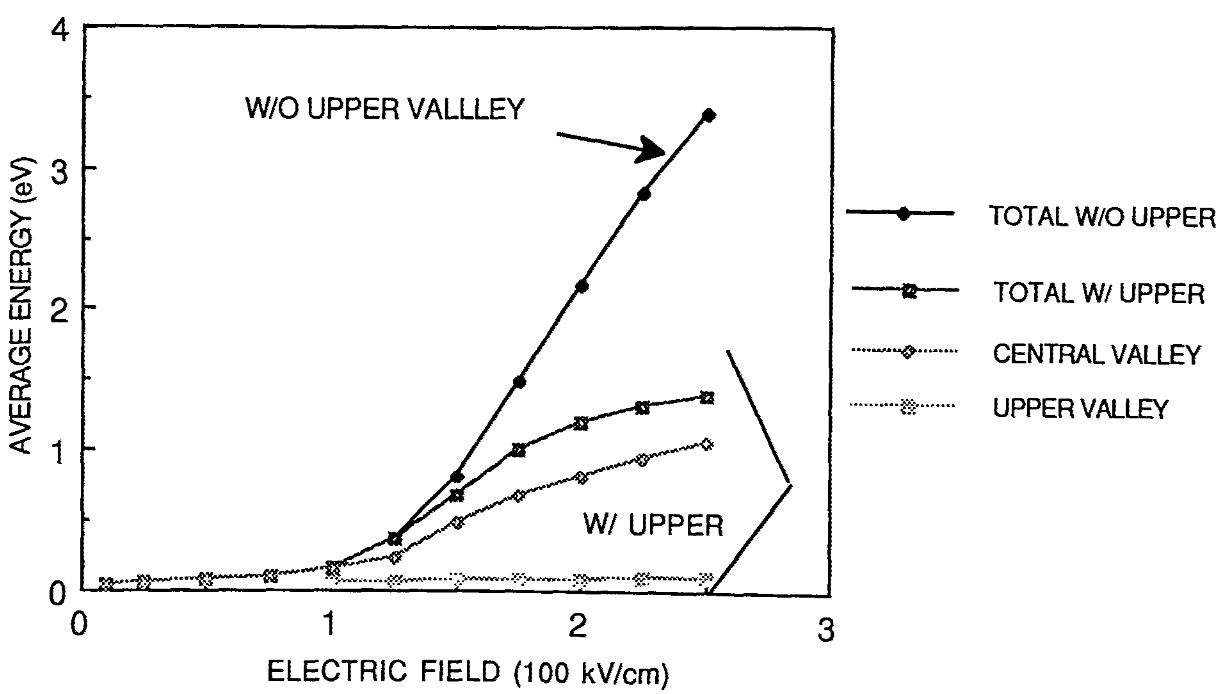

Fig.2 Average energy vs. electric field, excluding and including upper valleys.
The reference level for energy calculation in each valley is the minimum of each valley, while the references for the total energy calculation are the central valley bottom.

2). Such energies are considerably larger than the energy separation between the central and satellite The importance of the intervalley transfer can be clearly seen from Fig. 1 and 2. Not only, the average valleys in GaN. Hence, the intervalley transfer must be accounted for in the Monte Carlo simulations. electron energies in high electric fields are greatly diminished by the intervalley transfer but this transfer also results in the inversion of the energy occupation in the central valley caused by the intervalley scattering from the satellite valleys back into the central valley. A similar effect (even though not as much pronounced) also occurs in GaAs.

3. Velocity calculation.

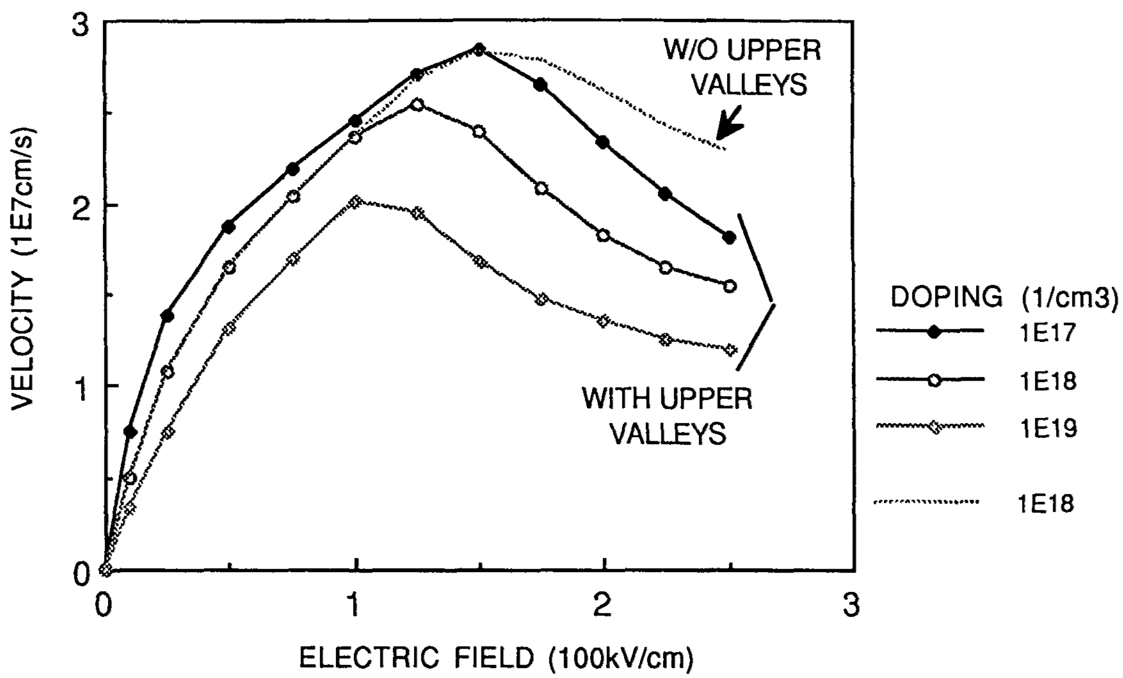

Fig.3 Velocity vs. electric field for different electron concentrations.

The non-parabolicity of the conduction band in GaN leads to a negative differential resistance in high electric fields even when the intervalley transfer is not accounted for [2]. However, the intervalley transfer leads to a much larger negative differential conductance as can be seen from Fig. 3. Even in high electric fields, he velocities show a noticeable dependence on ionized impurity concentration. This is because most electrons occupy the upper valleys where their kinetic energy is small, as can be seen from Fig. 2. We also notice that the negative differential conductance is fairly large even in very highly doped samples ($n=1x10^{19}$ cm^{-3}). We also repeated these calculations for a smaller value of the effective mass in the upper valleys ($meff=0.7m_o$). The negative conductance differential conductance was still large even though it decreased somewhat.

This work has been supported by the Office of Naval Research under contract # N00014-92-J-1580, and the Virginia Center for Innovative Technology. The Monte Carlo simulations have been made possible through a computer resource grant from the Minnesota Supercomputer Institute.

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