Monte-Carlo study of Velocity Overshoot and Terahertz Generation in GaN

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Abstract

We have theoretically investigated velocity overshoot phenomenon for both electrons and holes in bulk wurtzite GaN at 300K using one-particle Monte-Carlo method. The Boltzmann transport equation is solved incorporating deformation potential acoustic phonon, polar optical phonon, impurity and intervalley phonon scatterings. The velocity overshoot characteristics for electrons and holes at 300K reveal that higher peak drift velocities occur for higher electric field values. The variation of drift velocity with electric field shows a negative differential resistance (NDR) effect for electrons at 300K, but the NDR effect is not observed in case of hole transport. We have found that the self-oscillating frequencies of wurtzite GaN diodes are 2.62 THz, 1.74 THz and 1.31 THz corresponding to diode lengths 0.2μm, 0.3μm and 0.4μm respectively.

Keywords

Velocity overshoot; Monte-Carlo method; Negative differential effect

I. Introduction

GaN being a wide bandgap material has a high breakdown field and a high electron mobility, which make it a suitable material for optoelectronic devices like blue light-emitting diodes, photodiodes and other high frequency devices [1-2]. Monte Carlo methods have been widely used to study carrier transport in GaN because they provide a nearly exact solution of the Boltzmann transport equation by treating accurately the hot-electron effects in GaN. This cannot be accomplished by the drift diffusion models [3]. The transferred-electron (TE) effect at high electric fields due to inter-valley scattering gives rise to a negative differential resistance (NDR) in GaN [4]. The diode oscillators based on the NDR mechanism in GaN have self-oscillating frequencies in the terahertz (THz) frequency range depending on the author to whom any correspondence may be addressed. diode lengths. We have treoretically investigated the velocity-field characteristics in bulk wurtzite GaN by solving the Boltzmann transport equation using the Monte-Carlo method. The deformation potential acoustic phonon scattering, polar optical phonon scattering, inter-valley phonon scattering and impurity scattering have been taken into account in our calculations. In this report we have studied the velocity-field characteristics of electrons and holes in GaN assuming a two-valley band structure for wurtzite GaN using a one particle Monte-Carlo method. Our studies have revealed velocity overshoot phenomenon for both electrons and holes in wurtzite GaN at 300K. We have also theoretically computed the self-oscillating frequencies of several GaN diodes of submicron dimensions.

II. Theoretical Model

We have used the Monte-Carlo method to study the motion of one electron in momentum space encountering a large number of lattice scattering processes. In order to include a scattering rate in Monte-Carlo method, the formulation of the total scattering rate and the angular dependance of the scattering rate between the states k and k′ is required.

The scattering rate for polar mode scattering in parabolic band approximation is given as [5]:

$$\lambda_{po}(k) = \frac{e^2\, m^{*1/2}\, \omega_o}{4\sqrt{2}\,\pi\,\hbar\,\epsilon_o}\,(1/k_\infty - 1/k_o)\,E^{-1/2} \times F_o(E,E')\,H\begin{cases} N_o & \text{(absorption)} \\ (N_o+1) & \text{(emission)} \end{cases} \qquad (1)$$

$$\text{where } E' = \begin{cases} E + \hbar\omega_o & \text{(absorption)} \\ E - \hbar\omega_o & \text{(emission)} \end{cases} \qquad (2)$$

$$F_o(E,E') = \ln\left| (E^{1/2} + E'^{1/2}) / (E^{1/2} - E'^{1/2}) \right| \qquad (3)$$

The factor H is unity for absorption and is equal to the Heavyside unit function H $(E- \hbar\omega_o)$ for emission. The angle β between the initial state k and the final state k′ has been obtained from the angular probability distribution $P_A(\beta)$ given in [5]:

$$\text{Cos}\beta=[(1+f)-(1+2f)^r]/f \qquad (4)$$

$$\text{where } f=2(E\,E')^{1/2}(E^{1/2}-E'^{1/2})^{-2} \qquad (5)$$

and r is the random number uniformly distributed between 0 and 1. We have included in our calculations the expressions for deformation potential acoustic phonon scattering, ionized impurity scattering and intervalley scattering as given in [5].

III. Results and discussions

We have considered the effective mass for electrons in wurtzite GaN as $0.21m_0$, where m_0 is the rest mass of the electron. The band gap energy is taken as 3.39eV and inter-band (L-M) energy seperation as 2.1 eV [1]. The effective mass for holes has been taken from the paper reported by Shiyu Chen et al [1] as $1.8m_0$ and the spin-off parameter as 0.2 eV. The other parameters used in our computations have been given in Table 1.

Table 1 : Material parameters of wurtzite GaN.

Density (g/cm^3)	6.15
Acoustic deformation potential (eV)	8.3
Static dielectric constant	8.9
High frequency dielectric constant	5.35
Polar optical phonon energy (meV)	92
Inter-valley phonon energy (meV)	92
Inter-valley deformation potential (10^9 eV/cm)	1
Hole acoustic deformation potential (eV)	19.6
Hole inter-valley phonon energy (meV)	92
Hole inter-valley deformation potential (10^9 eV/cm)	1.5

We have theoretically investigated velocity overshoot characteristics for both electrons and holes in wurtzite GaN at 300K, which are depicted in Fig. 1 and Fig. 2 respectively. Fig. 1 shows simulated transient response characteristics of electrons for electric fields 100 kV/cm, 200 kV/cm and 400 kV/cm respectively. Similar transient response features for holes corresponding to the above mentioned electric fields have been shown in Fig. 2.

It is evident from Fig. 1 that velocity overshoot phenomenon does not occur at electric field lower than 200kV/cm. At 100 kV/cm the curve is nearly flat showing no effect of velocity overshoot. Fig. 1 shows that velocity overshoot of electrons occur at about 0.06 ps for electric field value of 400 kV/cm.

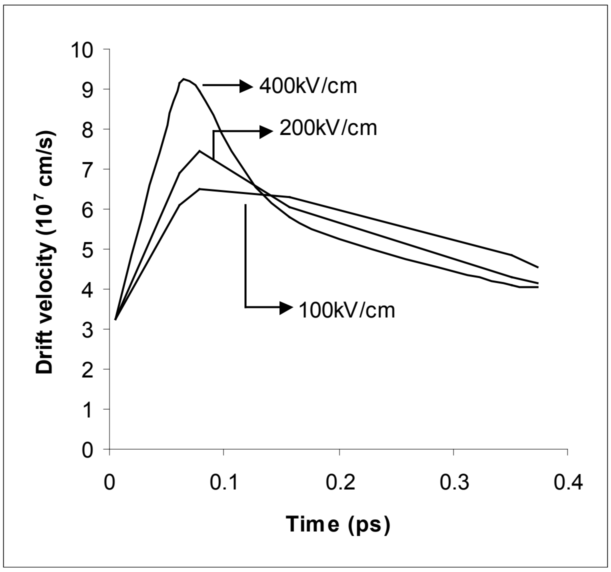

Fig. 1: Velocity overshoot phenomenon for electrons in bulk wurtzite GaN at 300K.

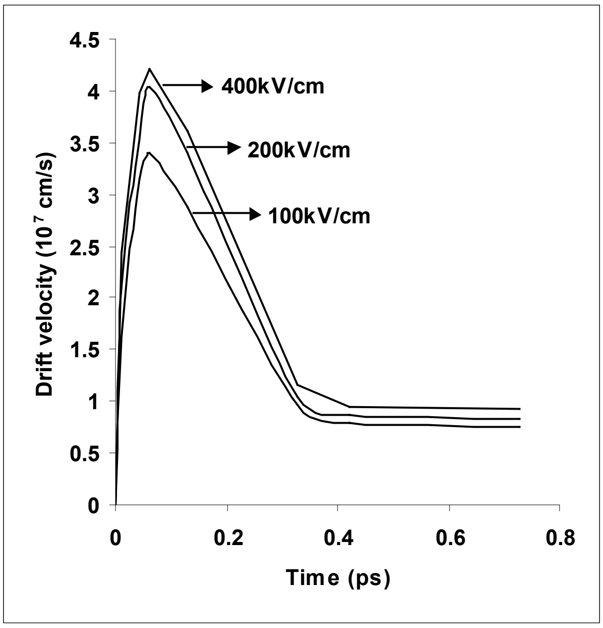

Fig. 2: Velocity overshoot phenomenon in case of holes in bulk wurzite GaN at 300K.

The transient response peak for holes occurs at about 0.06 ps which is shown in Fig.2. It is apparent from the characteristics that velocity peaks are more prominent at higher values of electric field, which is true for both electrons and holes. Our results agree with the results obtained by the workers as reported in [6].

Drift velocity variation with electric field under steady state condition in bulk wurtzite GaN at 300K for both electrons and holes is shown in Fig. 3. The drift velocity for the electrons reaches a peak of about 6.52 x 10^7 cm/s for an electric field of 100 kV/cm and then decreases and attains almost a saturation value. The peak drift velocities of the electrons at 200 kV/cm and 400 kV/cm are 7.46 x 10^7 cm/s and 9.17 x 10^7 cm/s respectively. This shows higher peak drift velocities are obtained at higher field values which is in agreement with the results reported by Zhiyuan Zheng et al [6]. A NDR effect is observed in the velocity-field characteristics, which is due to the intervalley transfer of electrons from the low effective mass high mobility central valley to the high effective mass low mobility higher satellite valleys. Based on this NDR mechanism, the self-oscillating frequencies (f) of the diodes of length l are calculated from the relation vp = f x l, where vp is the peak drift velocity of the electrons. The peak drift velocity for electrons as calculated from Fig. 3 has been found to be 5.23 x 10^7 cm/s at T=300K, the corresponding frequencies computed for diode lengths of 0.2μm, 0.3μm and 0.4μm are all in the Terahertz range as shown in Table 2 below:

Table 2: Self-oscillating frequencies at Terahertz range for wurtzite GaN diodes of submicron dimensions

Diode length (μm)	Self-oscillating frequency (THz)
0.2	2.62
0.3	1.74
0.4	1.31

In case of holes, which are mainly distributed in the heavy band the drift velocity at first increases and then nearly approaches a saturation value due to predominance of scattering rates and no NDR effect is observed.

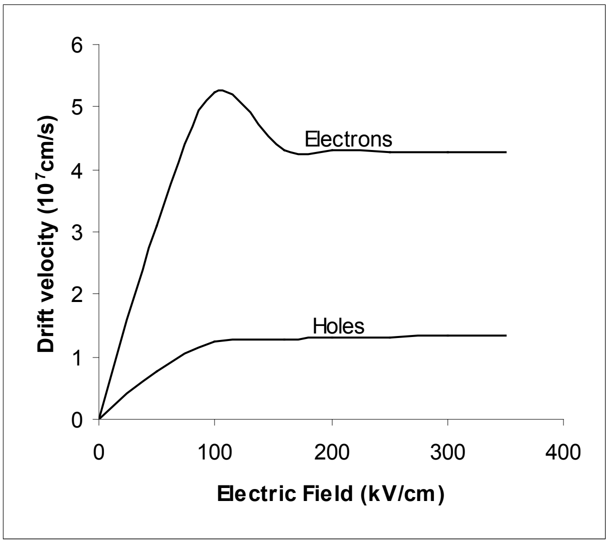

Fig. 3: Velocity-Electric field characteristics for electrons and holes under steady-state condition in bulk wurtzite GaN at 300K.

IV. Conclusion

Our study of transient response characteristics in bulk wurtzite GaN reveals velocity overshoot phenomenon for both electrons and holes at 300K. Velocity peaks are more prominent for higher electric field values. The drift velocity variation with electric fields for electrons as well as holes has also been investigated. The characteristics for electrons reveal a NDR effect at an electric field of 100 kV/cm at a temperature of 300K. Based on this NDR mechanism, GaN diode oscillators can be successfully designed in the terahertz frequency range using sub-micron diode lengths. The transport characteristics for holes show monotonic increase of drift velocity with electric field. The velocity at higher fields attain almost a saturation value due to the scattering effects.

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