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Comparison Between Three-Valley Model and Full Band Model in Monte Carlo Simulation of Bulk Wurtzite GaN

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Abstract: The Monte Carlo simulators with the three-valley model and the full band Monte Carlo model are used to explore electron transport in bulk wurtzite gallium nitride (GaN). Comparison of the results based on the two models is made. The results based on both models are basically the same at the lower field region, but exhibit some differences at the higher field region. The electron average energy exhibits obvious difference at the high field region between the two models. This difference further causes several other differences of GaN properties, such as the drift velocity versus field characteristics, the repopulation. Because of the complicated energy band structures at the high-energy region for wurtzite GaN, the analytical band structures in the three-valley model can not cover all properties of the band structures of wurtzite GaN, so the results based on the full band Monte Carlo model should be more exact.

Key words: Monte Carlo simulation; wurtzite GaN; transport properties; band structures
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1 Introuction

In the past decade, investigations of GaN material and GaN-based devices have been extensively carried out. Considerable progress has been made. Because of its wide band gap, GaN is a primary candidate for optoeletronic devices operating with blue to ultraviolet wavelengths and for electronic devices operating at high temperatures and high power levels. Many kinds of GaN-based structures and devices have been grown, such as superlattices[1], heterojunction[2,3], quantum well devices[4], blue laser[5], optoelectron detectors[6], light emitting diode[4,7].

It is essential for improvement and exploration of an advanced GaN device technology to best understanding of electronic transport properties of GaN. In recent years, several authors used Monte Carlo method to study electronic transport properties of wurtzite GaN. By Monte Carlo method, the steady-state drift velocity, and the electron average energy were obtained[8~11]. Most of the authors used the three-valley model and others used the full band Monte Carlo model. We noted that the results obtained by different authors are not agreement very well, even there are obvious differences among the results obtained by different authors. For example, at basically same parameters of wurtzite GaN, according to the results reported by Bhapkar *et al.*[9], the threshold field is approximately 150kV/cm, and the peak value of drift velocity is approximately 2.9×10^7cm/s. However, according to the results reported by Kolnik *et al.*[11], the corresponding values are approximately 180kV/cm and 2.5×10^7cm/s. There are also obvi-

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ous differences for some other properties such as the average energy and the repopulation.

In order to obtain more exact results of electronic transport properties in GaN and to find the reason of different results obtained by different authors, we use both the three-valley model with nonparalicity and the full band Monte Carlo model to calculate properties of bulk wurtzite GaN. Comparison of the results based on the two models has been made, and we also compare our results with the results reported by other authors. The results obtained based on both models are basically the same at the lower field region, but exhibit some differences at the higher field region. The average energy of electron exhibits obvious differences in the higher field region. Our studies indicate that these differences, we mentioned above, can be attributed to the different models adopted during the simulations.

The paper is organized in the following way. In Sec. 2, the details of both the three-valley model and the full band model are described. In Sec. 3, we report the calculated steady-state electron drift velocity, the average energy as a function of electric field strengths based on both models, and we compare the results obtained based on both methods; In Sec. 4, conclusions are drawn.

2 Model description

The Monte Carlo technique we employ to treat electron transport was described in some excellent reviews[12~14]. In our Monte Carlo simulation process, we adopt the same parameters as far as possible for both the three-valley model and the full band Monte Carlo model. In Table 1, we list the material parameters of wurtzite-phase GaN, which have been taken from Refs. [11, 14, 15].

For the three-valley model, Γ_1、Γ_2 and LM valley are included. In Table 2, we list the energy valley parameters of wurtzite GaN, which have been taken from Refs. [9, 11]. These parameters also very well agree with our band structure results.

Table 1 Material parameters of wurtzite GaN

Lattice constant, A/nm	0.38
Lattice constant, c/nm	0.5185
Dielectric constants, ϵ_0	9.5
Dielectric constants, ϵ_∞	5.35
Mass density, ρ/(g·cm^{-3})	6.095
Sound velocity/(cm·s^{-1})	4.33×10^5
Acoustic deformation potential/eV	10.1
Polar optical phonon energy/eV	0.092

Table 2 Valley parameters of wurtzite GaN

Valley	Γ_1	Γ_2	LM
Number of equiv. valley	1	1	6
Effect mass (m_i/m_0)	0.19	0.40	0.60
Nonparabolicity const. α/eV^{-1}	0.183	0.065	0.029
Intervalley energy separation/eV	0	1.98	2.15

For the full band Monte Carlo simulations, the full details of all of the eight bands for conduction band are included. In the present study, the energy band structures were calculated based on the first-principles total-energy pseudopotential method within the local-density-functional formalism. We have used norm-conserving separable pseudopotentials and a preconditioned conjugate gradient algorithm for minimizing the crystal energy with respect to the electronic as well as the ionic degrees of freedom. Compared with other methods, such as empirical pseudopotential method, this method can give reliable conduction band structures and valence band structures, but it can not give exact band gap. Minimum of conduction band, which is Γ_1 valley, sits in the symmetry point Γ. At the second conduction sub-band, there is another energy valley. That is Γ_2 valley, which also sits in the symmetry point Γ. Between symmetry point L and symmetry point M, there is another energy valley, which is LM valley. The separations between them are given in Table 2. These three lowest energy valleys play important role in transport properties of wurtzite GaN.

During the course of the Monte Carlo simulation, the energy of an electron is determined by the advanced interpolation technique, i. e. by using

mesh points within a finely spaced k-space grid spanning the irreducible wedge of the first Brillouin zone. The wave vectors are normalized by $4\pi/\sqrt{3}a$ in k_X and k_Y direction and $2\pi/c$ in k_Z direction (a and c are the lattice constants of wurtzite GaN), and equidistant spacing of the k points of 0.025 is chosen. This choice of k-point spacing, including those points located outside the irreducible wedge necessary for interpolation purposes, results in a mesh comprised of 4991 points. For some isotropic scattering process, such as intervalley phonon scattering, after scattering, the electron wave vectors are determined only by its energy. For this purpose, another fine band structure data is calculated. The k space region is the same as above, but spacing of k-point of 0.01 is chosen, resulting in 311,727 points.

For both models, the scattering mechanisms included in simulations are polar optical phonon scattering, ionized impurity scattering, acoustic phonon scattering, impact ionization as well as intervalley scattering. For the calculations of ionized impurity scattering rates, the donor concentration is set to $1\times10^{17}/cm^3$.

For the three-valley model, nonparabolic bands are assumed, and nonparabolicity constants for Γ_1, Γ_2, and LM valley are listed in table 2. The scattering rates in Γ_1, Γ_2, and LM valley are calculated, respectively. For example, for intervalley scattering, the scattering rates of, Γ_1 *to* Γ_2, Γ_1 to LM, LM to Γ_1, Γ_2 to Γ_1, LM to Γ_2, Γ_2 to LM as well as LM equivalent intervalley scattering are calculated, respectively.

For the full band Monte Carlo simulations, the electron energy is divided into two regions for the purpose of evaluating the scattering rates. The low energy region is defined to extend up to 2.5eV. At this region, the scattering rates, which depend on the wave vectors, are calculated by using Fermi's golden rule, so the final state of an electron, after scattering, can be determined exactly. For example, if an electron scatter from Γ_1 valley to LM valley, its wave vectors in LM valley can be determined by using the band structure data. For the high-energy region, the electron energy is strongly degenerated, so it is impossible to determine scattering rates by using the method mentioned above. Because the scattering rates are proportional to the density of states at the energy of final state, at the high energy region the scattering rates are obtained from normalizing low boundary scattering rates by the density of states of final state energy, which is obtained according to band structure data. Figure 1 shows the total scattering rate normalized by the density of states.

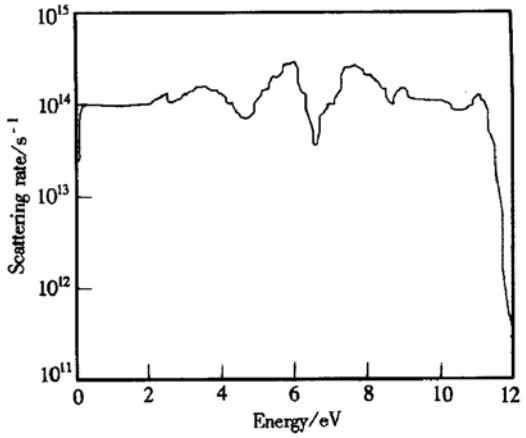

Fig. 1 Energy dependence of the total scattering rate at room temperature

The total scattering rate of the full band Monte Carlo simulation in Figure 1 is completely the same as that of the three-valley Monte Carlo at low energy region. At high-energy region, due to complicated band structure for wurtzite GaN, the variation of scattering rate with electron energy is very quick. Due to simple band model assumed in the three-valley model, the variation of scattering rate with electron energy is smooth.

In each simulation, the twenty thousand electrons are initially distributed in the sample according to equilibrium Maxwellian distribution. The time step is 2×10^{-15}s, and the number of time steps for each data point is 10,000.

3 Simulation results

Figure 2 shows the calculated steady-state electron drift velocities as a function of the applied electric field at room temperature in the three-valley model and the full band Monte Carlo model. Noted that in the three-valley model, due to assuming isotropic band valley, there is only one curve of the velocity versus field characteristic. Actually, the realistic band structures are anisotropy, so in the full band Monte Carlo simulations there are the three curves of the velocity versus field characteristics in the three main symmetry directions. The velocity-field characteristics exhibits three general regions. A deep linear slope is in the first region. For an electron to be able to emit a polar optical phonon its energy must be at least equal to the phonon energy. In this region, the average energy of electrons is lower, and polar optical phonon emissions are a rare event. The dominant scattering mechanisms are the ionized impurity scattering and the acoustic scattering, so the drift velocity increases very quickly with increasing the electric field. As the electric field reaches the value about (2~ 3) × 10^4V/cm, the polar optical emission scattering becomes the dominant scattering mechanism, so drift velocity versus electric field characteristics enter the region with easy slope. As the electric field is further increased, many electrons gain enough energy to transfer to the satellite valleys by intervalley phonon scattering. Because the electron effect mass is larger in satellite valleys than that in Γ1 valley, the peak drift velocities with certain value start to decrease.

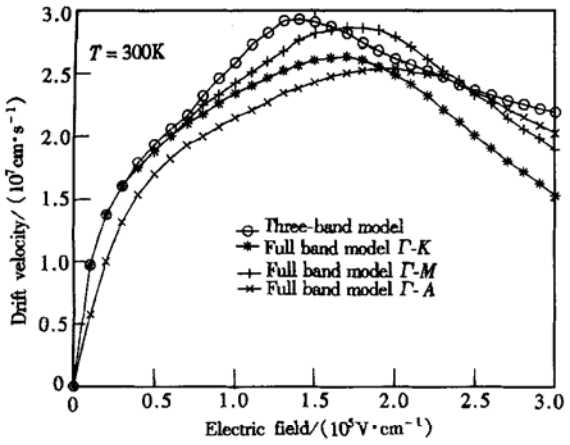

Fig. 2 Calculated steady-state electron drift velocity as a function of applied electric field in wurzite GaN obtained using two models In the full band model, the three curves are drawn for the field along the three major crystalline axes, Γ-*K*, Γ-*M* and Γ-*A* direction.

Figure 2 indicates that at lower electric fields the velocity-field characteristics obtained by the three-valley model and the full band Monte Carlo model are basically the same. This is because most of the electrons sit in the low energy position of Γ1 valley. In the three-valley model, the relation of dispersion of the nonparabolicity energy valley is described by

$$\hbar^2k^2/2m^* = E(1 + \alpha E) \qquad (1)$$

where $\hbar$ is Planck's constant, k is wave vector, m^* is the effect mass, α is a nonparabolic parameter and E is the electron energy. For Γ1 valley, α is equal to 0.183eV^{-1}. At the low energy region, most of the electrons sit in the low energy position of Γ1 valley. Equation (1) can describe band structure very well. However, for the realistic band structure of GaN, α is not a constant, but is a function of the electron energies. As the electric fields become larger, a large number of the electrons reach the high-energy region of Γ1 valley. In this situation, in the three-valley model treating α to be a constant may cause some errors, so the drift velocity increases faster in the three-valley model than in the full band model. Figure 3 shows the average energy of electrons as a function of applied electric field. In connection with the velocity-field curves, at the low field region the average energy of electrons increases very slowly with the increasing of electric field, and near the threshold filed the average energy of electrons increases abruptly. At the high field region, average electrons energies are obviously larger in the three-valley model than those in the full band Monte Carlo model. From our results and other authors' results, we can conclude that the

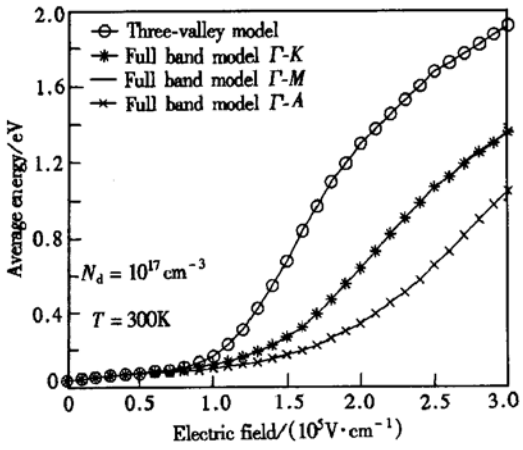

Fig. 3　Calculated average energy as a function of applied electric field in wurtize GaN based on the two models　For the full band model three curves are drawn in the field along the three major crystalline axes Γ-*K*, Γ-*M*, Γ-*A* direction. The curves in field along Γ-*K*, Γ-*M* are basically the same.

threshold field is 150~ 160kV/cm in the three-valley model, and 170 ~ 190kV/cm in the full band Monte Carlo model. These results can be explained by the average energy of electrons versus the electric field curve. For the three-valley model, α is assumed to be a constant. For the realistic band structures, α is larger in the high-energy region than that in the low-energy region. For this reason, for the case where the electron wave vectors are the same and the electron energy is large, the electron effect mass is larger in the full band model than that in the three-valley model. In the high field region with same electric field strength, the average energy of electrons are larger in the three-valley model than those in the full band Monte Carlo model. For higher fields, the number of the electrons those energies are above the transfer threshold energies (1.9eV for *LM* valley and 2.1eV for Γ_2 valley), is lager in the three-valley model than that in the full band Monte Carlo model. Therefore, the threshold field is smaller in the three-valley model than that in the full band Monte Carlo model.

The results of velocity-field characteristics in wurtzite GaN obtained with our Monte Carlo calculation exhibit the similar properties with typical compound semiconducting materials, such as GaAs. In these materials, due to intervalley transfer, there is a region of negative differential resistance. The negative differential resistance can further cause Gunn effect. But in our results no Gunn effect is observed. There are two reasons. First, our simulation is bulk simulation. In this simulation, we assume that the electric fields in the material are constants. That is, we assume the electrons are uniformally distributed in material, that is to say, additional electric fields does not exist. Secondly, our simulations are stable simulations. That is, we do not consider the variation of transport properties with time.

Figure 4(a) and (b) show the temperature dependence of velocity-field characteristics based on the three-valley model and the full band Monte Carlo model, respectively. Generally, as the temperature decreases, the number of phonons by the Bose-Einstein factor decreases and so the total scattering rates decrease, so the drift velocity increases with decreasing temperature. At the low field region, Figure 4(a) and (b) both show that the steady-state drift velocity increases as the temperature decreases. However, as high electric field above the threshold, due to scattering rate decreasing with decreasing temperature, so the average energy of electrons will increase, and much more electrons will gain enough energy to transfer to the satellite valleys. This effect will cause the drift velocity to decrease with decreasing temperature. Therefore, at high fields the two factors come into effect. By comparing Figure 4 (a) with (b), the effect of the latter is much larger in the full band Monte Carlo model than that in the three-valley model. In the three-valley model at high field region, the differences of the drift velocity in various temperature tend to disappear, but in the full band Monte Carlo model the curves of velocity versus electric field characteristics become crisscross. Specially, the curve of velocity versus electric field

characteristics in 77K is much lower than other curves in higher temperature.

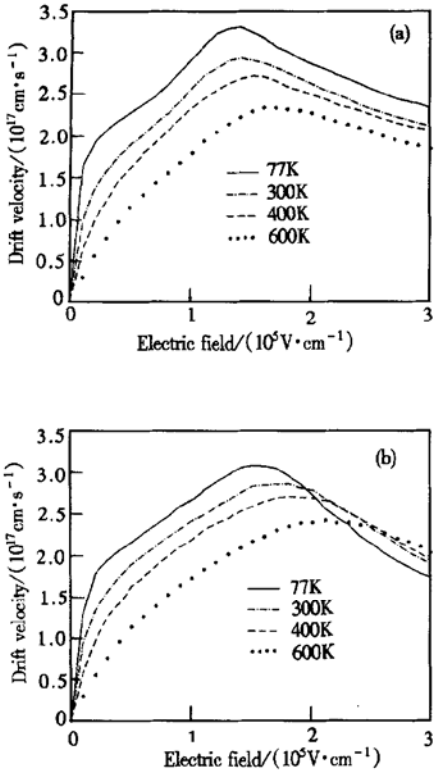

Fig. 4 Temperature dependence of velocity-field characteristics of GaN at $N_d = 10^{17}\,cm^{-3}$ (a) Three-valley model; (b) Full band Monte Carlo model(Γ-K direction)

4 Conclusions

In this paper, the Monte Carlo simulation results of the electron transport in bulk wurtzite GaN by using both the three-valley model and the full band Monte Carlo model have been presented. For the three-valley model, the analytical band structures are used, and the complicated calculations of band structures are not required. At the low electric field region the results of electron transport obtained by using this model are exact enough. At the high electric field region, due to assuming the simple band structures, the results will cause some errors. For the full band Monte Carlo simulations, the full band structures are used, and the complicated calculations of band structure are required. At both low and high electric field the results of electron transport obtained by using this model are exact enough. Due to complicated energy band structures in a high-energy region, the electron effect mass is larger than that obtained by using the analytical band structures. For this reason, at the higher field region, the average energy of electrons and the drift velocity are smaller in the full band Monte Carlo model than those in three-valley model. Due to the lower average energy, the threshold electric filed is larger in the full band Monte Carlo model than that in the three-valley model. Otherwise, in the three-valley model, the analytical band structures are treated as isotropy. Actually, the realistic band structures in wurtzite GaN are strongly anisotropy. The full band Monte Carlo simulations can obtain the transport properties in different directions.

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用三带和全带模型蒙特卡罗方法模拟纤锌矿相 GaN 体材料输运特性结果的比较

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摘要: 报道了分别用三带和全带模型蒙特卡罗方法模拟纤锌矿相 GaN 体材料输运特性的结果, 并对基于两种模型的模拟结果进行了比较. 在低场区, 基于两种模型获得的输运特性基本相同, 但在高场区却表现出明显的差别. 这是因为在高场区, 电子平均能量较高, 多数电子处于能带图中的高能态位置, 电子能量与波矢量的关系表现出明显的非椭圆特性. 由于三带模型假定了能量与波矢量简单关系, 故算得的平均能量, 高于由全带蒙特卡罗模拟算得的能量. 从而导致其它特性的差别. 全带模型包含了基于能带理论算得的能带结构的所有特性, 故模拟结果更加精确.

关键词: 蒙特卡罗模拟; 钎锌矿相氮化镓; 输运特性; 电子结构

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