Quasi Self-consistent Monte Carlo Particle Simulations of Local Heating Properties in Nano-scale Gallium Nitride FETs

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Abstract—In this paper, we report our novel Monte Carlo quasi self-consistent particle simulation method for both electron and phonon transport in nanometer-sized electron devices. We developed two kinds of simulation procedures for the Monte Carlo method. First, we made a program to estimate the local temperature from a phonon spatial distribution, where we used a Bose-Einstein distribution function, the phonon density of states, and the phonon generation rate. Second, we developed an algorithm that made it possible to calculate multiple time scale phenomena of electron and phonon transport by introducing different time steps for electron and phonon transport simulations. With these methods, we succeeded in executing quasi self-consistent simulations of both electron and phonon transport in nanometer-channel FETs in consideration of saving computer processing time. Using these methods, we simulated the local heating properties of nanometer-scale gallium nitride FETs for the first time. Our FET model includes highly doped source and drain regions near the electrodes. It was found that phonon generation takes place mainly in the highly doped drain region, rather than in the high electric field regions of the channel or between the gate and drain. We discuss the physical basis of the spatial distributions of heat generation and local temperature in the GaN channel.

Keywords—Phonons; Monte Carlo methods; Field effect transistors; Thermal management of electronics.

I. INTRODUCTION

Due to high density integration of LSIs and high power applications, the thermal management of electron devices has become more and more important. GaN has been expected for use for high-frequency and high-power applications due to its large bandgaps, high breakdown voltage, and high electron drift velocities. Previously, to simulate electric and heat transport phenomena in electron devices, a fluid model based on the Maxwell distribution functions was used. For an advanced electron device scaled below or comparable to the size of the electron mean-free-path, the Monte Carlo particle simulation method has been used as the most reliable and accurate method for calculating non-stationary electron transport [1]. Similarly, because the mean free path of a phonon also becomes comparable to or less than the size of a typical device, thermal properties should be analyzed for non-stationary state phonon transport. Using the Monte Carlo particle method for both electron and phonon transport [2]

should be the most accurate theoretical approach. However, there are two big problems. The first is that the simulation algorithm for local temperature estimation from phonon distributions has not yet been established. The second is that, because of a large difference in time scales between electron and phonon transport phenomena, performing a self-consistent simulation for both electrons and phonons in a realistic amount of computer processing time would be very difficult. Additionally, it is also important for future phonon engineering. In this paper, we report novel quasi self-consistent algorithms for the Monte Carlo method with a reasonable computing time [3] and report the electrical and thermal properties of GaN FETs calculated for the first time when using these methods.

II. SIMULATION METHOD

Figure 1 shows the algorithm of our simulation. It consists of two parts: an electron transport part to obtain the spatial distributions of phonon emission and absorption and a phonon transport part to estimate local heating in a device. By introducing the feedback of local heating information to the scattering rate in the electron transport part, our simulation model of electron and phonon transport becomes self-consistent. For this method, we developed two simulation procedures.

A. Algorithm for Local Temperature Distribution

We made a program to estimate the local temperature from a phonon spatial distribution, where we used a Bose-Einstein distribution function, the phonon density of states, and the phonon generation rate, which were obtained by Monte Carlo simulations. First, we calculate the Bose-Einstein distribution function for the temperature, T_1. By multiplying it by the phonon density of the states of the channel material, we can obtain the energy distribution of phonons at time t_1. Next, we implement a Monte Carlo particle simulation to obtain the numbers and locations of phonon scattering events in the channel during a time increment of Δt. By adding the generated phonons to the original one, we can obtain the revised phonon distribution at time t_2 (= $t + \Delta t$), where we assumed that the energy of phonons generated during Δt will be uniformly dispersed in the whole range of the acoustic phonon energy on the basis of the initial phonon energy distribution function (as shown in Fig. 2). Then, we obtain the revised Bose-Einstein distribution by dividing the revised phonon distribution by the
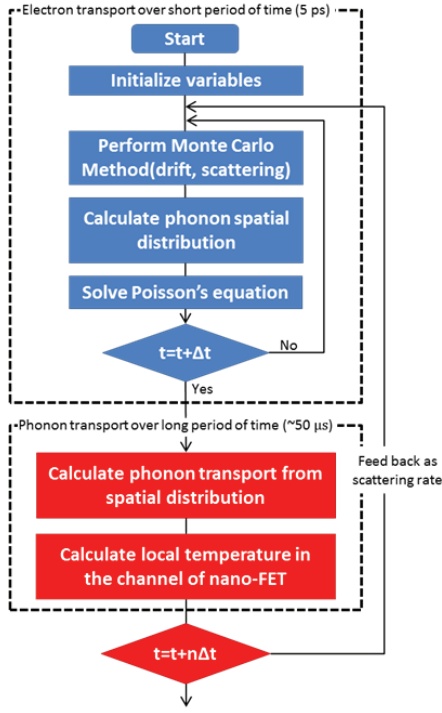
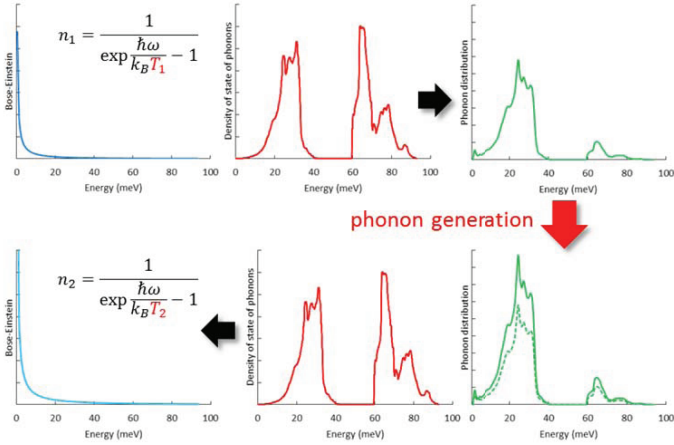Fig. 1 Algorithm of Quasi Self-consistent Monte Carlo method for electron and phonon transport

Fig. 2 Schematic of method for estimating local temperature from phonon population

density of states. Finally, the local temperature T_2 at time t_2 is determined. From this procedure, we established the following equations that enable us to estimate the local temperature in the channel from the phonon spatial distribution at time t_2.

$$T_2 = \frac{\hbar\omega_a}{k_B \ln\left(\frac{n_2+1}{n_2}\right)} \qquad (1),$$

$$n_2 = \frac{\hbar\omega_a n_1(\hbar\omega_a, T_1) A[D(\hbar\omega_a)] + m\hbar\omega_o P[n_1(\hbar\omega_a, T_1)D(\hbar\omega_a)]}{\hbar\omega_a A[D(\hbar\omega_a)]} \qquad (2),$$

where $\hbar\omega_a$ and $\hbar\omega_o$ are the energies of the representative acoustic and optical phonons, respectively, m is the number of optical phonon emissions during Δt and $D(\hbar\omega_a)$ is the phonon density of states at the energy of $\hbar\omega_a$. The n_i is the Bose-Einstein distribution function value for the acoustic phonon energy $\hbar\omega_a$ at time t_i. The term $P[n_1(\hbar\omega_a, T_1)D(\hbar\omega_a)]$ means the percentage of the number of acoustic phonons $\hbar\omega_a$ to the total numbers of phonons over the whole energy range. The term $A[D(\hbar\omega_a)]$ is the phonon density of states at the energy of $\hbar\omega_a$ normalized by the total numbers of oscillators (the product of the number of atoms in the region where the local temperature is defined and the degree of freedom). We emphasize that if we know the crystal structure and phonon dispersion of the material, this method can be applied for any material.

B. Dual Time-step Simulation Method

We introduce a calculation algorithm that separates the timescales of electron and phonon transport, which made it possible to calculate multiple time scale phenomena of electron and phonon transport (Figure 3). In the algorithm, first, we only calculate the electron transport for a short period of time Δt, enough to achieve electron relaxation and obtain phonon spatial distribution. Then, only phonon transport is calculated for a long period of time, where phonon particles are generated at each time step of Δt on the basis of the simulated spatial distribution of phonons. After that, we calculate a local temperature in the channel, and the temperature is fed back to the scattering rate calculation. By repeating this process, we can skip most of the calculation of electron transport and analyze phonon transport for a long period of time with an extremely short amount of computation time. With these methods, we succeeded in calculating both electron and phonon transport self-consistently with a reasonable amount of computation time. The phonon velocity is derived from the phonon dispersion curve [4]. The phonon-phonon scattering rate is assumed to be a constant value for each material. Our FET model includes a 2DEG GaN-channel and highly doped n+-source and drain regions near the source and drain electrodes. Both the heat dissipation through the substrate and the heat radiation from the surface were not taken into account.
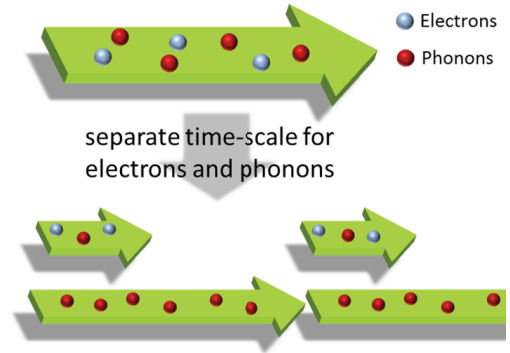

Fig. 3 Schematic of quasi self-consistent simulation procedure for both electron and phonon transport

C Two-dimensional FET Model

Figure 4 shows a two-dimensional model of an AlGaN/GaN high electron mobility transistor (HEMT). The gate length is 0.1 μm. The channel n-layer is sandwiched between two source and drain n+ layers. We assumed that the electron motions and phonon generations were limited to the n- and n+ layers. We will discuss the comparison between the confined phonon motion model and real space phonon transfer model.
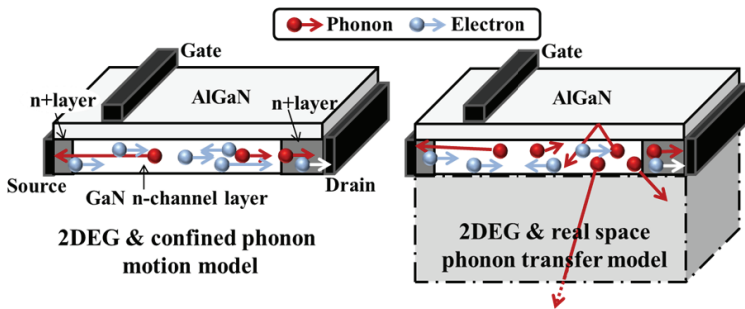

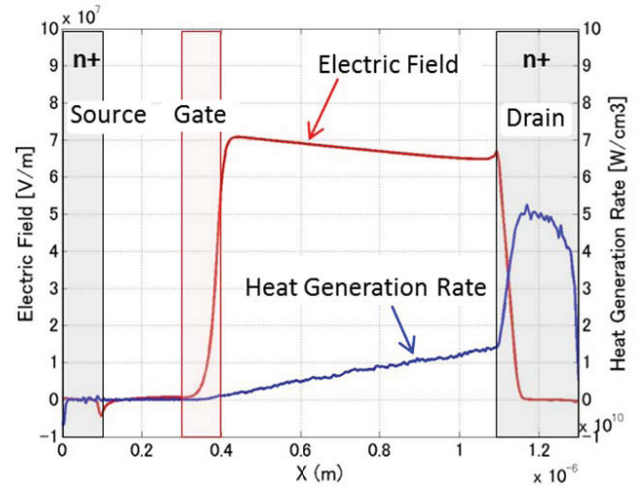
Fig. 4 Two-dimensional AlGaN/GaN HEMT models

Fig. 5   Distributions of electric field and heat generation rate in channel of 100-nm-gate GaN FET simulated with MC simulation method (at Δt after applying voltage Vds of 50 V)

III. RESULTS AND DISCUSSION

Using these methods, we succeeded in analyzing local heating phenomena in nano-scale GaN FETs quantitatively. Figure 5 shows the spatial distributions of the electric field and the heat generation rate calculated by calculating the phonon generation in the GaN FETs. The applied drain to source voltage (Vds) and gate voltage (Vgs) were 50 and 0 V, respectively. Note that the peak of the heat generation rate was located in the n+-drain region, rather than in the high field regions in the channel or between the gate and drain. This is probably because back-scattered high energy electrons have a longer transit time in the low field drain n+-region, which means many more chances for optical phonon emissions, compared with the electrons in the high field regions with a shorter transit time.

Figure 6 shows the local temperature distribution at 50 μs after applying voltage. Even if the distribution was not completely saturated, we succeeded in simulating phonon diffusion in the GaN channel from the drain n+-region towards the source. In this work, we used the confined phonon motion model. It is seen that the local temperature gradually decreased in the channel from the drain to the source and that the peak position of local heating was in the n+ drain region.

Figure 7 shows the local temperature distribution at 50 μs after applying the voltage obtained by using a model that included real space phonon transfer. In other words, it included heat removal through the substrate. We assumed that the thermal conductivity of AlGaN is the same as that of GaN. The temperature in the whole area of the channel became lower than that in the phonon confined model. Even so, remarkable local heating was still observed. Further
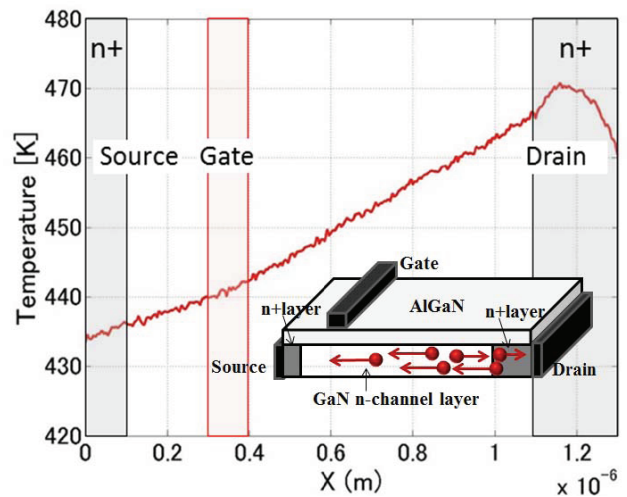

Fig. 6   Temperature distributions in channel of 100-nm-gate GaN FET simulated with quasi-self-consistent MC simulation method (at 50 μs after applying voltage Vds of 50 V)

simulation studies using this model are needed, in particular, to assess the quantitative accuracy of the simulation method and to investigate new heat removal technologies in terms of new device structures and materials.
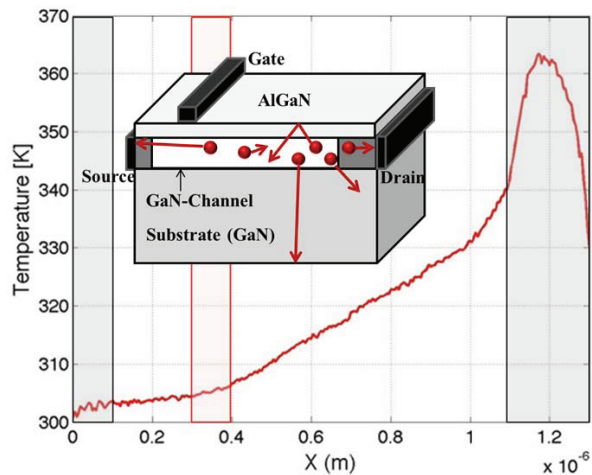
Fig. 7 Temperature distributions in channel of 100-nm-gate GaN FET simulated with quasi-self-consistent MC simulation method with real space phonon transfer model (at 50 µs after applying voltage Vds of 50 V)

IV. CONCLUSION

In conclusion, we developed two kinds of simulation procedures for the Monte Carlo method, which make it possible to realize quasi self-consistent simulation of electron and phonon transport in nano-scale devices with a reasonable amount of computing time. Using the method, we investigated the local self-heating phenomena of nano-scale GaN FETs. We confirmed that phonon generation takes places mainly in the highly doped and low electric field drain regions, rather than in the high field regions of the channel or between the gate and drain.

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