Simulation of Semiconductor Processes and Devices 2016
Edited by E. Bär, J. Lorenz, and P. Pichler

Advanced Quasi Self-consistent Monte Carlo Simulations of Electrical and Thermal Properties of Nanometer-scale Gallium Nitride HEMTs Considering Local Phonon Number Distribution

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***Abstract*— As a means of investigating both the electrical and thermal properties of nanometer-scale electron devices within a reasonable computing time, we previously proposed a quasi-self-consistent Monte Carlo simulation method that used two new procedures: (i) a local temperature determination using the simulated phonon spatial distribution and feedback to update the electron-phonon scattering rates and (ii) a new algorithm which calculates long-time phonon transport by introducing different time increments for the electron and phonon transport. In this paper, to improve the quantitative accuracy and self-consistency of the simulation, we investigate an advanced Monte Carlo method considering (i) spatially dependent electron-phonon scattering rates that are calculated directly using a simulated phonon distribution (not the local temperature) taking into account (ii) the energy dependence of the phonon group velocity and phonon-phonon scattering rate and (iii) positive polarization charges due to piezoelectricity at the AlGaN/GaN interface. Using this advanced Monte Carlo method, we succeeded in simulating the current-voltage characteristics and thermal resistance of GaN HEMTs (High Electron Mobility Transistors), with which a quantitative evaluation could be made using actual devices. We also examined the convergence of this self-consistent Monte Carlo model.**

Keywords—Phonons; Monte Carlo methods; High Electron Mobility Transistor; Thermal management of electronics.

I. Introduction

As the density of LSI integration increases and as demand for high-power applications grows, thermal management has become more and more important [1]. Gallium nitride (GaN) has been viewed as having great potential for such applications because of its large band gap, high breakdown voltage, and high electron drift velocity. Previously, a fluid model based on the Maxwell distribution functions was used to simulate electric and heat transport phenomena in electron devices [2]. On the other hand, the self-consistent Monte Carlo particle simulation method has been viewed as the most reliable and accurate way of calculating non-equilibrium electron and phonon transport properties of advanced electron devices with dimensions comparable to the electron and phonon mean free paths [3]. However, this approach consumes a lot of resources and has not been used to study realistic transistors. As a way of dealing with this problem, we developed a new quasi self-consistent algorithm that has a reasonably short computing time and used it to calculate long-time phonon transport by introducing dual time steps for the electron and phonon transport simulations (Fig. 1) [4, 5]. Here, to evaluate electrical and thermal properties more quantitatively, we should improve the calculation of the spatially dependent electron-phonon scattering rates and the modeling of phonon transport. Thus, in this study, we developed a more accurate model and used it to simulate the electrical and thermal properties of GaN HEMTs.

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II. Simulation Method

Our simulation model consists of two parts: an electron transport part to simulate electron transport and obtain the spatial distributions of phonon emission and absorption and a phonon transport part to simulate phonon motions and estimate local heating in the device. By feeding back local heating information to the electron-phonon scattering rate calculation in the electron transport part, our simulation model becomes self-consistent. The concept of the method is basically the same as that of our previous work [4, 5], but several new features have been included.

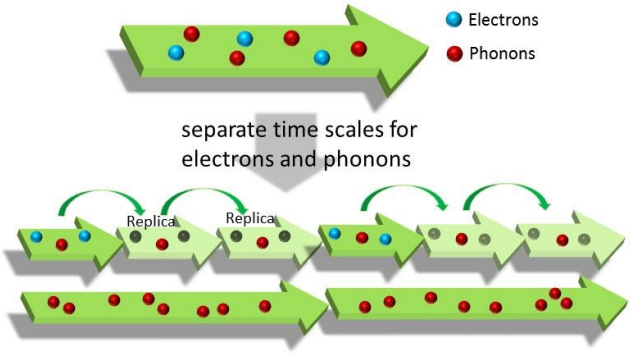

Fig. 1 Schematic diagram of dual time-step method for quasi self-consistent simulation procedure for electron and phonon transport

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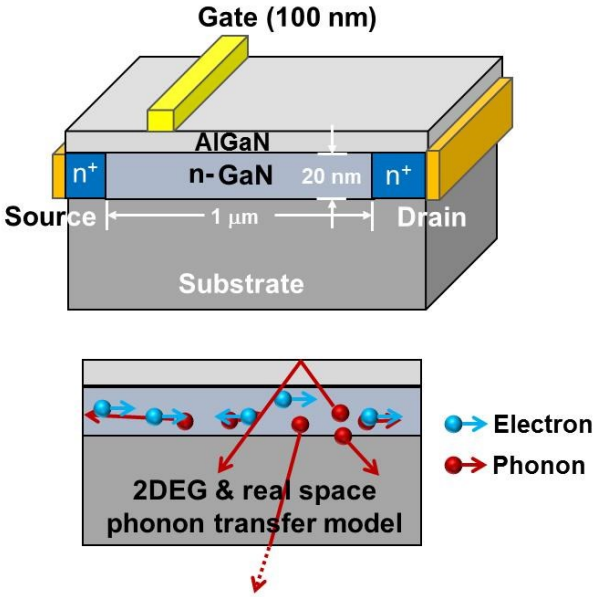

Fig. 2 AlGaN/GaN HEMT model and boundary conditions for electrons and phonons transport models

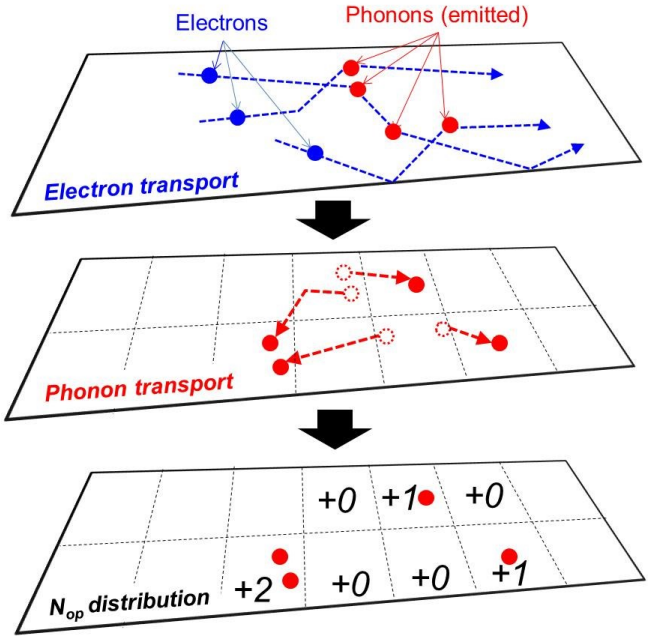

Fig. 3 Schematic diagram of a spatial and time-dependent phonon distribution determination

A. Device Model and Electron Transport Model

Fig. 2 shows the cross-section of a two-dimensional GaN/GaN HEMT model. The gate length is 0.1 μm. The channel n-layer is sandwiched between two source and drain n+ layers. The thickness of the channel layer is 20 nm. The doping densities of the n and n+ layers are assumed to be 10^{19} cm^{-3} and 10^{20} cm^{-3}, respectively. A GaN substrate is employed. In this model, the motions of the electrons are limited to the GaN channel layer. In order to give a realistic density to the two-dimensional electron gas (2DEG) at the AlGaN/GaN interface, we assume that there are additional positive polarization charges in the AlGaN-side of the interface [6]. Electron-phonon scattering (intra-valley and inter-valley) and ionized-impurity scattering are also included.

B. Phonon Transport Modeling

In order to simulate phonon transport in the device by using the Monte Carlo particle method, the dispersion relations of the longitudinal acoustic (LA) and transverse acoustic (TA) phonons are calculated using molecular dynamic software (ATK-Classic[7]). The energy dependence of the phonon-phonon scattering rates (Normal and Umklapp processes) and of the phonon group velocity are taken into account on the basis of these calculations. The Holland model is used to calculate the phonon-phonon interactions [8]. The life-time it takes for polar optical phonons (τ_{op}) emitted by electrons to decay into acoustic phonons is assumed to be a constant of 2.5 ps [9]. The model assumes that the GaN/substrate interface and AlGaN/GaN interface do not affect the motions of the phonons. Furthermore, heat dissipation through the GaN substrate (as a no reflection boundary) and heat insulation in the AlGaN surface (as a specular reflection boundary) are taken into account.

C. Direct Determination of Spatially Dependent Electron-phonon Scattering Rates

Our new model directly calculates the electron-phonon scattering rate based on local phonon numbers, whereas our previous model [4, 5] bases its calculation on the local temperature. For example, the polar optical phonon scattering rate can be expressed as

$$P_{vv',\mathrm{po}}(\boldsymbol{k},\Omega_{k\pm q}) = \frac{2\pi}{\hbar}|C(\boldsymbol{q})|^2|I(v,v';\boldsymbol{k},\boldsymbol{k}\pm\boldsymbol{q})|^2 \times D_{v'}(E',\Omega_{k'})\begin{Bmatrix} N_{op} \\ N_{op}+1 \end{Bmatrix},$$

where N_{op} is the phonon occupation number given by the Bose-Einstein distribution $N_{op} = \left[\exp(\hbar\omega_{op}/k_BT) - 1\right]^{-1}$ at equilibrium. $I(v,v';\boldsymbol{k},\boldsymbol{k}\pm\boldsymbol{q})$ is the overlap factor and $D_{v'}(E',\Omega_{k'})$ is the density of state as before. $C(\boldsymbol{q})$ is the electron-phonon coupling coefficient. Under non-equilibrium conditions, N_{op} must be determined using the local phonon distribution, not local temperature. Thus, in the new model, the local phonon occupation numbers obtained by the phonon transport simulation can be used directly to determine spatially dependent electron-phonon scattering rates (Fig. 3).

III. Results and Discussion

We used the new method to investigate the electrical and thermal properties of GaN HEMTs. Fig. 4 shows the spatial distributions of the electric field, heat generation rate, and local temperature. The drain to source voltage (Vds) and gate voltage (Vgs) were 20 V and 1 V, respectively. The heat generation rate was calculated as the phonon generation rate of electrons in the channel. We estimated the local temperature by using the Bose-Einstein distribution in the same way as in our

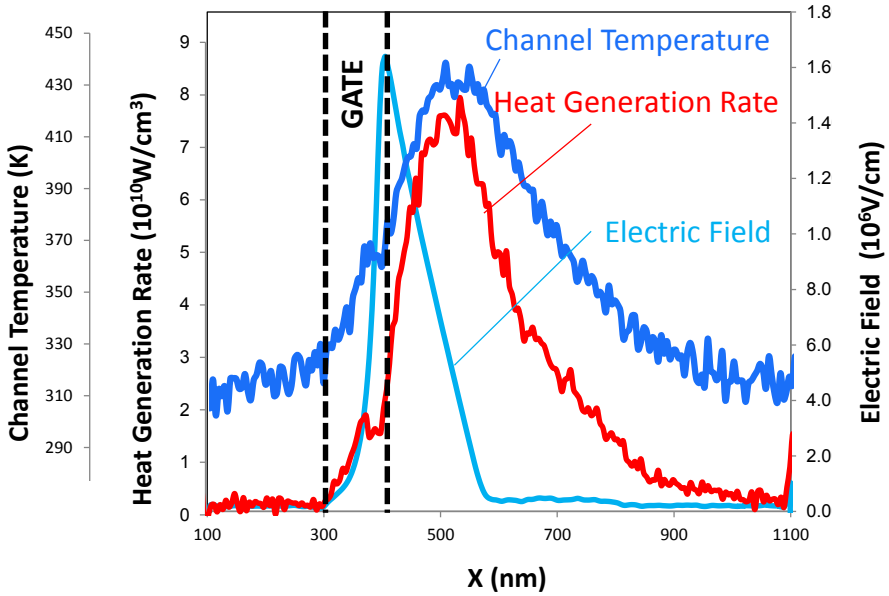

Fig. 4 Profiles of local channel temperature, heat generation rate, and electric field in the channel (Vgs=1 V, Vds=20 V)

previous model [4, 5]. The electric field reaches a maximum at the gate edge on the drain side. The peak temperature is 130 degrees C higher than room temperature. Note that the positions of the peaks of the local temperature and heat generation rate are almost the same, but are 150 nm closer to the drain than the peak of the electric field. This difference is due to the drift effect during the mean free time of the electron-phonon scattering with phonon emission. Fig. 5 shows the drain current (Ids) versus drain voltage (Vds) of the HEMT with and without local phonon distribution feedback. Ids becomes lower as Vds increases, showing negative resistance in the high current regime.

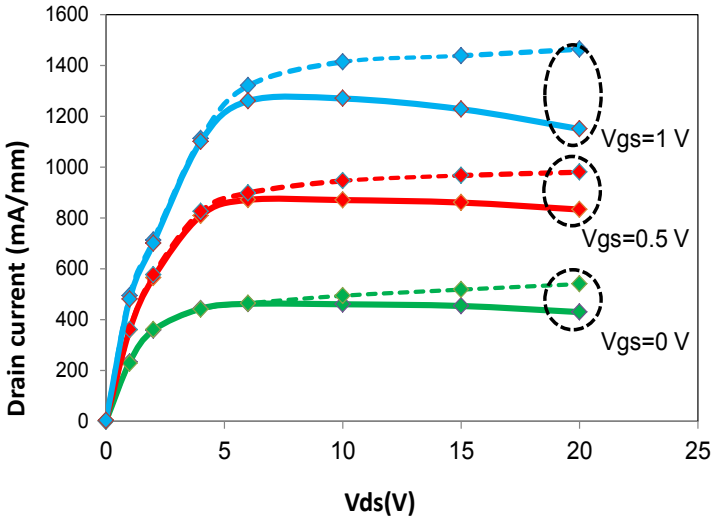

Fig. 5 Drain current (Ids) versus drain voltage (Vds) of the HEMT with (solid lines) and without (dashed lines) local phonon distribution feedback

Current decreases like this often occur in high-power transistors [10], and they are mainly because the increase in the phonon population or local heating (Fig. 6) leads to a higher electron-phonon scattering rate, and consequently, a decrease in electron velocity.

Fig. 7 shows the relation between peak temperature in the channel and power dissipation. Here, the power dissipation is normalized by the channel width. The slope of the line indicates a thermal resistance of 4.9 K· mm/W, which is very close to that of GaN. There is an experimental report indicating that the slope corresponds to the substrate's thermal resistance, although it used different substrates [11].

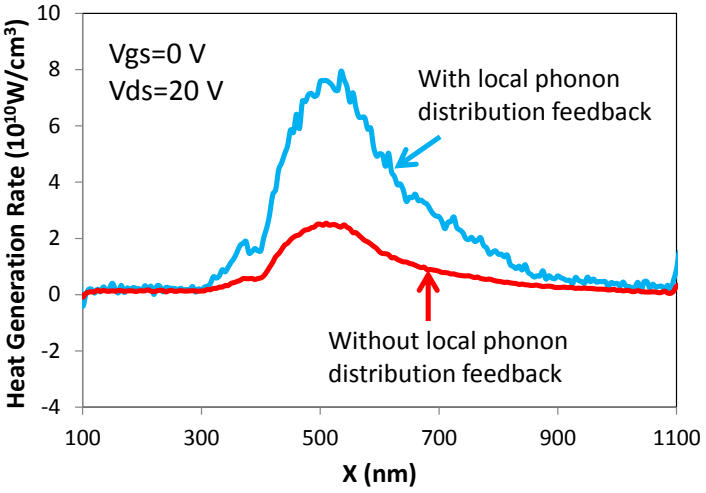

Fig. 6 Heat generation rate in the channel with and without local phonon distribution feedback (Vgs=0 V, Vds=20 V)

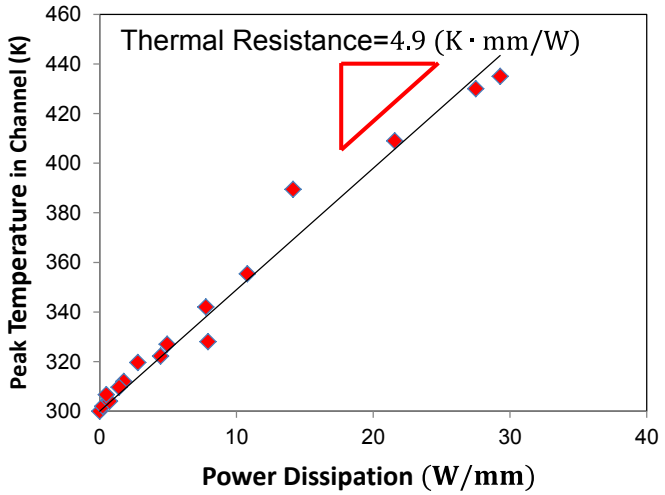

Fig. 7 Peak temperature in channel vs. power dissipation

Fig. 8 shows the time dependence of the simulated drain current and peak temperature in the channel. As mentioned before, an increase in the phonon population (or local heating) leads to a decrease in the electron velocity in the channel. The figure shows that as the peak temperature in the channel converges, the drain current also tends to saturate. This is mainly due to there being steady-state electron-phonon scattering rates, resulting from the steady-state of the local phonon number distributions in the device.

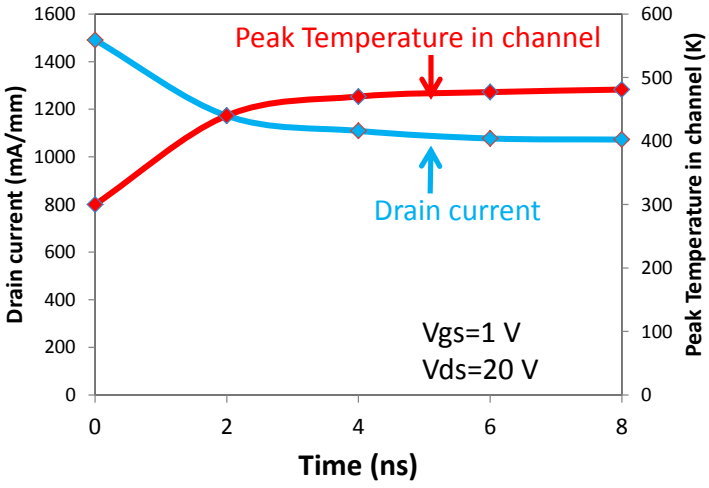

Fig. 8 Time dependence of drain current and peak temperature in an AlGaN/ GaN HEMT (Vgs=1 V, Vds=20 V)

IV. CONCLUSION

We developed a quasi-self-consistent Monte Carlo method for both electron and phonon transport in nanometer-sized electron devices. In the electron transport part, we determine the electron-phonon scattering rate on the basis of the local phonon distribution. Using the new method, we investigated electrical and thermal phenomena of nanometer-scaled GaN HEMTs. We found several interesting features. Firstly, the drain current decreases due to local heating phenomena. Secondly, the peak temperature in the channel is proportional to the power dissipation, and the slope of this relation is nearly equal to the thermal resistance of GaN. We also discussed the convergence of this quasi-self-consistent Monte Carlo model.

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