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HOT-PHONON-ASSISTED ADDITIONAL CORRELATION IN $Al_{0.23}Ga_{0.77}N/GaN$

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The hot-phonon effect is considered for an $Al_{0.23}Ga_{0.77}N/GaN$ structure with a two-dimensional electron gas subjected to an electric field applied in the plane of electron confinement. The hot-phonon accumulation is taken into account in the hot-phonon lifetime approximation for the quantum well model designed through a self-consistent solution of Schrödinger and Poisson equations. The field-dependent electron temperature and non-ohmic transport are obtained from the Monte Carlo simulation for a 3-subband model. The longitudinal tensor component of an additional correlation of electron velocities is estimated in the hot-electron temperature approximation and an essential dependence on the hot-phonon lifetime is demonstrated. The results are in a reasonable agreement with the experimental data for a similar structure with a two-dimensional electron gas.

Keywords: hot electrons, fluctuations, diffusion, hot phonons

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1. Introduction

Semiconductor heterostructures open wide possibilities to improve transistor performance, and a great variety of high-speed devices has been discussed [1]. A comparative analysis of different designs requires considering electron gas subjected to a strong electric field. The physical backgrounds include Schrödinger and Poisson equations coupled with kinetic equations for hot-electron transport and fluctuations [2]. A huge amount of processor time and memory is needed for numerical treatment of the kinetic equation [3], and simpler approaches also look attractive. In particular, a drift–diffusion equation is often used for approximate fast solution under different conditions of interest [4].

The electron drift velocity and diffusion coefficient are prerequisites for the drift–diffusion equation. At equilibrium, the kinetic coefficients are interrelated. In particular, the electron diffusion coefficient and the spectral intensity of velocity fluctuations can be obtained from the relations of Einstein and Nyquist once the electron density and mobility are known. Strictly speaking, these relations are no longer valid at high electric fields, but some of them survive under well specified conditions [5]. In particular, the hot-electron diffusion coefficient is proportional to the spectral intensity of velocity fluctuations at a low electron density [6]. This relation is violated at a high density of hot-electron gas where an intense electron–electron interaction causes an additional correlation of the final states after each two-electron collision [7]. The additional correlation also follows from a theoretic treatment of coupled kinetic equations for non-equilibrium electrons and non-equilibrium phonons [8]: a non-equilibrium phonon can assist an exchange of energy and momentum between two electrons in a similar way as it happens during their direct collision.

The kinetic coefficients at high electric fields are often obtained from either experiment or computer simulation. The Monte Carlo procedure is one of the best for simulation of hot-electron diffusion [9]. A standard way for measuring of the hot-electron drift velocity and diffusion coefficient is based on the time-of-flight experiment of a cloud of electrons injected into an insulating semiconductor subjected to a high electric field [10, 11]. Regretfully, this technique is not applicable to conductive materials and quantum well channels with a high density of electron gas.

Požela and his colleagues have proposed and tested the fluctuation technique for measuring the diffusion coefficient of majority carriers in semiconductors [12, 13]. The technique is applicable to uniformly doped semiconductors and channels with a two-dimensional electron gas (2DEG) [14–16]. No carrier density gradient is needed. The pioneering result for a p-type germanium [12] is in an excellent agreement with the results obtained for the same semiconductor more than half a decade later by the traditional time-of-flight technique [11].

As mentioned, the two-electron collisions destroy the simple fluctuation–diffusion relation. On the other hand, intense collisions validate the treatment of hot-electron effects in the electron temperature approximation. In this approach, an additional correlation, born by the two-electron collisions, can be expressed in terms of non-ohmic conductance and excess temperature [7]. The same expression is applicable to the proposed new source of the additional correlation due to the hot-phonon-assisted interaction [8]. The short term *hot phonons* stands for non-equilibrium longitudinal optical phonons (LO phonons) launched by hot electrons [17]. Under a strong coupling of hot-electron and hot-phonon gases in 2DEG channels, the electron temperature approximation is applicable [18]. An accumulation of hot phonons affects non-ohmic transport of hot electrons [19]. The experimental results on GaN-based 2DEG channels have been treated in the electron temperature approach [20].

Our goal is estimation of the additional correlation in the electron temperature approximation for a coupled hot-electron and hot-phonon gases confined in a quantum well subjected to an electric field. The hot-electron temperature and non-ohmic transport are obtained from the Monte Carlo simulation for a model of a GaN-based 2DEG channel. The shape of the well, the electron density profile, and subband energies are obtained from a self-consistent solution of coupled Schrödinger–Poisson equations. The repulsive force of two electrons during their direct collisions is ignored in order to resolve the effect of phonon-assisted exchange of two-electron energies and momenta.

2. Model

The coupled kinetic equations for hot electrons and hot phonons are solved numerically by the Monte Carlo technique for an AlGaN/GaN 2DEG model in a standard way [21]. The model has been recently used to interpret the experimental results on hot-electron noise, transport, and hot-phonon decay in $Al_{0.23}Ga_{0.77}N$/GaN structures [22]. According to the self-consistent numerical solution of coupled one-dimensional Schrödinger–Poisson equations, the 2DEG channel is formed in the quantum well located in the nominally undoped GaN layer at the heterojunction with the AlGaN barrier layer. The conduction band splits into subbands in the well. Figure 1 illustrates the bottom energies of the three lowest subbands at the assumed 2DEG density of 7.4×10^{12} cm^{-2}. This density corresponds to polarization and piezoelectric charges of 1.02×10^{13} cm^{-2} and fits the experimental data [22].

A three-subband model is used to calculate the electron–phonon scattering rates. No impurity scattering is considered. The direct two-electron collisions are ignored in order not to mask the concurrent effect caused by the exchange of two-electron energies and momenta during the LO-phonon-assisted scattering event. The hot-phonon decay into other vibrations is treated in the hot-phonon lifetime approximation [21]. No dependence of the lifetime on hot-phonon mode occupancy is taken into account.

The 2DEG channel is subjected to the electric field E applied in the channel plane. The hot-electron distribution function is extracted from the Monte Carlo simulation. The result at E = 8 kV/cm is shown in Fig. 1 (inset, squares). The Fermi–Dirac function (solid red curve) fits the simulation data and suggests that the hot-electron temperature approximation is acceptable. The electron temperature of T_e = 440 K is extracted in this way. The fitting confirms the statement that the hot phonons support the temperature approximation in the GaN-based 2DEG channels [18, 19] – the phonon-assisted intense energy exchange among the hot electrons together with a weak contribution of acoustic phonons tend to form an almost isolated hot subsystem characterised with its own temperature. The results of the Monte Carlo simulation and the fitting provide the hot-electron temperature at any chosen electric field strength.

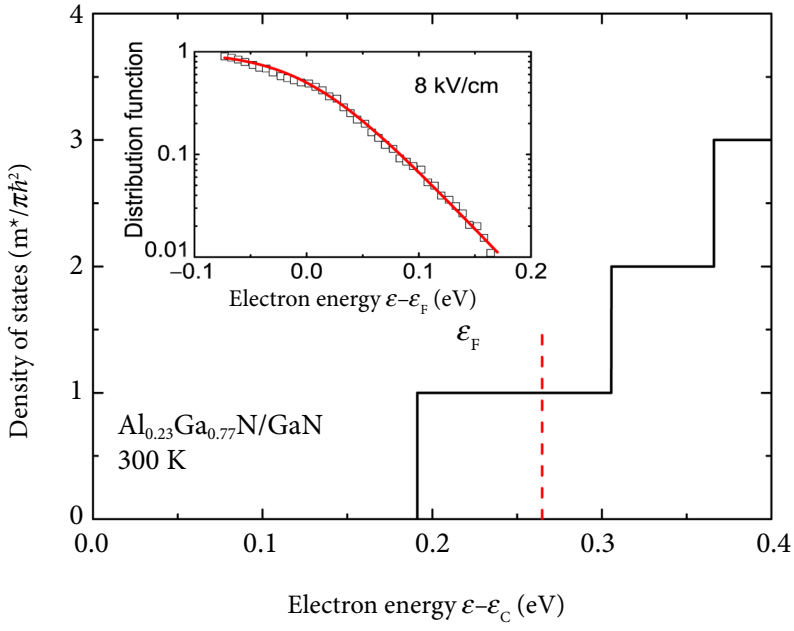

Fig. 1. Density of states for subbands in $Al_{0.23}Ga_{0.77}N$/GaN at temperature of 300 K. Red online dashed line stands for the Fermi energy. Inset illustrates the electron distribution function in the lowest subband at electric field of 8 kV/cm: the Fermi–Dirac approximation at hot-electron temperature of 440 K (red online curve) fits the results of Monte Carlo simulation (squares).

3. Additional correlation

The tensor of the additional correlation $\Delta_{\alpha\beta}$ enters the fluctuation–diffusion relation [7]

$$S_{\alpha\beta} = D_{\alpha\beta} + D_{\beta\alpha} - \Delta_{\alpha\beta}, \tag{1}$$

where $S_{\alpha\beta}$ is the spectral intensity of velocity fluctuations, $D_{\alpha\beta}$ is the tensor component of the electron diffusion coefficient.

The hot-electron temperature approximation for an isotropic channel yields simple expressions for the tensor components of the additional correlation $\Delta_{||}$ in the current direction and $\Delta_{\perp}$ in the transverse direction, respectively [2, 20]:

$$\Delta_{||}(\omega) = -\frac{D_{\perp}}{1+\omega^2\tau_T^2}\left(\frac{\sigma_{||}}{\sigma}-1\right)\left[\frac{T_e}{2(T_e-T_0)}\left(\frac{\sigma_{||}}{\sigma}-1\right)-\frac{\partial\ln\sigma}{\partial\ln T_e}\right], \tag{2}$$

$$\Delta_{\perp}(\omega) = 0,$$

where T_e is the electron temperature, $\sigma(T_e)$ and $\sigma_{||}(T_e)$ are the temperature dependent static and differential conductances, $\partial\ln\sigma/\partial\ln T_e$ is the dimensionless function of electric sensitivity to electron heating, $D_{\perp}$ is the transverse diffusion coefficient, and τ_T is the temperature (energy) relaxation time. The frequency dependence is not important if $\omega\tau_T \ll 1$. The Ohm law leads to $\Delta_{||} = 0$ because $\sigma = \sigma_{||}$. The expression $(\sigma_{||}/\sigma - 1)$ is the measure of deviation from the Ohm law. The coefficient $D_{\perp}$ can be expressed in the standard way:

$$D_{\perp} = k_B T_e \sigma/(e^2 n), \tag{3}$$

where e is the elementary charge and n is the electron density.

The results of the Monte Carlo simulation provide sufficient data for estimating the additional correlation according to Eq. (2) at $\omega\tau_T \ll 1$. The electron temperature approximation together with the results of the simulation for the 3-subband model lead to $\partial\ln\sigma/\partial\ln T_e$ and $\sigma_{||}/\sigma - 1$ as functions of E shown in Fig. 2 for the assumed values of the hot-phonon lifetime: 100 fs (blue online dotted curves), 370 fs (black solid curves), and 3000 fs (red online dashed curves). The results demonstrate an essential dependence on the hot-phonon lifetime. The sensitivity $\partial\ln\sigma/\partial\ln T_e$ decreases and the factor $\sigma_{||}/\sigma - 1$ tends to saturation at high electric fields. The hot-phonon effect on $\partial\ln\sigma/\partial\ln T_e$ and $\sigma_{||}/\sigma - 1$ is best resolved at moderate electric fields. The effect is stronger if the lifetime is longer.

Expression (3) is used to obtain the $D_{\perp}(E)$ dependence illustrated in Fig. 3, where D_0 is the diffusion coefficient at equilibrium. The non-ohmic transport means that the conductance σ decreases when the electric field and the electron temperature T_e increase (Fig. 2). As a result, the transverse diffusion coefficient increases (until the deviation from the Ohm law is weak), reaches the maximum value, and decreases as the electric field continues increasing. A longer hot-phonon lifetime supports

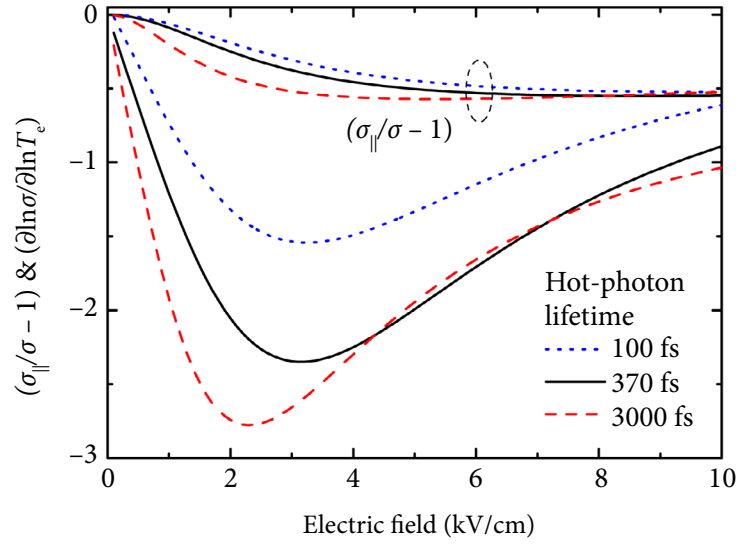

Fig. 2. Dependence of the steady-state electric sensitivity $\partial\ln\sigma/\partial\ln T_e$ and the measure of non-ohmic behaviour $\sigma_{\|}/\sigma - 1$ on the electric field obtained from the analysis of Monte Carlo results for the model shown in Fig. 1 for three values of hot-phonon lifetime: 100 fs (blue online dotted curve), 370 fs (solid black curve), and 3000 fs (red online dashed curve).

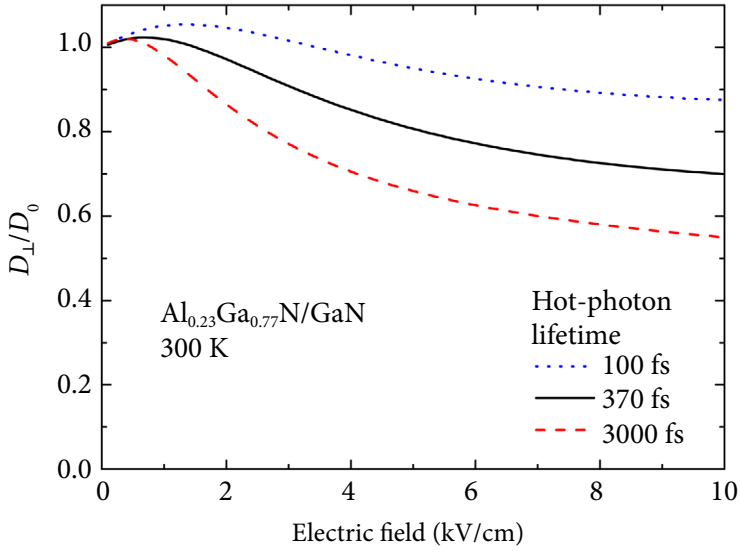

Fig. 3. The coefficient of steady-state transverse diffusion for the $Al_{0.23}Ga_{0.77}N/GaN$ model at 300 K based on the Monte Carlo simulation for three assumed values of hot-phonon lifetime: 100 fs (blue online dotted curve), 370 fs (solid black curve), and 3000 fs (red online dashed curve).

a stronger deviation from the Ohm law, and, consequently, the maximum of $D_{\perp}$ forms at a lower electric field (red online dashed curve). The diffusion coeffcient $D_{\perp}(E)$ decreases when the non-ohmic behaviour prevails over the increase in the electron temperature T_e.

Figure 4 shows the additional correlation coefficient $\Delta_{\|}$ estimated according to Eq. (2) at low frequencies, $\omega\tau_T \ll 1$. It is zero at the thermal equilibrium and slowly increases with the electric field E as long as the deviation from the Ohm law remains unimportant. The maximum forms in the combined action of the transverse diffusion $D_{\perp}$, the non-ohmic transport $\sigma_{\|}/\sigma - 1$, and the electric sensitivity $\partial\ln\sigma/\partial\ln T_e$. The hot-phonon effect is evident – the additional correlation $\Delta_{\|}$ is higher when a longer hot-phonon lifetime is assumed.

4. Discussion

Let us compare the results based on simulation with those available from the experiment [20, 23]. The experimental results on noise and transport for an $Al_{0.15}Ga_{0.85}N/GaN$ structure with a 2DEG channel were treated in the electron temperature approximation at 80 K ambient temperature [23], and the additional correlation $\Delta_{\|}$ was estimated according to Eq. (2) [20]. The result is illustrated in Fig. 4 (open circles). A high value of $\Delta_{\|}$ at an electric field of 3 kV/cm is not consistent with the model

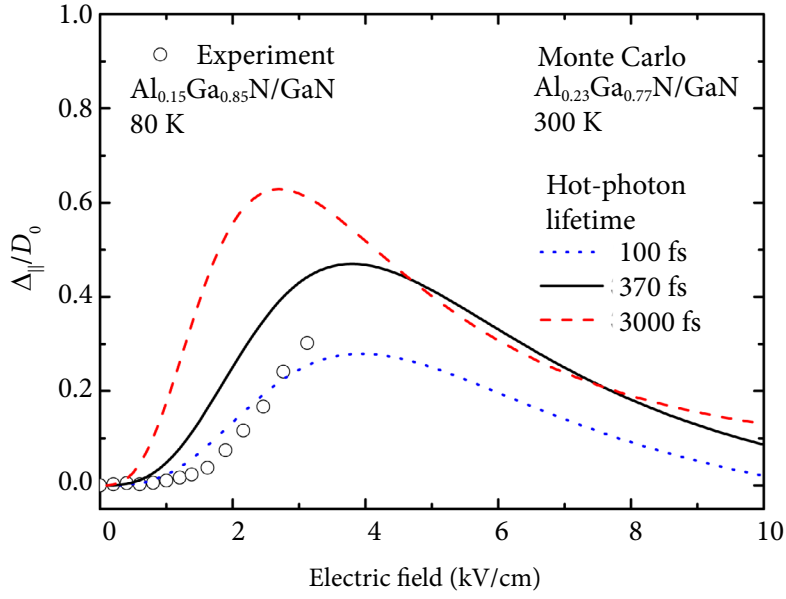

Fig. 4. The coefficient of additional correlation in the electron temperature approximation for the $Al_{0.23}Ga_{0.77}N/GaN$ model at 300 K based on the Monte Carlo simulation for three assumed values of hot-phonon lifetime: 100 fs (blue online dotted curve), 370 fs (solid black curve), and 3000 fs (red online dashed curve). Open circles stand for experimental data at 80 K for the $Al_{0.15}Ga_{0.85}N/GaN$ structure [20].

of direct two-electron collisions treated in terms of the screened Coulomb interaction of the involved electrons [2]. This interaction is known to decrease rapidly as the electric field increases; the associated effects can be ignored at electric fields above 2 kV/cm in GaN [24]. The Monte Carlo technique was also used for estimating the additional correlation in doped GaAs in the electron temperature approximation for the model of the dominant screened Coulomb interaction of two electrons [25]. The electron density was high enough for a considerable effect of the two-electron collisions on the electron transport. The model was fitted to the experimental data, and the required functions $T_e(E)$, $\sigma(T_e)$ and $\sigma_{||}(T_e)$ were extracted. The values of $\Delta_{||}$ obtained according to Eq. (2) from the simulation [25] were an order of magnitude lower than those extracted from the experiment [20] in the same approximation.

The additional correlation (Fig. 4, open circles) obtained according to Eq. (2) from the experimental data on the $Al_{0.15}Ga_{0.85}N/GaN$ structure can be associated with the proposed new source of the additional correlation due to the hot-phonon-assisted interaction [8]. Our Monte Carlo simulation includes the hot-phonon effects while the concurrent direct two-electron collisions are ignored. This opens a possibility to propose the hot-phonon mechanism [8] for an interpretation of the experimental data on the additional correlation [20]. The comparable values for $\Delta_{||}$ are obtained from the simulation (Fig. 4, curves) and the experiment (open circles) when the values for hot-phonon lifetime are close: the lifetime values of 350 fs and 370 fs have been estimated for the 2DEG in the $Al_{0.15}Ga_{0.85}N/GaN$ [19] and $Al_{0.23}Ga_{0.77}N/GaN$ structures [22], respectively. Note that the lifetime is almost independent of the ambient temperature in the $Al_{0.15}Ga_{0.85}N/GaN$ channels [26]. On the other hand, the experiment shows that the lifetime decreases as the hot-electron temperature increases in $Al_{0.23}Ga_{0.77}N/GaN$ [22].

5. Summary

The additional correlation of electron velocities is considered in the hot-electron temperature approximation for the undoped $Al_{0.23}Ga_{0.77}N/GaN$ structure with the two-dimensional electron gas subjected to the electric field applied in the plane of electron confinement. The quantum well model is obtained through the solution of the Schrödinger–Poisson equations. The electron–phonon scattering is considered in the framework of the 3-subband model. The hot-phonon decay is treated in terms of the hot-phonon lifetime. The direct two-electron collisions are ignored in order not to mask the concurrent effect caused by the hot-phonon-assisted two-electron scattering events. The hot-electron energy distribution and transport are simulated by the Monte Carlo technique. The electron temperature approximation is found applicable and is used to estimate the longitudinal tensor component of the additional correlation. The simulated highest values of the additional correlation are in a reasonable agreement with the experimental data for a similar $Al_{0.15}Ga_{0.85}N/GaN$ structure.

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KARŠTŲJŲ FONONŲ PALAIKOMA PAPILDOMA KORELIACIJA $Al_{0,23}Ga_{0,77}N$/GaN DARINYJE

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Santrauka

Išnagrinėtas karštųjų fononų vaidmuo sukuriant papildomą elektronų greičių koreliaciją $Al_{0,23}Ga_{0,77}N$/GaN darinyje su dvimatėmis elektronų dujomis, veikiamomis stipriu elektriniu lauku, sudarytu dvimatės kvantinės protakos plokštumoje. Karštaisiais fononais įprasta vadinti išilginius optinius fononus, kuriuos išspinduliuoja karštieji elektronai taip atsikratydami savo perteklinės energijos. Kaupdamiesi dvimatėje protakoje, karštieji fononai trukdo elektronams judėti ir dalyvauja sukuriant papildomą koreliaciją. Šrėdingerio ir Puasono lygčių sistemos skaitmeninis sprendimas panaudotas sudarant juostų sandaros ir elektronų sklaidos modelį, kuris sprendžiamas Monte Karlo metodu. Papildomos koreliacijos tenzoriaus sandas elektrinio lauko kryptimi įvertinamas karštųjų elektronų temperatūros artinyje. Parodyta, kad ilgesnės karštųjų fononų pusėjimo trukmės lemia reikšmingesnę papildomą koreliaciją. Skaitmeninis įvertinimas neblogai dera su eksperimentiniais panašaus darinio tyrimo rezultatais.