Spherical Harmonics Solver for Coupled Hot-Electron–Hot-Phonon System

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***Abstract*—In polar semiconductors with intensive electron–optical-phonon interaction excess energy of non-equilibrium (hot) electrons, supplied by the external electric field, is transferred to longitudinal optical (LO) phonons. LO phonons are displaced from equilibrium with the thermal bath, and hot-phonon effects take place. The kinetics of such a non-equilibrium electron/optical-phonon system is described by two coupled non-linear Boltzmann-type equations for the non-equilibrium electron and LO phonon distribution functions. Here, to our knowledge for the first time, we present a spherical harmonics expansion (SHE) method for the coupled system for electrons and LO phonons. The nonlinear system of coupled equations is solved with a Gummel type iterative scheme and the Newton-Raphson method. Simulation results are verified against a Monte Carlo model and good agreement is obtained. Hot phonon effects increase the mean energy of electrons and decrease the drift velocity.**

I. Introduction

Non-equilibrium distributions of quasi-particles can be relatively easy induced in semiconductor materials under the action of external electric fields or optical excitation [1]. The energy obtained by the electrons from an external excitation is transferred via lattice vibrations to the remote heat sink. Hot electron scattering by acoustic phonons is almost elastic and excess electron energy is mainly dissipated through the emission of optical phonons. The spectrum of generated optical phonons is defined by energy and momentum conservation during the electron-phonon scattering event. The occupation of phonon modes in those parts of the Brillouin zone, where the electron-phonon interaction is strongest, is displaced from the equilibrium Bose distribution. The electronically active non-equilibrium phonons are called hot phonons.

The influence of hot phonons on steady state electron transport under strong external electrical fields is widely investigated [1], [2]. Hot phonons are recognized as the main reason of slow energy relaxation of photoexcited electrons in AlGaAs/GaAs quantum wells [3]. During the last decade the influence of hot phonons on high frequency performance of GaN-based heterostructure field-effect transistors (HEMT's) was intensively investigated. The buildup of non-equilibrium phonons accelerates degradation of power devices, and limits the high frequency performance of transistors [4], [5].

The standard approach of theoretical treatment for such a coupled hot-electron–hot-phonon system is the Monte Carlo method [6], [7]. It is fast in implementation and requires no assumptions on the form of the distribution functions. However, the main disadvantage of the Monte Carlo method hides in it's transient and stochastic nature: it takes prohibitive amounts of computational time to achieve results within reasonable accuracy in case of low currents in the device or in systems with different time scales. To overcome this difficulty deterministic methods are used [8], [9].

II. Theory

The kinetics of the non-equilibrium electron/optical-phonon system is described by two coupled nonlinear Boltzmann-type equations for the electron $f(\vec{k},t)$ and optical phonon $n(\vec{q},t)$ distribution functions. The kinetic equation for the electron distribution function has the form:

$$\frac{\partial f(\vec{k},t)}{\partial t} - \frac{e}{\hbar}\vec{E}\nabla_k f(\vec{k},t) + \mathrm{I}_k[f] + \Pi_k^{(\mathrm{lo})}[f,n] = 0, \quad (1)$$

here e is the positive electron charge, $\hbar$ the Planck constant, $\vec{E}$ the applied electric field, operator $\mathrm{I}_k[f]$ describes the electron interaction (scattering) with acoustic phonons, and operator $\Pi_k^{(\mathrm{lo})}[f,n]$ the electron interaction (scattering) with non-equilibrium longitudinal optical phonons. The kinetic equation for the optical-phonon distribution function has the form:

$$\frac{\partial n(\vec{q},t)}{\partial t} + \mathrm{I}_q^{(\mathrm{th})}[n] + \Pi_q^{(\mathrm{el})}[n,f] = 0, \quad (2)$$

where the operator $\mathrm{I}_q^{(\mathrm{th})}[n]$ represents decay of the optical phonons into other modes of crystal lattice vibrations (thermal bath), and $\Pi_q^{(\mathrm{el})}[n,f]$ describes phonon net generation by electrons. The coupling is introduced through the optical phonon scattering term in the electron Boltzmann equation, and the optical phonon net generation rate by electrons in the Boltzmann equation for phonons. We proceed with the investigation of the stationary system and the time derivatives in (1), (2) are skipped.

The deterministic solver discussed in the present paper is based on the spherical harmonics expansion method [10]. The electron distribution function is expanded on equienergy surfaces and the generalized electron distribution function is introduced:

$$g(\epsilon,\theta_k) = \sum_l g_l(\epsilon)Y_l(\theta_k) = f(\epsilon,\theta_k)Z_{\mathrm{el}}(\epsilon), \quad (3)$$

where $Z_{\mathrm{el}}(\epsilon) = 2/(2\pi)^3 k^2 dk/d\epsilon$ is the (reduced) density of states for electrons, and $Y_l(\theta_k)$ the l-th spherical harmonic

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assuming rotational symmetry w.r.t. the electric field. The electron transport equation (1) is expanded in the same way as the distribution function and balance equations for the coefficients $g_l(\epsilon)$ are obtained. The expansion in spherical harmonics of the drift term in (1) is described in [10].

The scattering term of the Boltzmann transport equation consists of two parts, out-scattering and in-scattering:

$$\Pi_k^{(\mathrm{lo})}[f,n] = \frac{V_0}{(2\pi)^3}\sum_\nu \int \{W^\nu_{\mathrm{out}}(n,\vec{k},\vec{k'})f(\vec{k}) - W^\nu_{\mathrm{in}}(n,\vec{k'},\vec{k})f(\vec{k'})\}d^3k'. \tag{4}$$

Here summation is performed over different scattering mechanisms $W^\nu(n,\vec{k},\vec{k'})$. Expansion in spherical harmonics of elastic scattering by acoustic phonons is described in [8], and we will focus on expansion of polar optical scattering in case of a non-equilibrium phonon distribution. In general, the optical phonon scattering rate can be expressed as the product of the interaction function $C^\nu(n,\epsilon,\epsilon',\theta_k,\theta_{k'})$ and Dirac delta function for energy conservation:

$$W^\nu(n,\vec{k},\vec{k'}) = C^\nu(n,\epsilon,\epsilon',\theta_k,\theta_{k'})\delta(\epsilon-\epsilon'\mp\hbar w(\epsilon,\epsilon',\theta_k,\theta_{k'})). \tag{5}$$

The upper sign stands for phonon emission and the lower for absorption. In case of scattering by longitudinal polar optical phonons in III-V semiconductors, usually the cubic approximation is used. Phonons are assumed to be dispersionless with constant energy $\hbar w_0$. The interaction function is anisotropic:

$$C^\nu(n,\epsilon,\epsilon',\theta_k,\theta_{k'}) = C_0\frac{1}{q^2}\left[n(\vec{q})+\frac{1}{2}\pm\frac{1}{2}\right]. \tag{6}$$

Here C_0 is the interaction constant. In our case phonons are assumed to be driven out of equilibrium, and the phonon distribution function depends on the phonon wave-vector. For the sake of brevity we will discuss only phonon absorption and the case of phonon emission is similar. After the expansion of the generalized electron and phonon distribution functions in spherical harmonics, the income term for LO phonon absorption is expressed as:

$$S^{ll'}_{\mathrm{in}}(\epsilon) = \frac{1}{2}Z_{\mathrm{el}}(\epsilon)C_0\sum_r K^{ll'r}_{\mathrm{in}}(\epsilon,\epsilon-\hbar w_0), \tag{7}$$

with:

$$K^{ll'r}_{\mathrm{in}}(\epsilon,\epsilon') = \int\int \frac{n_r(q)}{q^2}Y_l(\theta_k)Y_{l'}(\theta_{k'})Y_r(\theta_q)d\Omega_k d\Omega_{k'}, \tag{8}$$

where $n_r(q)$ is r-th spherical harmonic of the phonon distribution function. For the outcome term we get:

$$S^{ll'}_{\mathrm{out}}(\epsilon) = \frac{1}{2}Z_{\mathrm{el}}(\epsilon+\hbar w_0)C_0\sum_r K^{ll'r}_{\mathrm{out}}(\epsilon,\epsilon+\hbar w_0), \tag{9}$$

with:

$$K^{ll'r}_{\mathrm{out}}(\epsilon,\epsilon') = \int\int \frac{n_r(q)}{q^2}Y_l(\theta_k)Y_{l'}(\theta_k)Y_r(\theta_q)d\Omega_k d\Omega_{k'}. \tag{10}$$

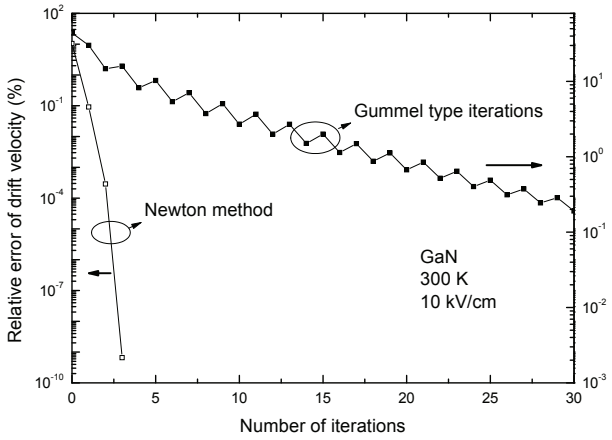


Fig. 1. Relative error of the electron drift velocity versus the number of iterations: closed rectangles- Gummel type iterations, open rectangles- Newton method.

The spherical harmonics expansion of the scattering term for the electron Boltzmann transport equation is given by:

$$\sum_{l'} S^{ll'}_{\mathrm{out}}(\epsilon)g_{l'}(\epsilon) - \sum_{l'} S^{ll'}_{\mathrm{in}}(\epsilon)g_{l'}(\epsilon-\hbar w_0). \tag{11}$$

The Boltzmann equation for the LO-phonon distribution is usually solved in the relaxation time approximation under assumption of dispersionless LO phonons with zero group velocity:

$$\Pi_q^{(\mathrm{th})}[n] = \frac{n(\vec{q})-n_{\mathrm{eq}}}{\tau_{\mathrm{ph}}}. \tag{12}$$

Here n_{eq} stands for the equilibrium Bose distribution with the lattice temperature (temperature of the thermal bath), and τ_{ph} is the non-equilibrium phonon decay time. Coupling with the electron system is expressed as:

$$\Pi_q^{(\mathrm{el})}[n,f] = 2\sum_{\vec{k}}\left[W_{\mathrm{abs}}(n,\vec{k},\vec{q}) - W_{\mathrm{em}}(n,\vec{k},\vec{q})\right]f(\vec{k}), \tag{13}$$

where $W_{\mathrm{abs}}(n,\vec{k},\vec{q})$ stands for optical phonon absorption by electrons (phonon annihilation) and $W_{\mathrm{em}}(n,\vec{k},\vec{q})$ for optical phonon emission by electrons (phonon generation); and both depend on the phonon distribution function.

After the expansion of the phonon transport equation into spherical harmonics and introduction of the generalized phonon distribution function:

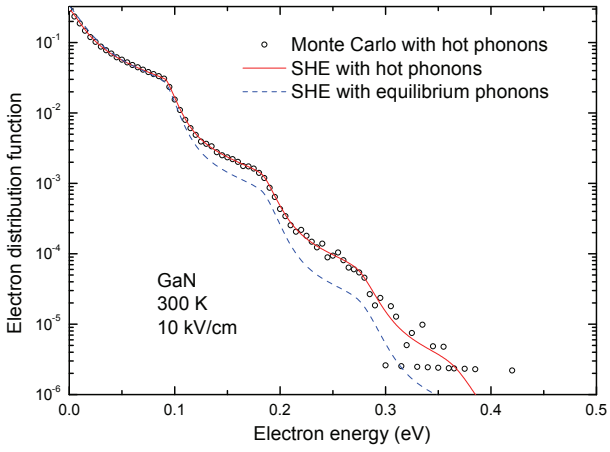
$$p(q,\theta_q) = \sum_r p_r(q)Y_r(\theta_q) = n(q,\theta_q)Z_{\mathrm{ph}}(q), \tag{14}$$

with $Z_{\mathrm{ph}}(q) = q^2/(2\pi)^3$, we get for the relaxation term:

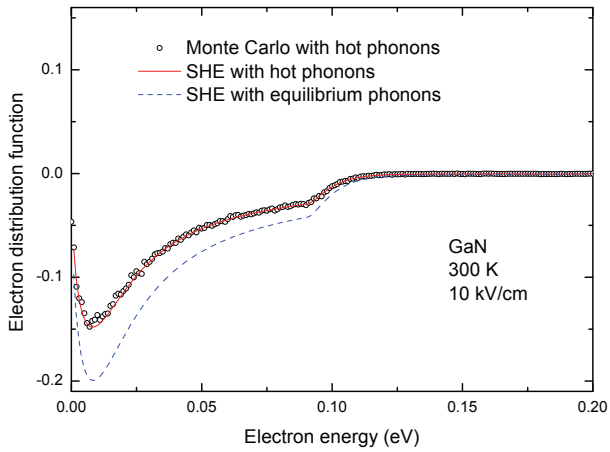
$$\frac{p_r(q)-p^0_{\mathrm{eq}}\delta_{r,0}}{\tau_{\mathrm{ph}}}, \tag{15}$$

with $p^0_{\mathrm{eq}} = Y_0 p_{\mathrm{eq}}$.

The coupling term (13) consists of two parts: phonon annihilation (absorption) and generation (emission). After expansion of both generalized distribution functions (3), (14),

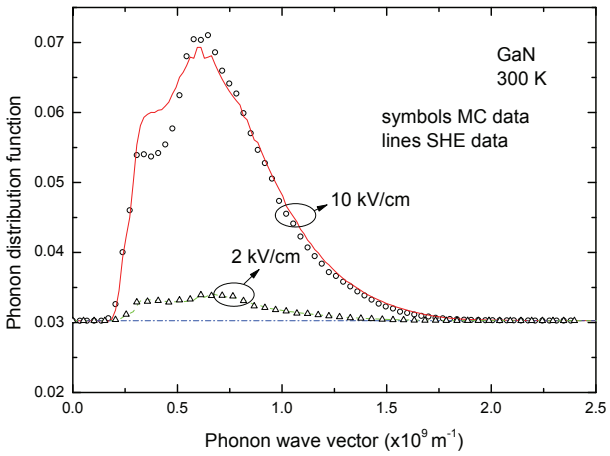


(a)

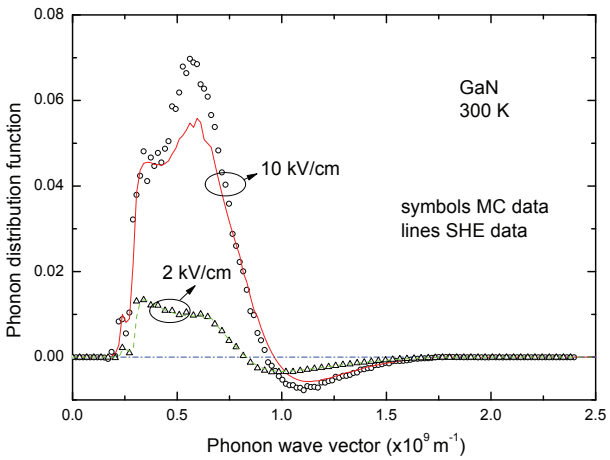


(b)

Fig. 2. Zeroth (a) and first (b) order harmonics of the electron distribution function for GaN at 10 kV/cm. Solid line- SHE results with hot phonons; dashed line- SHE results with equilibrium phonons; symbols- Monte Carlo simulation with hot phonons.



(a)



(b)

Fig. 3. Zeroth (a) and first (b) order harmonics of the phonon distribution function for GaN. 10 kV/cm: solid line- SHE results, open circles- Monte Carlo data; 2 kV/cm: dashed line- SHE results, and open triangles- Monte Carlo data. Dash-dotted line shows the equilibrium distribution.

the absorption term is expressed as:

$$A_r(q) = C_0 \frac{m_{\rm el}}{\hbar^2 q^3} \sum_{l,r'} \int_0^\infty \frac{1}{k} g_l(\epsilon) p_{r'}(q) I_{lrr'}(\epsilon, q) d\epsilon, \quad (16)$$

with:

$$I_{lrr'}(\epsilon, q) = \int \delta \left(\cos(\theta_{kq}) - \frac{q}{2k} - \frac{m_{\rm el} w_0}{\hbar k q} \right) \times Y_l(\theta_k) Y_r(\theta_q) Y_{r'}(\theta_q) d\Omega_k d\Omega_q. \quad (17)$$

For the emission term a similar expression can be obtained. The box integration method is used to discretize the balance equations for $g_l(\epsilon)$ and $p_r(q)$. In case of the electron transport equation a staggered grid is used.

III. Model and Results

As a model system, bulk wurtzite GaN at 300 K lattice temperature is selected, where the longitudinal optical (LO) phonon energy is high and electron–LO-phonon interaction is intense at high electric fields. Electron distribution functions and transport parameters are calculated within the one-valley spherical parabolic conduction band approximation.

In the range of electric fields under investigation electron scattering into the upper valleys is expected to be negligible. $10^{18}\mathrm{cm}^{-3}$ electron gas density is considered, and 1 ps LO phonon lifetime is used. Acoustic phonon scattering via deformation potential and LO phonon polar scattering (cubic approximation) are taken into account. The electron effective mass and scattering parameters are the same as in [11]. Eight spherical harmonics are considered for electrons and two for phonons.

The system of equations describing the non-equilibrium electron/optical-phonon system is nonlinear in electron scattering due to the LO phonon term in (1) and phonon net generation by electrons in (2). To obtain a solution of such a nonlinear system of equations, iterative schemes should be used. We have implemented both the Gummel type iterative scheme and the full Newton-Raphson method.

In the Gummel scheme first the Boltzmann transport equation for electrons is solved using the equilibrium phonon

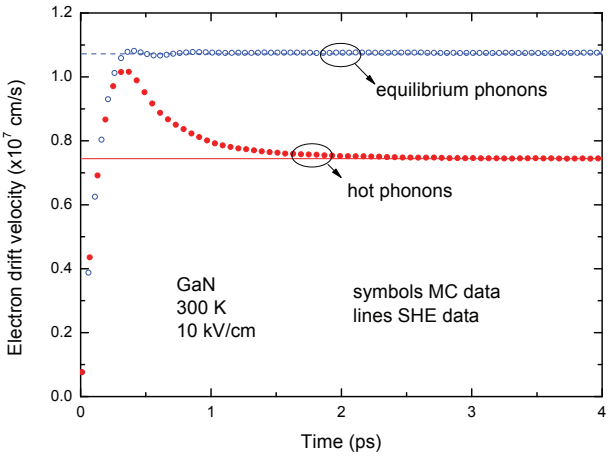


Fig. 4. The time dependent electron drift velocity for the first 4 ps of electron motion in GaN at 10 kV/cm: open circles stand for Monte Carlo data with equilibrium phonons and closed circles with hot phonons. Lines represent stationary values obtained by the SHE solver.

distribution. the resultant electron distribution is used to calculate the net phonon generation and from it the new phonon distribution. The new phonon distribution is used again in the electron transport equation and subsequent iterations yield the final self-consistent solutions for the electron and phonon distribution functions. In addition, a Newton-Raphson method for the full system of coupled nonlinear equations has been implemented. Fig. 1 shows the convergence behavior for both methods. In case of the full Newton-Raphson method quadratic convergence is obtained and three or four iterations are sufficient to achieve convergence (Fig. 1, open squares).

Semiclassical ensemble Monte Carlo simulation [7] is performed for the wurtzite GaN using the same material parameters, band structure and scattering mechanisms to verify the results of the spherical harmonics solver. The Monte Carlo procedure takes into account each LO-phonon generation/annihilation event due to their interaction with the electrons (LO phonon emission/absorption). The resultant histogram is used to calculate the non-equilibrium (hot) phonon distribution. Figure 2 presents zeroth (a) and first (b) order harmonics of the electron distribution function, and Figure 3 for the LO phonon distribution. Good agreement with Monte Carlo results is obtained for both zeroth and first order harmonics of the electron distribution function. Hot phonon effects increase the mean energy of the system and decrease the drift velocity (solid and dashed lines in Fig. 2 and Fig. 4).

The stronger the applied electric field is, the bigger is the displacement of the phonon distribution from equilibrium (compare solid, dashed and dash-dotted lines in Fig. 3). Good agreement with Monte Carlo results is obtained for both zeroth and first order harmonics of the phonon distribution function at 2 kV/cm electric field. The discrepancy between Monte Carlo and SHE results for the phonon distribution at 10 kV/cm may be attributed to stronger anisotropy of the distribution function at a stronger electric field.

Figure 4 shows Monte Carlo simulation results for the electron drift velocity during the first 4 ps of electron motion. It takes 2.5 ps for the non-equilibrium phonon distribution to build up and for the electron drift velocity to reach its stationary value (closed circles in Fig. 4), whereas the SHE simulator gives the stationary value of electron drift velocity directly (solid line in Fig. 4).

IV. Conclusion

Spherical harmonics expansion method for the coupled system for electrons and LO phonons is presented. In case of the full Newton-Raphson method quadratic convergence is obtained. Good agreement with a consistent Monte Carlo model is obtained. Hot phonon effects increase the mean energy of electrons and decrease the drift velocity.

Acknowledgments

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