TIME-DEPENDENT ANALYSIS OF THE COUPLED HOT-CARRIER–HOT-PHONON BOLTZMANN EQUATIONS

L. Hlou, J. C. Vaissiere, J. P. Nougier, L. Varani, P. Houlet
Centre d'Electronique de Montpellier,
Université Montpellier II, 34095 Montpellier Cedex 5, France

L. Reggiani
Dipartimento di Fisica, Università di Modena,
Via Campi 213/A, 41100 Modena, Italy

M. Fadel
Faculté des Sciences d'Agadir,
Agadir, Morocco

P. Kocevar
Institut für Theoretische Physik, Universität Graz,
Universitätsplatz 5, A-8010 Graz, Austria

Abstract

We present a detailed investigation of the transient transport regime in InP at room temperature based on an original method to solve numerically the coupled hot-phonon–hot-carrier time-dependent Boltzmann Equations. The method enables a study of the perturbation of the phonon distribution function induced by hot carriers and the corresponding modifications of the carrier distribution function. As a consequence of the high numerical accuracy of the method, the time behavior of the main transport parameters can be investigated in great detail.

I. INTRODUCTION

The influence of hot phonons on carrier transport parameters in polar semiconductors has been theoretically studied in relation with non-ohmic transport [1], laser photoexcitation [2], and noise phenomena [3]. As concerning the transient regime, the influence of non-equilibrium phonons has been recently investigated in Ref. [1] by means of a Monte Carlo simulation in n-type GaAs. However, a detailed and extensive investigation of the effect of a non-equilibrium phonon population on the carrier distribution function (CDF), phonon distribution function (PDF) and main transport parameters is still lacking in the literature. In this communication we present a detailed analysis of the transient transport regime in InP at room temperature under spatially homogeneous conditions. We take advantage of an original method to solve numerically the coupled hot-phonon–hot-carrier Boltzmann Equations (BE) in the time domain. The method enables a study of the perturbation of the longitudinal-optical (LO) PDF induced by hot carriers and the corresponding modifications of the CDF. As a consequence, the time behavior of the main transport parameters can be investigated in great detail with an accuracy far beyond other existing numerical methods.

II. THE SYSTEM OF COUPLED EQUATIONS

To take into account the perturbation of the LO phonon population, it is convenient to write the time dependent BE for the CDF $f(\mathbf{k},t)$ in the following form:

$$\frac{\partial f(\mathbf{k},t)}{\partial t} = \hat{C}_{nc} f(\mathbf{k},t) + \hat{C}_{po} f(\mathbf{k},t) - \frac{f(\mathbf{k},t)}{\tau_{po}(\mathbf{k})} \tag{1}$$

Here $\hat{C}_{nc}$ is the operator including the external field term and collisions with acoustic deformation potential, piezoelectric, impurity, intervalley and intravalley non-polar optical phonon scatterings; $\hat{C}_{po}$ is the input term for polar-optic LO-phonon scattering and $[f(\mathbf{k},t)/\tau_{po}(\mathbf{k})]$ the output term, $1/\tau_{po}(\mathbf{k})$ being the polar-optic scattering rate. The detailed expressions for the above operators

can be found in Ref.[4]. We remark that $\hat{C}_{po}$ and τ_{po} depend on the PDF and, as a consequence, Eq. (1) becomes non-linear since its solution requires the knowledge of the PDF.

The time dependent phonon BE gives the time variation of the PDF $N(\mathbf{q},t)$. This variation is the result of the balance between two terms: the former is associated with the phonon appearance and disappearance due to carrier emission and absorption and the latter is associated with the nonelectronic lattice relaxation of the phonons. Therefore, we write the phonon BE in the following form:

$$\frac{\partial N(\mathbf{q},t)}{\partial t} = \hat{C}_{ph}N(\mathbf{q},t) - \hat{D}_{ph}N(\mathbf{q},t) - \frac{[N(\mathbf{q},t) - N_L]}{\tau_L} \tag{2}$$

where $\hat{C}_{ph}$ and $\hat{D}_{ph}$ are the gain and loss operators related to emission and absorption of phonons by carriers, respectively, N_L is the thermal-equilibrium Bose-Einstein distribution and τ_L the non-electronic phonon relaxation time.

III. NUMERICAL SIMULATION

The main task is now to solve the system of coupled equations (1) and (2). To do that, we have devised the following procedure:

(i) The CDF and PDF at thermal equilibrium are introduced in Eqs. (1) and (2) thus calculating $[\partial f(\mathbf{k},t)/\partial t]_{t=0}$ and $[\partial N(\mathbf{q},t)/\partial t]_{t=0}$.

(ii) From the knowledge of these quantities we determine $f(\mathbf{k},\Delta t)$ and $N(\mathbf{q},\Delta t)$ by Taylor expansion.

(iii) The new CDF and PDF at time Δt are introduced in Eqs. (1) and (2) thus calculating $[\partial f(\mathbf{k},t)/\partial t]_{t=\Delta t}$ and $[\partial N(\mathbf{q},t)/\partial t]_{t=\Delta t}$.

(iv) From the knowledge of these quantities we determine $f(\mathbf{k},2\Delta t)$ and $N(\mathbf{q},2\Delta t)$.

(v) Steps (iii) and (iv) are iteratively repeated until the stationary regime is reached.

This selfconsistent procedure has been found to present some numerical problems. As a matter of fact, when solving the usual BE (not coupled with the phonon BE) the different operators which appear are independent of time: this enables their associated matrix to be calculated only at the beginning of the simulation. In the present case the operator associated with the LO-phonon interaction depends on the PDF, which is a time dependent quantity: therefore $\hat{C}_{po}$ must be recalculated at each time step. Furthermore, the inclusion of the equation for the time evolution of the PDF has been found to increase significantly the duration of the transient regime. This leads to the necessity of adopting some kind of optimization of the numerical algorithm in order to save computer time.

As concerning the carrier BE we notice that Eq. (1) can be written in matrix form as:

$$\left[\frac{\partial f}{\partial t}\right] = [C]_{nc}[f] + [C]_{po}[f] + \left[\frac{1}{\tau_{po}}\right][f] \tag{3}$$

where $[C]_{po}$ and $[1/\tau_{po}]$ are the matrices associated with the LO operator depending on time through the PDF, and $[C]_{nc}$ is the time-independent matrix associated with the operator $\hat{C}_{nc}$. The calculation of the first two matrices is the part of the program which requires most of the computer time. To try to avoid this problem we have verified that the increase in the time-duration of the transient is due to the slow time variation of the PDF. Therefore, we have calculated the time-dependent matrices ONLY when one value of $N(\mathbf{q},t)$ has undergone a significative variation (about 1 %).

As concerning the phonon BE, Eq. (2) can be written in the following form:

$$\frac{\partial N_i(t)}{\partial t} = \left[\sum_j E_{ij}f_j(t)\right] N_i(t) + \sum_j F_{ij}f_j(t) - \frac{N_i(t)}{\tau_L} + \frac{N_L}{\tau_L} \tag{4}$$

The coefficients E_{ij} and F_{ij} are independent of the CDF and therefore independent of time: this enables to calculate the matrices $[E]$ and $[F]$ only at the beginning of the simulation, thus saving a significant amount of computer time.

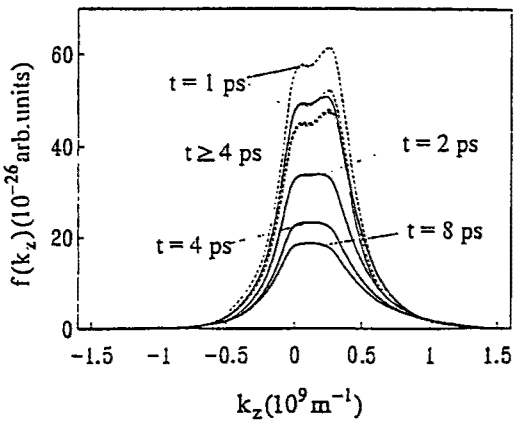

Fig. 1 - *Carrier distribution function* $f(k_z) = f(k_x = 0, k_y = 0, k_z)$ *along the electric field as a function of* k_z, *in the* Γ *valley of InP, for* $T_L = 300\ K$, $N_D = 10^{17}\ cm^{-3}$, $E = 10\ kV/cm$ *and the reported times. Solid lines: calculations taking into account hot-phonons; dashed lines: calculations assuming phonons to be at thermal equilibrium.*

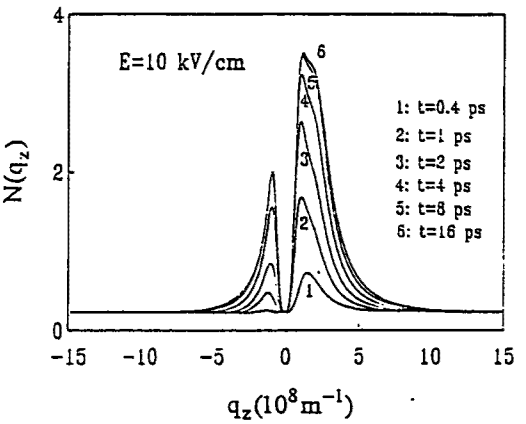

Fig. 2 - *Phonon distribution function* $N(q, \theta = 0)$ *along the electric field in InP, for* $T_L = 300\ K$, $N_D = 10^{17}\ cm^{-3}$, $E = 10\ kV/cm$ *and the reported times from the beginning of the transient.*

To evaluate the gain in computer time some tests have been performed on an IBM 3090. By using the optimization procedure here described we were able to reduce the CPU time of a typical simulation from 120 hours to about 6 hours, thus gaining a factor of about 20.

IV. RESULTS

The theory is applied to the case of n-type InP at a temperature $T_L = 300\ K$, a doping concentration $N_D = 10^{17}\ cm^{-3}$ and with the same material parameters as reported in the Appendix B of Ref. [4]. Two spherical and non-parabolic bands (one Γ and four equivalent L valleys) are taken into account. The simulation includes the following intra and intervalley scattering mechanisms: acoustic deformation potential (in elastic approximation), piezoelectric (in elastic approximation), polar optical, impurity (in Brooks-Herring model including a screened Coulomb potential) and non-polar optical intervalley. The LO-phonon relaxation time τ_L has been taken as 5.8 *ps*.

Figure 1 reports the CDF in the Γ valley, at different times from the beginning of the transient and for an abruptly applied electric field of 10 *kV/cm*. Since some time is required in order to perturb the PDF from its equilibrium value, for times shorter than 0.4 *ps* no significant difference is observed between the values of the CDF assuming phonons to be perturbed or at thermal equilibrium. For times longer than 0.4 *ps* the two CDF begin to differ one from each other, the difference becoming more evident at increasing times. We notice also that the presence of a non-equilibrium phonon population is responsible for an increase in the time duration of the transient.

Figure 2 reports the results for the PDF at different times from the beginning of the transient and for an electric field of 10 *kV/cm*. The appearance of the perturbation of the PDF is related to the displacement of the carriers in the high energy region [4]. At the beginning of the transient the CDF is displaced under the action of the electric field; as a consequence the PDF develops a peak at small positive phonon wave-vectors associated with the phonons emitted by carriers at high energy. This peak progressively increases with time due to the enhanced LO-phonon emission by the carriers.

Figure 3 reports the results for the drift-velocity at three electric fields of 5, 10 and 20 *kV/cm*. For very short times ($\lesssim 0.4\ ps$) there is nearly no difference between the values of the drift-velocity obtained with and without hot-phonons. For an intermediate electric field of 10 *kV/cm*, a second overshoot is observed which is related to the perturbation of the PDF.

Figure 4 reports the results concerning the average carrier energy for the same electric fields

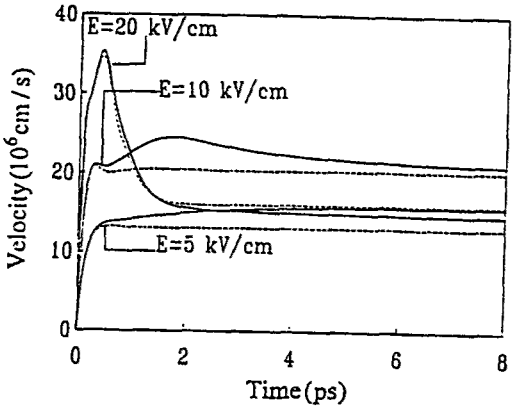

Fig. 3 - *Mean-carrier drift-velocity as a function of time in InP, for* $T_L = 300\ K$, $N_D = 10^{17}\ cm^{-3}$, *and the reported electric fields. The solid lines refer to calculations taking into account hot-phonons and the dashed lines to calculations obtained assuming phonons to be at thermal equilibrium.*

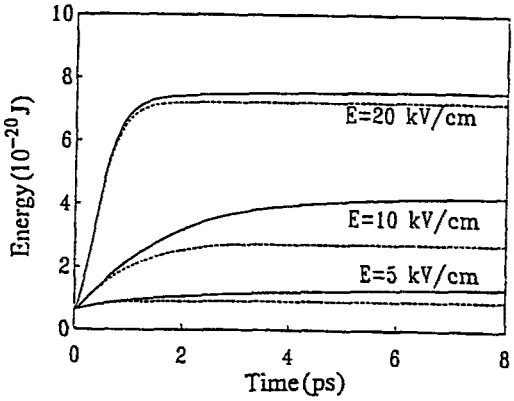

Fig. 4 - *Mean-carrier energy as a function of time in InP, for* $T_L = 300\ K$, $N_D = 10^{17}\ cm^{-3}$, *and the reported electric fields. The solid lines refer to calculations taking into account hot-phonons and the dashed lines to calculations obtained assuming phonons to be at thermal equilibrium.*

as in Fig. 3. Also in this case we observe that the presence of non-equilibrium phonons is found to be responsible for modifications in the transient regime. As already noticed for the case of the drift-velocity, these modifications appear after a time required for the perturbation of the PDF to take place.

V. CONCLUSIONS

We have presented a detailed investigation of the transient transport regime in InP at room temperature. We take advantage of a numerically extremely efficient method for solving the coupled hot-phonon–hot-carrier Boltzmann Equations in both the linear and non-linear regime. The accuracy of the method is particularly evident during the transient which is fundamental to the performances of high-frequency semiconductor devices. The non-linearity introduced by the phonon disturbance is responsible for a great complexity in looking for a solution of the whole problem and noticeable effort has been made in order to optimize the code and obtain a reasonable CPU time. Modifications of the transient regime at low and intermediate electric fields are observed.

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