Transient hot-electron transport in GaAs with a Γ-L-X band structure

1989 J. Phys.: Condens. Matter 1 407

(http://iopscience.iop.org/0953-8984/1/2/009)

J. Phys.: Condens. Matter 1 (1989) 407–418. Printed in the UK

Transient hot-electron transport in GaAs with a Γ–L–X band structure

M Liu†‡, D Y Xing†§ and C S Ting†

† Department of Physics and Space Vacuum Epitaxy Center, University of Houston, Houston, TX 77004, USA

‡ Department of Physics and Chemistry, Nanjing Institute of Technology, Nanjing, People's Republic of China

§ Department of Physics, Nanjing University, Nanjing, People's Republic of China

Received 24 June 1988, in final form 17 August 1988

Abstract. The method of non-equilibrium statistical operators developed by Zubarev has been extended to study transient hot-electron transport in many-valley semiconductors. A set of coupled evolution equations with memory effect are derived to determine the time-dependent drift velocities $v_\alpha(t)$, hot-electron temperatures $T_\alpha(t)$ and populations $N_\alpha(t)$ of various valleys under time-dependent electric fields. In the classical approximation these non-linear differential equations are applied to study the transient transport of GaAs with a Γ–L–X band structure under electric fields with several configurations:

(i) time-step;
(ii) rectangular time pulse;
(iii) high-frequency sinusoid.

Using the same set of parameters, our calculated results for $v_d(t) = \Sigma_\alpha N_\alpha(t) v_\alpha(t) / \Sigma_\alpha N_\alpha(t)$ compare quantitatively with those in Monte Carlo calculations.

1. Introduction

Current interest in studying the transport properties of conducting material with an ultra-small size has been stimulated with the development of submicrometre semiconductor devices (for a general review, see [1]). The features characterising carrier transport in semiconductors for a submicrometre scale can be very different from those obtained in the usual steady-state transport. These new features occur either when the semiconductor sample is submitted to a very fast time variation in the electric field or when the electric field is characterised by a small spatial scale. For an ultra-small sample the drift velocity v_d is time dependent and the measured current density $Nev_d(t)$ depends on the distance between the source and the drain. This transport property is very important and will govern the behaviour of a device. In the present paper, we shall study the transient drift velocity of electrons by submitting a GaAs sample to a time step or a time pulse configuration of electric field, or to a high-frequency sinusoidal electric field superimposed on an applied steady field.

Although several classical and quantum mechanical formulations for high-field transient transport have been proposed, in realistic calculation, one has to employ methods based on either the phenomenological Boltzmann equation in the relaxation time approximation [2] or the Monte Carlo simulation [3, 4]. Since an ensemble of electrons in a strong electric field is far from the equilibrium state, the method of non-equilibrium statistical operator (NSO) developed in [5] seems to be a useful tool for studying hot-electron transport in high electric fields. We have generalised this method to the steady-state hot-electron transport for both simple-band [6] and many-valley [7] semiconductors, as well as to the transient hot-electron transport for a single-valley semiconductor [8]. In this paper, we shall extend the NSO method to the study of transient hot-electron transport of many-valley semiconductors. Considering n-type GaAs with a Γ–L–X valley ordering, we shall derive a set of non-linear time-differential equations for momenta, energies and populations of various valleys, from which the drift velocities $v_\alpha(t)$, the electron temperatures $T_\alpha(t)$ and the populations $N_\alpha(y)$ ($\alpha \equiv \Gamma$, L, X) can be determined self-consistently as functions of time t and electric field $E(t)$. Using these equations, we shall calculate transient current waveform $I(t) = Nev_{\mathrm{d}}(t)$ with $v_{\mathrm{d}} = \Sigma_\alpha N_\alpha(t) v_\alpha(t)/N$ in various time-dependent electric fields. We show that the results obtained are in reasonable agreement with those of the Monte Carlo simulations.

In § 2 the Hamiltonian of a many-valley electron–phonon system in a time-dependent electric field is described. The NSO for a many-valley system is introduced to perform statistical averages over the centre-of-mass momenta, Hamiltonians and population operators in the non-equilibrium state. In § 3 a set of evolution equations with memory effect are derived to calculate the drift velocities, electron temperatures and populations of various valleys. In § 4 the explicit expressions for these non-linear differential equations in the classical approximation are given. In § 5, our formulation is applied to calculate the transient hot-electron transport in GaAs with a Γ–L–X valley structure in several time-dependent electric fields. The results are discussed and compared with those of the Monte Carlo calculations. The final section, § 6, contains a brief summary.

2. The non-equilibrium statistical operator method

We consider an ensemble of electrons in a semiconductor with an n-valley band structure in a time-dependent electric field $\boldsymbol{E}(t)$. The electrons are accelerated by the applied electric field and scattered by phonons, forming a transient flow of current. The total Hamiltonian of the system can be written in terms of the centre-of-mass variables and electron variables in the relative coordinates [9]:

$$H = H_{\mathrm{c}} + H_{\mathrm{e}} + H_{\mathrm{ph}} + H_{\mathrm{e\text{-}ph}} \tag{1}$$

where

$$H_{\mathrm{c}} = \sum_{\alpha=1}^{n} \left(\frac{\boldsymbol{P}_\alpha^2}{2N_\alpha m_\alpha} - N_\alpha e\boldsymbol{E} \cdot \boldsymbol{R}_\alpha \right)$$

$$H_{\mathrm{e}} = \sum_{\alpha=1}^{n} H_{\mathrm{e}\alpha}$$

$$H_{\mathrm{e}\alpha} = \sum_{k} \varepsilon_{\alpha k} c_{\alpha k}^{+} c_{\alpha k}$$

$$H_{\mathrm{ph}} = \sum_{q,\lambda} \Omega_{q\lambda} b_{q\lambda}^{+} b_{q\lambda}$$

$$H_{\text{e-ph}} = \sum_{\alpha,\gamma=1}^{n} \sum_{k,q,\lambda} M_{\alpha\gamma}(q,\lambda)(b_{q\lambda} + b^{+}_{-q\lambda})c^{+}_{\alpha,k+q}c_{\gamma,k}E_{\alpha\gamma}(k,q) + \text{HC}$$

with

$$E_{\alpha\gamma}(k,q) = \exp[(\boldsymbol{k}+\boldsymbol{q})\cdot\boldsymbol{R}_{\alpha} - \boldsymbol{k}\cdot\boldsymbol{R}_{\gamma}].$$

Here H_c is the centre-of-mass part of the Hamiltonian. $\boldsymbol{P}_\alpha$ and $\boldsymbol{R}_\alpha$ are the momentum and coordinate of the centre of mass respectively, for the αth valley, N_α is the population of electrons for the αth valley and m_α is the single-electron effective mass. $H_{e\alpha}$ is the free-electron Hamiltonian in the relative coordinate of the αth valley, and H_{ph} is the phonon Hamiltonian. $H_{\text{e-ph}}$ stands for the intra-valley ($\alpha=\gamma$) and inter-valley ($\alpha\neq\gamma$) electron–phonon interaction terms with $M_{\alpha\gamma}(q,\lambda)$ as the electron–phonon matrix elements. The electron–impurity and electron–electron interactions can easily be included in the present method [7], for simplicity, they are not considered here. The above Hamiltonian features the separations of H_c from $H_{e\alpha}$. The advantage of such variable separations is that the current ($\langle \boldsymbol{P}_\alpha\rangle \neq 0$) is carried only by the centre of mass, while electrons in the relative coordinates, which constitute n many-body systems, are not directly influenced by the electric field and do not carry current ($\Sigma_i\langle P_{\alpha i}\rangle = 0$). Since our approach depends on the separations of the centre of mass from the relative motions of electrons, the valleys of electrons must be assumed to be parabolic (isotropic or anisotropic).

The current density is defined as $I(t) = Nev_{\text{d}}(t)$ with $v_{\text{d}}(t) = \Sigma_\alpha n_\alpha(t)v_\alpha(t)$, where $v_\alpha(t)$ is the drift velocity of electrons for the αth valley, and $n_\alpha(t) = N(t)/N$ is the corresponding fraction of electron population. In order to study the transient behaviour of the current, one needs to investigate the equations of motion for operators $\boldsymbol{P}_\alpha$, $H_{e\alpha}$, N_α ($\alpha = 1, 2, \ldots, n$) and H_{ph}. According to the formula $\dot{\boldsymbol{P}} = -\text{i}[\boldsymbol{P}H]$, one obtains

$$\begin{aligned}
\dot{\boldsymbol{P}}_{\alpha x} &= N_\alpha eE - \text{i}\sum_{\gamma,k,q,\lambda}(k_x+q_x)M_{\alpha\gamma}(q,\lambda)(b_{q\lambda}+b^{+}_{-q\lambda})c^{+}_{\alpha,k+q}c_{\gamma,k}E_{\alpha\gamma}(k,q) + \text{HC} \\
\dot{H}_{e\alpha} &= -\text{i}\sum_{\gamma,k,q,\lambda}\varepsilon_{\alpha,k+q}M_{\alpha\gamma}(q,\lambda)(b_{q\lambda}+b^{+}_{-q\lambda})c^{+}_{\alpha,k+q}c_{\gamma,k}E_{\alpha\gamma}(k,q) + \text{HC} \\
\dot{N}_\alpha &= -\text{i}\sum_{\gamma,k,q,\lambda}M_{\alpha\gamma}(q,\lambda)(b_{q\lambda}+b^{+}_{-q\lambda})c^{+}_{\alpha,k+q}c_{\gamma,k}E_{\alpha\gamma}(k,q) + \text{HC} \\
\dot{H}_{\text{ph}} &= \text{i}\sum_{\alpha,\gamma}\sum_{k,q,\lambda}\Omega_{q\lambda}M_{\alpha\gamma}(q,\lambda)(b_{q\lambda}-b^{+}_{-q\lambda})c^{+}_{\alpha,k+q}c_{\gamma,k}E_{\alpha\gamma}(k,q).
\end{aligned} \tag{2}$$

The next step is to take the statistical average of operator Q (Q stands for $\dot{P}_{\alpha x}$, $\dot{H}_{a\alpha}$, $\dot{N}_\alpha$ and $\dot{H}_{\text{ph}}$) with respect to a time-dependent density matrix $\rho(t)$:

$$\langle\Omega\rangle = \text{Tr}[\rho(t)\Omega]. \tag{3}$$

Following to [5] and [8], we can write the NSO in the following form:

$$\rho(t) = \exp\left(-s(t,0) + \int_{-\infty}^{0}\text{d}t'\exp(\varepsilon t')\,\dot{s}(t+t',t')\right) \tag{4}$$

where

$$s(t,0) = \varphi(t) + \sum_{\alpha=1}^{n} \beta_\alpha(t) K_\alpha + \beta H_{\mathrm{ph}}$$
$$\varphi(t) = \ln\left[\mathrm{Tr}\left(\sum_{\alpha=1}^{n} -\beta_\alpha(t) K_\alpha - \beta H_{\mathrm{ph}}\right)\right] \tag{5}$$

with $K_\alpha = [H_{e\alpha} - \mu_\alpha(t) N_\alpha]$. Here $H_{e\alpha}$, N_α and H_{ph} are chosen as basis dynamic quantities, and their thermodynamically conjugate forces are $\beta_\alpha(t)$, $\beta_\alpha(t)\mu_\alpha(t)$ and β with $\beta_\alpha(t)$ and $\mu_\alpha(t)$ as the inverse of temperature and chemical potential for the αth valley, respectively, and β the inverse of temperature for the phonon system. From equation (5), we find that

$$\dot{s}(t,0) = \beta \dot{H}_{\mathrm{ph}} + \sum_{\alpha=1}^{n} [\beta_\alpha(t) \dot{K}_\alpha + \dot{\beta}_\alpha(t)(K_\alpha - \langle K_\alpha \rangle_t^1)] \tag{6}$$

$$\dot{s}(t,t') = \exp(\mathrm{i}Ht')\, \dot{s}(t,0) \exp(-\mathrm{i}Ht') \tag{7}$$

where $\langle K_\alpha \rangle_t^1 = \mathrm{Tr}[K_\alpha \rho_1(t)]$ with $\rho_1(t) = \exp[-s(t,0)]$ as the time-dependent quasi-equilibrium statistical operator corresponding to the isolated carrier distribution without electron–phonon interaction at the time t. It has been shown [5] that $\rho(t)$ defined in equation (4) satisfies Liouville's equation in the limit of $\varepsilon \to 0$ and can be used to describe the non-equilibrium transport process. Since the energy exchange rate between the electron and phonon systems is generally assumed to be small in hot-electron transport theory, we shall use the following perturbative expression for $\rho(t)$ to lowest order in $H_{\text{e-ph}}$ [6, 10]:

$$\rho(t) = \rho_1(t)\left[1 + \int_{-\infty}^{0} \mathrm{d}t' \exp(\varepsilon t') \int_0^1 \mathrm{d}\tau \left(\sum_{\alpha=1}^{n} \beta_\alpha(t+t') \dot{K}_\alpha(t', \mathrm{i}\tau) + \beta \dot{H}_{\mathrm{ph}}(t', \mathrm{i}\tau)\right)\right] \tag{8}$$

with

$$\dot{K}_\alpha(t', \mathrm{i}\tau) = \exp[-\tau s(t,0)] \exp(\mathrm{i}Ht') [\dot{H}_{e\alpha} + \mu_\alpha(t+t') \dot{N}_\alpha] \exp(-\mathrm{i}Ht') \exp[\tau s(t,0)] \tag{9}$$

$$\dot{H}_{\mathrm{ph}}(t, \mathrm{i}\tau) = \exp[-\tau s(t,0)] \exp(\mathrm{i}Ht') \dot{H}_{\mathrm{ph}} \exp(-\mathrm{i}Ht') \exp[\tau s(t,0)]. \tag{10}$$

In deriving the above perturbative expression for $\rho(t)$, we have neglected the last term on the right-hand side of equation (6) which is of the second order of magnitude in $H_{\text{e-ph}}$ [8]. This corresponds to neglecting energy and population fluctuations in many-electron systems. Substituting the expressions for $\dot{H}_{e\alpha}$, $\dot{N}_\alpha$ and $\dot{H}_{\mathrm{ph}}$ into (8), using the relations

$$b_{q\lambda}(t', \mathrm{i}\tau) = \exp(\beta\tau\Omega_{q\lambda})\, b_{q\lambda}(t')$$
$$b_{q\lambda}^+(t', \mathrm{i}\tau) = \exp(-\beta\tau\Omega_{q\lambda})\, b_{q\lambda}^+(t') \tag{11}$$
$$\rho_{\alpha\gamma,kq}(t', \mathrm{i}\tau) = \exp\{-\beta_\alpha(t)\tau[\xi_{\alpha,k+q}(t) - \xi_{\gamma,k}(t)]\}\, \rho_{\alpha\gamma,kq}(t')$$

with $\rho_{\alpha\gamma,kq}(t') \equiv c_{\alpha,k+q}^+(t') c_{\gamma,k}(t')$ and $\xi_{\alpha,k}(t) \equiv \varepsilon_{\alpha,k} - \mu_\alpha(t)$ and performing the integration over τ in equation (8), we obtain

$$\rho(t) - \rho_1(t) = \mathrm{i}\rho_1(t) \int_{-\infty}^{0} \mathrm{d}t' \exp(\varepsilon t') \sum_{\alpha,\gamma} \sum_{k,q,\lambda} M_{\alpha\gamma}(q,\lambda) E_{\alpha\gamma}(k,q)$$

$$\times \left(\frac{A_{\alpha\gamma}(t+t')}{A_{\alpha\gamma}(t)} [\exp(-A_{\alpha\gamma}(t) - 1] \rho_{\alpha\gamma,kq}(t') b_{q\lambda}(t') \right.$$

$$\left. + \frac{B_{\alpha\gamma}(t+t')}{B_{\alpha\gamma}(t)} [\exp(-B_{\alpha\gamma}(t) - 1] \rho_{\alpha\gamma,kq}(t') b^{+}_{q\lambda}(t') \right) \tag{12}$$

where $A_{\alpha\gamma}(t) = \beta_\alpha(t)[\xi_{\alpha,k+q}(t) - \xi_{\gamma,k}(t)] - \beta\Omega_q$ and

$$B_{\alpha\gamma}(t) = \beta_\alpha(t)[\xi_{\alpha,k+q}(t) - \xi_{\gamma,k}(t)] + \beta\Omega_q. \tag{13}$$

From equations (3) and (8) the statistical average of a dynamic variable Ω at time t can be written as

$$\langle\Omega\rangle^t = \langle\Omega\rangle_1^t + \mathrm{Tr}\{\Omega[\rho(t) - \rho_1(t)]\}. \tag{14}$$

In § 3, we shall apply equations (12) and (14) to derive the evolution equations for $v_\alpha(t)$, $T_\alpha(t)$ and $n_\alpha(t)$.

3. The evolution equations

Substituting equation (2) for $\dot{P}_\alpha$ into equation (14) and using the relations

$$\begin{aligned} \langle \dot{P}_\alpha b_{q\lambda}(t')\rho_{\alpha\gamma,kq}(t')\rangle_1^t \{\exp[-A_{\alpha\gamma}(t)] - 1\} &= \langle [b_{q\lambda}(t')\rho_{\alpha\gamma,kq}(t'), \dot{P}_\alpha]\rangle_1^t \\ \langle \dot{P}_\alpha b^{\pm}_{-q\lambda}(t')\rho_{\alpha\gamma,kq}(t')\rangle_1^t \{\exp[-B_{\alpha\gamma}(t)] - 1\} &= \langle [b^{\pm}_{-q\lambda}(t')\rho_{\alpha\gamma,kq}(t'), \dot{P}_\alpha]\rangle_1^t \end{aligned} \tag{15}$$

with $[C, D] \equiv CD - DC$, we obtain the average value of the time derivative of operator $\boldsymbol{P}_{\alpha x}$ as

$$\langle \dot{\boldsymbol{P}}_{\alpha x}\rangle = N_\alpha e E(t) - \mathrm{i}\sum_{\gamma}\sum_{k,q,\lambda} (k_x + q_x)|M_{\alpha\gamma}(q,\lambda)|^2 \int_{-\infty}^{\infty} \mathrm{d}t' \, E_{\alpha\gamma}(t,t') \exp[\varepsilon(t'-t)]$$

$$\times \left(\frac{A_{\alpha\gamma}(t')}{A_{\alpha\gamma}(t)} \Lambda^{-}_{t,\alpha\gamma}(k,q,\lambda,t-t') + \frac{B_{\alpha\gamma}(t')}{B_{\alpha\gamma}(t)} \Lambda^{+}_{t,\alpha\gamma}(k,q,\lambda,t-t') \right) \tag{16}$$

where $\Lambda^{-}_{t,\alpha\gamma}(k,q,\lambda,t-t')$ and $\Lambda^{+}_{t,\alpha\gamma}(k,q,\lambda,t-t')$ are the retarded Green functions which are respectively defined as

$$\begin{aligned} \Lambda^{-}_{t,\alpha\gamma}(k,q,\lambda,t-t') &= -\mathrm{i}\theta(t-t')\langle [b_{q\lambda}\rho_{\alpha\gamma,kq'} \, b^{+}_{q\lambda}(t'-t)\rho^{*}_{\alpha,kq}(t'-t)]\rangle_1^t \\ \Lambda^{+}_{t,\alpha\gamma}(k,q,\lambda,t-t') &= -\mathrm{i}\theta(t-t')\langle [b^{\pm}_{-q\lambda}\rho_{\alpha\gamma,kq'} \, b_{-q\lambda}(t'-t)\rho^{*}_{\alpha,kq}(t'-t)]\rangle_1^t \end{aligned} \tag{17}$$

and $E_{\alpha\gamma}(t,t')$ is defined as

$$E_{\alpha\gamma}(t,t') = \exp\left(\mathrm{i}(k_x + q_x)\int_{t'}^{t} v_\alpha(s)\,\mathrm{d}s - \mathrm{i}k_x \int_{t'}^{t} v_\gamma(s)\,\mathrm{d}s \right). \tag{18}$$

Similarly, we can obtain the average values of the time derivations of H_α and N_α:

$$\langle \dot{H}_{e\alpha} \rangle = -\mathrm{i} \sum_{\gamma} \sum_{k,q,\lambda} \varepsilon_{k+q} |M_{\alpha\gamma}(q,\lambda)|^2 \int_{-\infty}^{\infty} \mathrm{d}t' \, E_{\alpha\gamma}(t,t') \exp[\varepsilon(t'-t)]$$

$$\times \left(\frac{A_{\alpha\gamma}(t')}{A_{\alpha\gamma}(t)} \Lambda^{-}_{t,\alpha\gamma}(k,q,\lambda,t-t') + \frac{B_{\alpha\gamma}(t')}{B_{\alpha\gamma}(t)} \Lambda^{+}_{t,\alpha\gamma}(k,q,\lambda,t-t') \right) \tag{19}$$

$$\langle \dot{N}_\alpha \rangle = -\mathrm{i} \sum_{\gamma} \sum_{k,q,\lambda} |M_{\alpha\gamma}(q,\lambda)|^2 \int_{-\infty}^{\infty} \mathrm{d}t' \, E_{\alpha\gamma}(t,t') \exp[\varepsilon(t'-t)]$$

$$\times \left(\frac{A_{\alpha\gamma}(t')}{A_{\alpha\gamma}(t)} \Lambda^{-}_{t,\alpha\gamma}(k,q,\lambda,t-t') + \frac{B_{\alpha\gamma}(t')}{B_{\alpha\gamma}(t)} \Lambda^{+}_{t,\alpha\gamma}(k,q,\lambda,t-t') \right). \tag{20}$$

Equation (16), (19) and (20) are the main formulae in this paper. With the relations $\langle \dot{P}_\alpha \rangle = N_\alpha m_\alpha (\mathrm{d}v_\alpha/\mathrm{d}t)$, $\langle \dot{H}_{e\alpha} \rangle = N_\alpha c_e (\mathrm{d}T_\alpha/\mathrm{d}T) + T_\alpha c_e (\mathrm{d}N_\alpha/\mathrm{d}t)$ and $\langle \dot{N}_\alpha \rangle = \mathrm{d}N_\alpha/\mathrm{d}t$ ($c_e = \frac{3}{2}k_B$ is the single-electron specific heat), these equations form a complete set of evolution equations to determine the transient value of the drift velocities v_α, effective temperatures T_α and populations N_α of electrons for various valleys in a time-dependent electric field. These evolution equations derived above are non-Boltzmann type and go beyond the semi-classical approximation because of the memory effect included in them.

4. Non-linear equations in the classical approximation

In equations (16), (19) and (20) the memory effect is included in the factors $A_{\beta\gamma}(t')$ and $B_{\alpha\gamma}(t')$ as well as $E_{\alpha\gamma}(t,t')$. It has been shown [8] that for single-valley case the transient currents obtained by the Langevin-type equations with memory and without memory are almost identical with each other in electric fields of moderate strengths. This result means that in such fields the memory effect is not important and can be neglected. We expect that this conclusion is still valid for many-valley systems. The classical approximation without a memory effect has been used extensively for studying the transient behaviour of laser-induced hot electrons in GaAs [11, 12]. Omitting memory effects from the evolution equations (16), (19) and (20) is equivalent to the following approximation:

$$A(t')/A(t) \simeq B(t')/B(t) \simeq 1$$

and

$$E_{\alpha\gamma}(t,t') \simeq \exp\{\mathrm{i}[(k_x+q_x)v_\alpha(t) - k_x v_\gamma(t)](t-t')]\}. \tag{21}$$

Under this approximation the integrals over t' in equations (16), (19) and (20) can easily be performed. In terms of the standard Green function technique [13], we obtain a set of classical equations which can easily be employed to calculate the transient hot-electron transport for a many-valley semiconductor:

$$N_\alpha m_\alpha \frac{\mathrm{d}v_\alpha}{\mathrm{d}t} = N_\alpha e E(t) + \sum_{\gamma} \sum_{k,q} (k_x+q_x) |M_{\alpha\gamma}(q,\lambda)|^2 \Lambda_{\alpha\gamma}(k,q,\lambda,\omega_{\alpha\gamma})$$

$$N_\alpha c_e \frac{\mathrm{d}T_\alpha}{\mathrm{d}t} = \sum_{\gamma} \sum_{k,q} (\varepsilon_{k+q} - c_e T_\alpha) |M_{\alpha\gamma}(q,\lambda)|^2 \Lambda_{\alpha\gamma}(k,q,\lambda,\omega_{\alpha\gamma}) \tag{22}$$

$$\frac{\mathrm{d}N_\alpha}{\mathrm{d}t} = \sum_{\gamma\neq\alpha}\sum_{k,q} |M_{\alpha\gamma}(q,\lambda)|^2 \Lambda_{\alpha\gamma}(k,q,\lambda,\omega_{\alpha\gamma})$$

where $\Lambda_{\alpha\gamma}(k,q,\lambda,\omega_{\alpha\gamma})$ is the imaginary part of the Fourier transform of $[\Lambda^-_{t,\alpha\gamma}(k,q,\lambda,t-t') + \Lambda^+_{t,\alpha\gamma}(k,q,\lambda,t-t')]$. Its expression [14] is

$$\Lambda_{\alpha\alpha}(k,q,\lambda,\omega_{\alpha\alpha}) = 2d_\alpha \Pi_{\alpha\alpha}(k,q,\omega_{\alpha\alpha})\{n(\Omega_{q\lambda}/T) - n[(\omega_{\alpha\alpha}+\Omega_{q\lambda})/T_\alpha]\} \tag{23}$$

$$\begin{aligned}\Lambda_{\alpha\gamma}(k,q,\lambda,\omega_{\alpha\gamma}) = 2d_\alpha d_\gamma\{&\Pi_{\alpha\gamma}(k,q,\omega_{\alpha\gamma}-\Omega_{q\lambda})[n(\Omega_{q\lambda}/T) \\ &- n(\xi_{\alpha,k+q}/T_\alpha - \xi_{\gamma k}/T_\gamma)] \\ &+ \Pi_{\alpha\gamma}(k,q,\omega_{\alpha\gamma}+\Omega_{q\lambda})[n(\Omega_{q\lambda}/T) - n(\xi_{\gamma k}/T_\gamma - \xi_{\alpha,k+q}/T_\alpha)]\}\end{aligned} \tag{24}$$

with

$$\Pi_{\alpha\gamma}(k,q,\omega) = -2\pi[f(\xi_{\alpha,k+q}/T_\alpha) - f(\xi_{\gamma k}/T_\gamma)]\delta(\varepsilon_{\alpha,k+q} - \varepsilon_{\gamma k} + \omega) \tag{25}$$

$$\omega_{\alpha\gamma} = (k_x+q_x)v_\alpha - K_x v_\gamma + m_\alpha v_\alpha^2/2 - m_\gamma v_\gamma^2/2 \tag{26}$$

where $f(\xi_{\alpha k}/T_\alpha) = 1/[\exp(\varepsilon_{\alpha k} - \mu_\alpha)/T_\alpha) + 1]$ is the Fermi–Dirac distribution function with $\xi_{\alpha k} = \varepsilon_{\alpha k} - \mu_\alpha$, and $n(x) = 1/[\exp(x) - 1]$ is the Bose–Einstein distribution function. In deriving equations (23)–(26), we have assumed that there are d_α equivalent valleys for the type-α carriers, and d_γ equivalent valleys for the type-γ carriers. For GaAs with a Γ–L–X band structure, the set of equations in (22) is composed of eight non-linear differential equations ($\alpha = \Gamma$, L, X, with $N_\Gamma + N_L + N_X = N$). It is well known that, for many-valley semiconductors, the carriers of various valleys in thermal equilibrium obey the Maxwell–Boltzmann distribution at room temperature. In such a case $f(\xi_{\alpha k}/T_\alpha) \simeq \exp[-(\varepsilon_{\alpha k} - \mu_\alpha)/T_\alpha]$ and $\exp(\mu_\alpha/T_\alpha) = (N_\alpha/2d_\alpha)(2\pi/m_\alpha T_\alpha)^{3/2}$, so that $\Pi_{\alpha\gamma}(k,q,\omega)$ and $\Lambda_{\alpha\gamma}(k,q,\omega_{\alpha\gamma})$ reduce to the expressions which have already been given in the Appendix of [14].

It is interesting to compare the evolution equations obtained above with those from the approximate treatments of the Boltzmann equation. Although the present method is non-Boltzmann, the results seem to be close to those obtained from the drifted Maxwellian approximation in solving the Boltzmann equation. A detailed discussion of this point has been given in [15]. As pointed out in [15], the carrier distribution function in the present method is not a drifted Maxwellian type and the exact carrier distribution function is not needed in calculating v_d as a function of E.

5. Numerical results

In this section, we apply those equations in (22) obtained above to calculate the drift velocity of carriers in an n-type GaAs sample in time-dependent electric fields at room temperature. For an n-type GaAs semiconductor, we consider the complexity of the conducting band structure by assuming that the system is composed of three parabolic valleys (one Γ valley, four equivalent L valleys and three equivalent X valleys). Carriers in different valleys have different effective masses, drift velocities and electron temperatures. Scatterings due to acoustic, polar optic and non-polar optic phonons are considered. For each valley the acoustic electron–phonon interaction matrix element is taken to be

$$|M_{\alpha\alpha}(q,\lambda)|^2 = E_\alpha^2 q/2dv_s. \tag{27}$$

For the Γ valley the polar optic electron–phonon interaction matrix element is taken to be

$$|M_{\Gamma\Gamma}(q,\lambda)|^2 = (e^2\Omega_{LO}/2\varepsilon_0 q^2)(1/\kappa_\infty - 1/\kappa_0). \tag{27}$$

For L valleys the non-polar optic electron–phonon matrix element is

$$|M_{LL}(q,\lambda)|^2 = D_{LL}^2/2d\Omega_{op}. \tag{28}$$

Between both equivalent and non-equivalent valleys, the non-polar optic electron–phonon interaction matrix element is

$$|M_{\alpha\gamma}(q,\lambda)|^2 = D_{\alpha\gamma}^2/2d\Omega. \tag{30}$$

The definitions of the parameters which appear in these electron–phonon interaction matrices are explained in table 1. For comparison, we use the same values for all parameters in GaAs as those in the Monte Carlo method (see table 8.2 of [1]), except that the non-parabolicity effect is not considered, in calculating the transient $v_\alpha(t)$, $T_\alpha(t)$ and $N_\alpha(t)$ for various valleys.

From equation (22), we first calculate the transient drift velocity in an external electric field with a time step configuration ($E = 0$ for $t < 0$, and $E = 5, 15, 40$ kV cm^{-1} for $t \geqslant 0$). The drift velocity as a function of time at $T = 300$ K is shown in figure 1. The time dependences of the mean velocity, temperature and the fraction of carriers in the Γ valley at $E = 15$ kV cm^{-1} are plotted in figure 2. The essential feature of the transient velocity is the overshoot behaviour. Owing to the inter-valley scattering in a many-valley system the overshoot effect is stronger than that in single-valley case [8]. As shown in figure 1, the higher the field is, the stronger the overshoot effect. Our calculated results for $E = 40$ kV cm^{-1} after $t = 0$ is very close to that of the Monte Carlo calculation which is shown in figure 8.4 of [1]. The overshoot effect can be understood in view of the

Table 1. The parameters of n-type GaAs.

Symbol	Parameter (units)	Value		
d	Density (g cm^{-3})	5.36		
v_s	Velocity of sound (cm s^{-1})	5.24×10^5		
κ	Static dielectric constant	12.90		
κ_∞	Optical dielectric constant	10.92		
Ω_{LO}	Longitudinal optical phonon energy (eV)	0.03536		
		Γ(000)	L(111)	X(100)
m_α/m_0	Effective mass	0.063	0.222	0.58
$\varepsilon_{\alpha 0}$	Energy band gap (eV) (relative to valence band)	1.439	1.769	1.961
E_α	Acoustic deformation potential (eV)	7.0	9.2	9.27
Ω_{op}	Optical phonon energy (meV)	0.0	34.3	0.0
D_{LL}	Optical deformation potential (10^9 eV cm^{-1})	—	0.3	—
$D_{\alpha\beta}$	Inter-valley coupling constant (10^9 eV cm^{-1})			
	from Γ	0	1	1
	from L	1	1	0.5
	from X	1	0.5	0.7
Ω	Inter-valley phonon energy (meV)			
	from Γ	0	27.8	29.9
	from L	27.8	29.0	29.3
	from X	29.9	29.3	29.9
d_α	Number of equivalent valleys	1	4	3

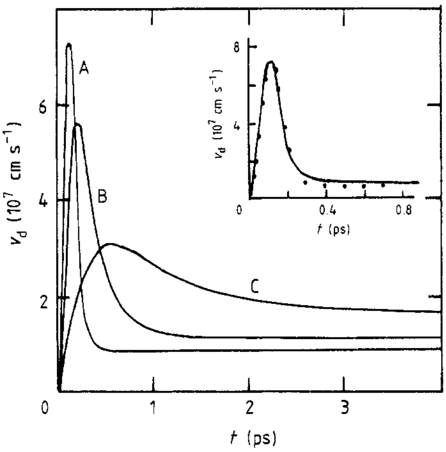

Figure 1. Transient drift velocity $v_d(t)$ against time when a time step of the electric field is applied to a GaAs sample at $T = 300$ K: curve A, calculated results for $E = 40$ kV cm^{-1}; curve B, calculated results for 15 kV cm^{-1}; curve C, calculated results for 5 kV cm^{-1}. Comparison between curve A and the results obtained in [1] with a Monte Carlo procedure (●) is shown in the inset.

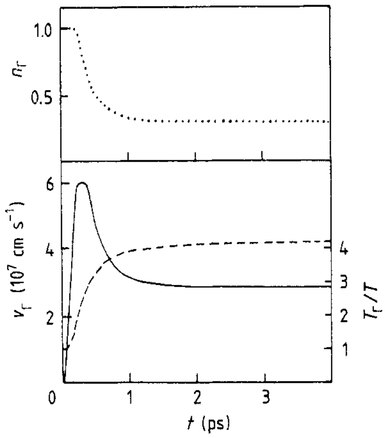

Figure 2. Mean velocity $v_\Gamma(t)$ (——), temperature ratio $T_\Gamma(t)/T$ (– – –) and fraction $n_\Gamma(t)$ (· · · · ·) of carriers in the Γ valley against time when a time step of the electric field ($E = 15$ kV cm^{-1}) is applied to a GaAs sample at $T = 300$ K.

disparity of the relaxation times for momentum, energy and carrier transfer. Since the momentum relaxation time is shorter than the energy and population relaxation times, as shown in figure 2, in the first 0.3 ps after the application of a constant electric field, while most of the carriers still stay in the Γ valley and the carrier temperature increases slowly, the mean velocity of carriers in the Γ valley increases rapidly, causing the overshoot behaviour. After about 0.3 ps has passed, the inter-valley scattering and hot-electron effect begin to play a leading role.

(i) Many carriers in the Γ valley with higher mean velocity transit to the satellite valleys (L and X) with lower velocities.

(ii) The drift velocities of various valleys decrease with the increase in hot-carrier temperatures.

Thus, the total drift velocity first decreases rapidly and then gradually reaches its steady-state value. In small devices with high operating frequencies an interesting problem is research on the optimum electric field configuration which make electrons go as fast as possible. By using the simple relation

$$s = \int_0^t v_d(t)\,dt \tag{31}$$

the average distance s travelled by the carriers over a time t can be obtained and is shown in figure 3. For a GaAs short channel field-effect transistor (FET), the separation between source and drain is in the micrometre range; the cold electrons injected at the source may never reach their steady-state velocity before being collected at the drain but travel at a overshoot velocity $v_d(t)$. From figure 3, it seems that in small-size devices (feature sizes in the range 0.1–0.5 μm) the optimised field for obtaining the maximum distance of high-velocity propagation depends on the overshoot velocity rather than the steady-state velocity.

Next we calculate the transient drift velocity when a time pulse of electric field is applied to a GaAs sample. The calculated result is shown by the full curve in figure 4, and that of the Monte Carlo calculation by the dotted curve. Both calculated results of the two methods are in good agreement with each other except for some discrepancies near state C and D. Both overshoot and undershoot effects are obtained. To clarify the reason for producing both overshoot and undershoot phenomena, the fraction of carriers in the Γ valley is plotted by the broken curve in figure 4. State A is the transient drift velocity in a time step of the field ($E = 0\ \mathrm{kV\ cm^{-1}}$ for $t < 0$ ps and $E = 2\mathrm{kV\ cm^{-1}}$ for $2\ \mathrm{ps} > t > 0\ \mathrm{ps}$). Before $t = 2$ ps, it has reached the steady-state value of $v_d = 1.48 \times 10^7\ \mathrm{cm\ s^{-1}}$. State B refers to a few tenths of a picosecond after the application of the high-electric-field pulse ($E = 20\ \mathrm{kV\ cm^{-1}}$). The drift velocity increase linearly with time and has a strong overshoot effect as discussed above. State C refers to 1 ps after the application of the pulse; although the electric field remains very high, the transient drift velocity $v_d(t) = \Sigma_\alpha v_\alpha(t) n_\alpha(t)$ decreases quickly because a great number of carriers are scattered into the L and X valleys from the Γ valley, and the transient velocity $v_\alpha(t)$ for various valleys drops quickly and develops the lower steady-state values. State D refers to a few tenths of a picosecond after the applied electric field E returns to $2\ \mathrm{kV\ cm^{-1}}$. At this moment, while the instantaneous energies of various valleys have not yet been reduced and the population in the Γ valley still remains of very small value, the mean velocities in various valleys decrease quickly owing to the low value of the electric field. Therefore, there is a drastic decrease in the total drift velocity. Such a phenomenon is called the undershoot velocity effect. With increasing time, most carriers will return to the Γ valley, T_Γ will decrease, and the drift velocity v_d will increase and tend towards the steady-state value corresponding to $E = 2\ \mathrm{kV\ cm^{-1}}$. Our calculated values for $v_d(t)$ near state C are higher than those of the Monte Carlo calculation (see figure 8.8 in [1]) where it is claimed that there is undershoot phenomenon at state C due to the Rees effect. In

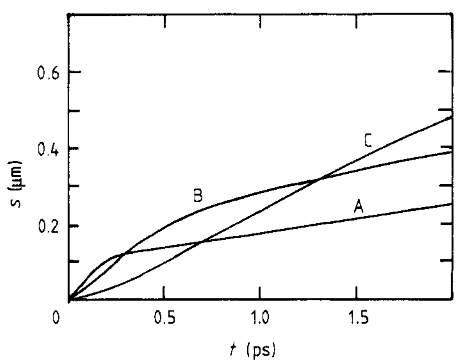

Figure 3. Average distance s travelled by the carriers over a time t when a time step of the electric field is applied to a GaAs sample at $T = 300$ K: curve A, $E = 40\ \mathrm{kV\ cm^{-1}}$; curve B, $E = 15\ \mathrm{kV\ cm^{-1}}$; curve C, $E = 5\ \mathrm{kV\ cm^{-1}}$.

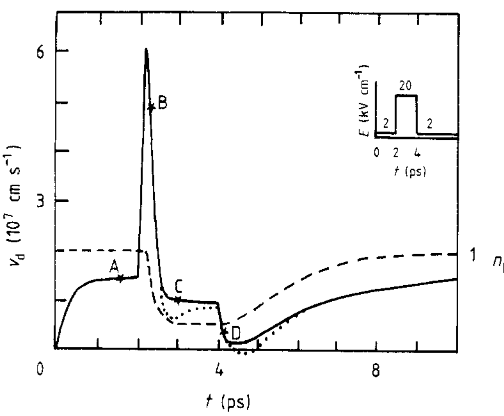

Figure 4. Transient drift velocity $v_d(t)$ (——) and fraction $n_\Gamma(t)$ (–––) of carriers in the Γ valley against time when a time pulse of electric field is applied to a GaAs sample at $T = 300$ K; ·····, Monte Carlo calculation [1].

our opinion the transient behaviour of the drift velocity near state C before $t = 4$ ps in a time pulse electric field should be same as that in a time step field because different configurations of the fields after $t = 4$ ps cannot affect the transient drift velocity before $t = 4$ps. It is inconsistent to assert that the undershoot phenomenon shows up at state C with a time pulse field ($E = 20$ kV cm^{-1}) from the Monte Carlo calculation in figure 4, while the transient drift velocity in a time step field with $E = 20\theta(t)$ kV cm^{-1} has no undershoot effect from both our and Monte Carlo results. Near state D the undershoot effect in our calculation is slightly weaker than that in the Monte Carlo calculation. The origin of this discrepancy is not clear. The undershoot phenomenon near state D is called the Rees effect. This effect was explained in [16, 17].

Finally we study the time responses of the drift velocity for a long sample submitted to a high-frequency sinusoidal electric field superimposed to an applied steady field: $E = E_0 + E_1 \cos(\omega t)$ with $E_0 = 18$ kV cm^{-1}, $E_1 = 14$ kV cm^{-1}, and $f = 100$ GHz. The calculated result for the time-dependent drift velocity waveform is shown by the full curve in figure 5(a), where a stable pulse current waveform with a time delay has been obtained. In order to show the transient transport behaviour in a high-frequency field, the steady-state values of the drift velocities in the same fields are plotted as the broken curve. It is easily seen that for the first half-period (5 ps $> t >$ 0 ps) the calculated drift velocities are lower than their corresponding steady-state ones owing to the undershoot effect in a field whose strength decreases with time, and for the last half-period (10 ps $> t >$ 5 ps) the overshoot behaviour dominates the drift velocity waveform in a increasing field with time. Figure 5(b) gives the time-varying mean velocities and populations of electrons for various valleys. From that both the undershoot and the

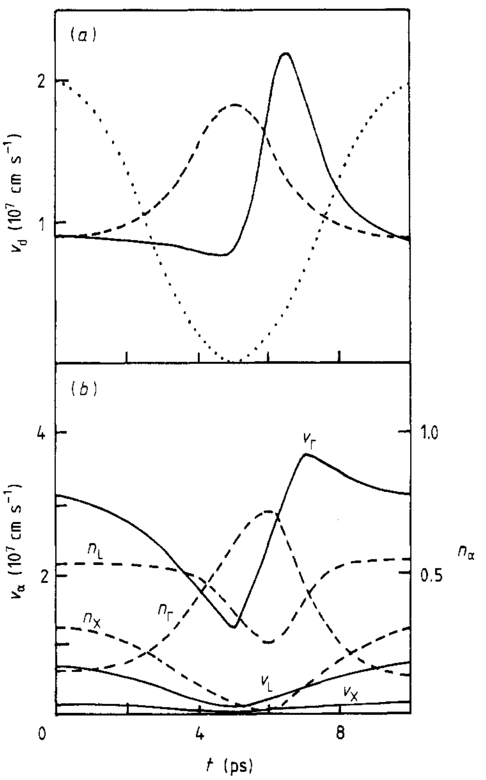

Figure 5. (a) Drift velocity $v_d(t)$ against time when a uniform electric field ($E = E_0 + E_1 \cos(\omega t)$ with $E_0 = 18$ kV cm^{-1}, $E_1 = 14$ kV cm^{-1} and $f = 100$ GHz) is applied to a GaAs sample at $T = 300$ K. ---, steady-state drift velocity for the corresponding electric fields; ·····, electric field strength waveform. (b) Corresponding mean velocities $v_\alpha(t)$ and fractions $n_\alpha(t)$ of carriers, where $\alpha \equiv \Gamma$, L, X, against time.

overshoot effects which dominate the current waveform can be understood, the peak of $v_d(t)$ corresponds to a high mean velocity v_Γ and a large population n_Γ of electrons at the Γ valley, and the valley of $v_d(t)$ near $t = 5$ ps is due to the minimum mean velocities of electrons for various valleys.

6. Conclusion

We have studied the transient hot-electron transport in many-valley semiconductors by employing the method of the NSO. A set of coupled evolution equations with memory effect are derived to determine the time-dependent drift velocity. In the classical approximation, non-linear differential equations for $v_\alpha(t)$, $T_\alpha(t)$ and $n_\alpha(t)$ in a numerically calculable form are obtained. By using the same parameters as those in the Monte Carlo simulation, the time-dependent drift velocity, hot-electron temperatures and populations of carriers are calculated from these differential equations when the sample is put in various time-dependent electric fields. The results obtained are comparable with those of Monte Carlo calculations, but the mathematical structure of the present method is quite simple and the required computational effort is minor, a set of differential equations being solved on a Micro-VAX II computer. Furthermore, the physical origin of both overshoot and undershoot behaviours which govern the transient transport in the small region of semiconductor devices can be understood in terms of the hot-electron effect and inter-valley scattering in a many-valley system. Using the present method, we can easily study transient transport property in many-valley semiconductors within any shape of time-dependent electric field.

Acknowledgments

This work is supported by the Space Vacuum Epitaxy Center through a grant from the National Aeronautics and Space Administration and the Texas Advanced Technological Research Program.

References

[1] Reggiani L 1985 *Hot-Electron Transport in Semiconductors* (Berlin: Springer)
[2] Carnez B, Cappy A, Kaszynski A, Constant E and Salmer G 1980 *J. Appl. Phys.* **51** 784
[3] Maloney T J and Jeffrey F 1977 *J. Appl. Phys.* **48** 781
[4] Ruch J G 1972 *IEEE Trans. Electron Devices* **ED-19** 652
[5] Zubarev D N 1974 *Nonequilibrium Statistical Thermodynamics* (New York: Consultants Bureau)
[6] Xing D Y, Hu P and Ting C S 1987 *Phys. Rev.* B **35** 6379
[7] Liu M, Xing D Y, Ting C S and Xu W T 1988 *Phys. Rev.* B **37** 2997
[8] Xing D Y and Ting C S 1987 *Phys. Rev.* B **35** 3971
[9] Lei X L, Xing D Y, Liu M, Ting C S and Birman J L 1987 *Phys. Rev.* B **36** 9134
[10] Kalashnikov V P 1970 *Physica* **48** 93
[11] Vasconcellos A R and Luzzi R 1983 *Phys. Rev.* B **27** 3874
Algarte A C S and Luzzi R 1983 *Phys. Rev.* B **27** 7563
[12] Cai W, Marchetti M C and Lax M 1987 *Phys. Rev.* B **35** 1369
[13] Lei X L and Ting C S 1985 *Phys. Rev.* B **32** 1112
[14] Xing D Y, Liu M and Ting C S 1988 *Phys. Rev.* B **37** 10283
[15] Lei L X and Ting C S 1987 *Phys. Rev.* B **36** 8162
[16] Fawcett W and Rees H D 1969 *Phys. Lett.* **39A** 578
[17] Boittianx B, Constant E, Reggiani L, Brunetti R and Jacoboni C 1982 *Appl. Phys. Lett.* **40** 407