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Hot intervalley phonons in GaAs

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Abstract. A novel ensemble Monte Carlo method for hot intervalley phonon problems is proposed. The dynamics of the non-equilibrium electron–intervalley phonon system is simulated under the conditions of high photoexcitation in GaAs. It is obtained that hot intervalley phonons insignificantly affect the electron-cooling dynamics and intervalley transfer even at high photoexcitation energies and photoexcited plasma densities.

1. Introduction

Hot-longitudinal-optical (LO)-phonon dynamics in polar semiconductors has been widely investigated experimentally [1–5] and by the ensemble Monte Carlo technique (EMC) [6–12]. It is found that hot LO phonons significantly influence the photoexcited carrier cooling process [4, 7] and high-field transport [10, 11] in GaAs as well as interband impact ionisation in InSb [12]. The electron intervalley scattering in many-valley polar semiconductors (as does any phonon-assisted process) generates non-thermal short-wave (intervalley) phonons. Hot intervalley phonons can affect the carrier relaxation and intervalley transfer, but the degree to which this happens is not yet known for certain [13].

In the present paper we have developed the previously proposed [6] EMC method for hot-intervalley-phonon problems. The method is applied to the simulation of the non-equilibrium electron–phonon system in GaAs under high photoexcitation conditions. The effects of hot intervalley phonons on the electron-cooling and intervalley transfer dynamics are investigated. Some of the results were briefly reported in [14].

2. Method

Because of momentum conservation, the electron intervalley transfer between the Γ, L and X valleys in GaAs (and other III–V semiconductors) is associated with electron interaction with short-wave phonons. Group theory selection rules applied to a cubic zinc-blende structure of III–V semiconductors show that the LO and longitudinal acoustic (LA) phonons can assist the intervalley transitions [15]. Owing to energy conservation, the electron scattering from the Γ to the upper valleys occurs only when the electron energy exceeds the threshold energy for intervalley transfer. The selection rules at such energies, however, do not apply [16, 17]. Therefore, all phonon branches including

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transverse optical (TO) and transverse acoustic (TA) can contribute to intervalley scattering. The LO, TO and LA phonons in GaAs have comparable energies at the zone edge [17, 18]. Therefore, the intervalley scattering can be considered by grouping together the scatterings assisted by these phonons and using the average phonon energy and the total coupling constant. The intervalley transitions assisted by TA phonons must be considered as a separate process, because the TA phonon energy is about three times lower [17, 18]. However, the estimations made by Herbert [16] have shown that the electron coupling with the TA branch is weak, and intervalley scattering by TA phonons can be neglected. Consistent with this simple model of the intervalley scattering, the total intervalley coupling constant D_{ij} between the i and j valleys and the total phonon occupation number N_{ij} can be introduced. Then the intervalley scattering rate from the state $\boldsymbol{k}_i$ in the i valley to any state in the j valley can be expressed as [19]

$$\bar{\lambda}(\boldsymbol{k}_i) = \frac{V}{8\pi^2}\frac{Z_j D_{ij}^2}{\rho\omega_{ij}} \int \mathrm{d}\boldsymbol{k}_j \, (N_{ij} + \tfrac{1}{2} \mp \tfrac{1}{2}) G(\boldsymbol{k}_i, \boldsymbol{k}_j) \delta[\varepsilon_j(\boldsymbol{k}_j) - \varepsilon_i(\boldsymbol{k}_i) - \Delta\varepsilon_{ij} \pm \hbar\omega_{ij}] \tag{1}$$

where $\hbar\omega_{ij}$ is the intervalley phonon energy, ρ is the density of the material, Z_j is the number of the j valleys, G is the overlap integral between states $\boldsymbol{k}_i$ and $\boldsymbol{k}_j$ in the i and j valleys, respectively, and $\Delta\varepsilon_{ij}$ is the energy separation between the i and j valleys (can also be negative).

In the case of the equilibrium phonon distribution, the phonon occupation number N_{ij} is usually assumed to be independent of the phonon wavevector $\boldsymbol{q}$. Within this assumption, equation (1) can easily be integrated. However, in the general case of the non-equilibrium phonon distribution the phonon occupation number depends on $\boldsymbol{q}$. The phonon wavevector can be expressed as $\boldsymbol{q} = \pm(\boldsymbol{k}_j - \boldsymbol{k}_i + \boldsymbol{k}_{ij})$ (where $\boldsymbol{k}_{ij}$ is the wavevector between the minima of the i and j valleys); therefore, the analytical integration of (1) is generally impossible. Because of this, we use a procedure similar to that proposed in [6]. Let us introduce some fictitious scattering rate

$$\tilde{\lambda}(\boldsymbol{k}_i, \boldsymbol{k}_j^*) = \frac{V}{8\pi^2}\frac{Z_j D_{ij}^2}{\rho\omega_{ij}} [N_{ij}(\boldsymbol{q}^*) + \tfrac{1}{2} \mp \tfrac{1}{2}] \int \mathrm{d}\boldsymbol{k}_j \, G(\boldsymbol{k}_i, \boldsymbol{k}_j) \times \delta[\varepsilon_j(\boldsymbol{k}_j) - \varepsilon_i(\boldsymbol{k}_i) - \Delta\varepsilon_{ij} \pm \hbar\omega_{ij}] \tag{2}$$

where $\boldsymbol{q}^* = \pm(\boldsymbol{k}_j^* - \boldsymbol{k}_i + \boldsymbol{k}_{ij})$ is the wavevector of the phonon assisting the particular intervalley transition to the state $\boldsymbol{k}_j^*$ in the j valley. It can be demonstrated that, if we choose $\boldsymbol{k}_j^*$ randomly with the distribution $G(\boldsymbol{k}_i, \boldsymbol{k}_j)\delta[\varepsilon_j(\boldsymbol{k}_j) - \varepsilon_i(\boldsymbol{k}_i) - \Delta\varepsilon_{ij} \pm \hbar\omega_{ij}]$ (the expression under the integral in (2)), then fictitious $\tilde{\lambda}$ averaged over many random choices of $\boldsymbol{k}_j^*$ is equal to $\bar{\lambda}$, i.e.

$$\langle\tilde{\lambda}(\boldsymbol{k}_i, \boldsymbol{k}_j^*)\rangle_{\boldsymbol{k}_j^*} = \bar{\lambda}(\boldsymbol{k}_i). \tag{3}$$

This means that we can choose random $\boldsymbol{k}_j^*$ and use $\tilde{\lambda}$ given by equation (2) instead of (1) in our Monte Carlo procedure. The integration of (2) yields the conventional expression for the intervalley scattering rate [19] only with N_{ij} as a function of the parameter $\boldsymbol{q}^*(\boldsymbol{k}_j^*)$.

Now let us analyse in more detail how to choose random $\boldsymbol{k}_j^*$. In spherical coordinates we have $\boldsymbol{k}_j^* = \{k_j^*, \cos\theta^*, \varphi^*\}$, where θ^* is the angle between $\boldsymbol{k}_i$ and $\boldsymbol{k}_j^*$. The integral in equation (2) can be rewritten in spherical coordinates as

$$\int G(\boldsymbol{k}_i, \boldsymbol{k}_j)\delta[\varepsilon_j(\boldsymbol{k}_j) - \varepsilon_i(\boldsymbol{k}_i) - \Delta\varepsilon_{ij} \pm \hbar\omega_{ij}] k_j^2 \, \mathrm{d}k_j \, \mathrm{d}(\cos\theta) \, \mathrm{d}\varphi. \tag{4}$$

k_j is always determined by energy conservation; therefore, we need to choose randomly

only $\cos\theta^*$ and φ^*. However, neither G nor the δ-function contain θ and φ (G is usually a function of only modules k_i and k_j); therefore, we choose them with uniform distribution:

$$\varphi^* = 2\pi r_1 \qquad \cos\theta^* = 1 - 2r_2 \tag{5}$$

where random r_1 and r_2 are uniformly distributed in the interval (0, 1).

N_{ij} as a function of $\boldsymbol{q}$ is evaluated during the simulation. Since every possible $i \rightarrow j$ intervalley scattering is usually treated as a separate mechanism, we must calculate the separate functions $N_{ij}(\boldsymbol{q})$ and produce the corresponding histograms. Owing to the Brillouin zone structure of III–V semiconductors, the phonons assisting the $i \rightarrow j$ transition cannot assist any other $i' \rightarrow j'$ transition except the reverse $j \rightarrow i$ transition. Therefore, five independent histograms corresponding to every intervalley coupling must be produced for the three-valley model of GaAs (and other III–V semiconductors).

Let us consider now the case where electric and magnetic fields are absent. Then axial symmetry of every intervalley $i \rightarrow j$ transition allows us to use two-dimensional N_{ij} histograms. The most convenient form of these histograms is $N_{ij}(K, \alpha)$, where $K^2 = k_i^2 + k_j^2 - 2k_ik_j\cos\theta$, $\cos\alpha = (q^2 - K^2 - k_{ij}^2)/2Kk_{ij}$. Using such a grid the $\boldsymbol{q}$-cells compactly fill the $\boldsymbol{q}$-space volume populated by intervalley phonons. The intervalley phonon wavenumber can be expressed as

$$q^2 = k_i^2 + k_j^2 + k_{ij}^2 - 2k_ik_j\cos\theta - 2k_ik_{ij}\cos\beta + 2k_jk_{ij}(\cos\theta\cos\beta + \sin\theta\sin\beta\cos\varphi) \tag{6}$$

where β is the angle between $\boldsymbol{k}_i$ and $\boldsymbol{k}_{ij}$. In the absence of the fields, electrons are distributed isotropically in the valleys; therefore, $\cos\beta$ is a random parameter uniformly distributed in the interval $(-1, 1)$: $\cos\beta^* = 1 - 2r_3$. Taking into account this fact as well as the uniform distributions of $\cos\theta$ and φ (see equation (5)), it can be demonstrated that $\cos\alpha$ is also a random number uniformly distributed in the interval $(-1, 1)$. Consequently, we can use a spherical grid in $\boldsymbol{q}$-space and produce one-dimensional histograms $N_{ij}(K)$. The $\boldsymbol{q}$-cell volume for the i–j coupling can be expressed as $V_q(K) = Z_{ij}[4\pi K\,\Delta K\,(K + \Delta K) + 4/3\pi\,\Delta K^3]$, where Z_{ij} is the number of possible $i \rightarrow j$ and $j \rightarrow i$ transition directions (taking into consideration equivalent valleys). In III–V semiconductors symmetry yields $Z_{\Gamma L} = 4$, $Z_{\Gamma X} = 3$, $Z_{LL} = 8$, $Z_{XX} = 6$ and $Z_{LX} = 10$.

The histogram $N_{ij}(K)$ is updated after every electron–phonon scattering event adding to $N_{ij}(K^*)$ the quantity

$$\pm\,[8\pi^3/V_q(K^*)]\,(n/N_e) \tag{7}$$

where n is the electron concentration, N_e is the number of simulated particles, and the signs plus and minus correspond to the phonon emission and absorption, respectively. After each time step, $N_{ij}(K)$ is recalculated according to phonon thermalisation [6].

In summary, the simulation procedure for the isotropic electron and phonon distributions is the following:

(i) choice of random $\cos\theta^*$ according to (5);
(ii) calculation of K^* and $N_{ij}(K^*)$, and its substitution into $\tilde{\lambda}$ given by equation (2);
(iii) choice of the scattering mechanism;

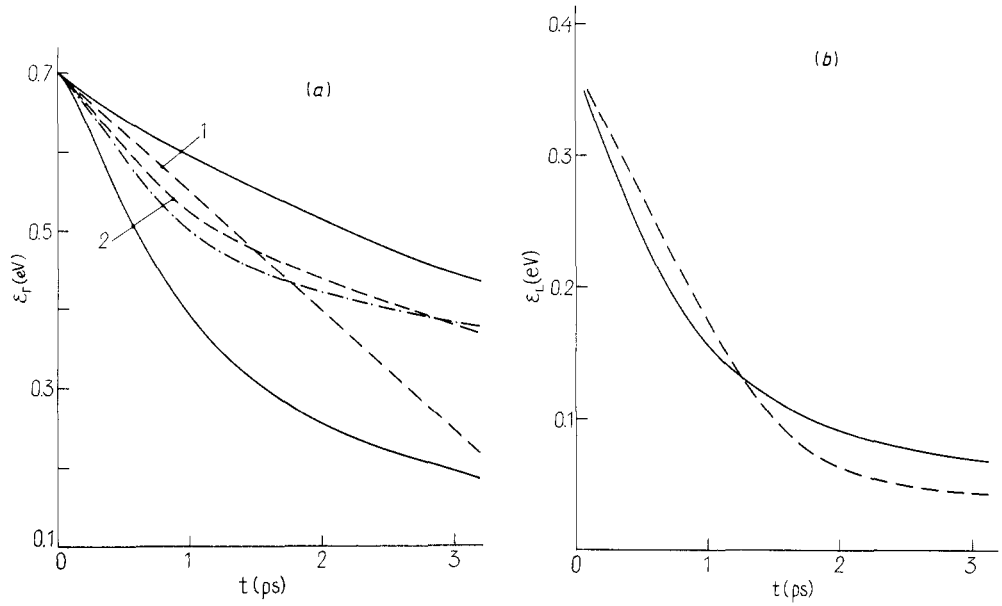

Figure 1. Time evolution of the mean electron energy (*a*) in the Γ valley and (*b*) in the L valleys ($T = 77$ K; $n = 2 \times 10^{18}$ cm^{-3}): curve 1, one-valley GaAs; curve 2, two-valley GaAs; ——, with hot phonons; – – –, without hot phonons; —·—, with hot intervalley phonons but without hot LO phonons.

(iv) if it is an intervalley scattering, the histogram $N_{ij}(K^*)$ is updated by the quantity, given by equation (7);

(v) after every time step N_{ij} is recalculated according to phonon thermalisation.

3. Model

We have used the simplified two-valley Γ–L model of GaAs with strong intervalley coupling: $D_{\Gamma L} = D_{LL} = 10^9$ eV cm^{-1}. In order to achieve high intervalley scattering intensities the excitation energy ε was chosen as 0.7 eV, which was much higher than intervalley energy separation $\Delta\varepsilon_{\Gamma L}$ of 0.3 eV. The photoexcited plasma density n was 2×10^{18} cm^{-3}. The relaxation dynamics of preliminary excited carriers were simulated after the photoexcitation had been switched off.

The Debye-screened polar optical scattering, the deformation acoustic scattering and the intervalley scattering of electrons were taken into account. Hot LO phonons and hot intervalley phonons were also considered. Carrier–carrier scattering was not taken into consideration.

The thermalisation time τ_{LO} of long-wave intravalley LO phonons was assumed to be dependent on the equilibrium lattice temperature [11] and equal to 7 ps at $T = 77$ K. The thermalisation of intervalley phonons is a much more complicated process because various intervalley phonon branches may have different thermalisation times that are not known yet. However, we have simulated only the initial stage of electron relaxation (0–3 ps). In such a time scale the thermalisation of hot intervalley phonons is expected

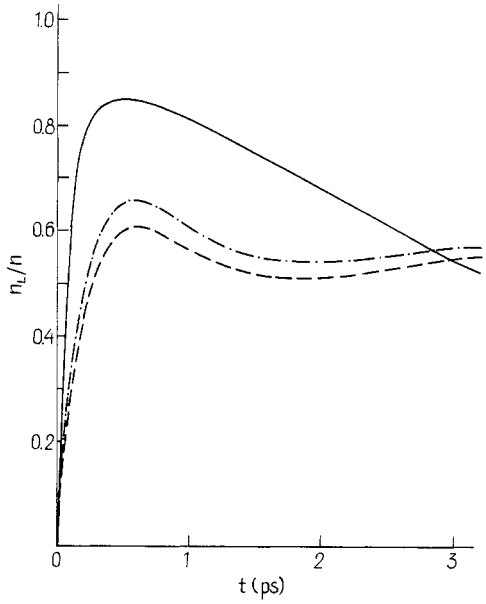

Figure 2. Electron intervalley transfer dynamics (relative L valley population versus time). The notation and parameter values are the same as in figure 1.

to be not very important. We have used the simplified thermalisation model with average intervalley phonon thermalisation time τ_{iv} of 7 ps.

4. Results and discussion

First let us study the role of the upper L valleys in the relaxation of hot electrons. Figures 1 and 2 show some of the simulation results. One can see from figure 1(*a*) that hot LO phonons reduce significantly the electron relaxation rate in one-valley semiconductors, which is in agreement with the previous results [4, 7]. However, the two-valley GaAs model predicts that hot LO phonons increase the relaxation rate in the central Γ valley. This can be explained in terms of valley repopulation dynamics. Figure 2 demonstrates that hot LO phonons lead to the stronger electron transfer to the L valleys in the initial stage of the relaxation. The electron cooling in the L valleys is faster (figure 1(*b*)) and electrons return to the central Γ valley as they are colder than those which relax in the Γ valley. Thus this faster electron relaxation channel is opened wider by hot LO phonons. However, in the second stage of the relaxation ($t > 2$ ps), electron cooling in the L valleys becomes slower (figure 1(*b*)) and electrons return to the Γ valley with higher energies. Therefore, the L valleys in the second stage of the relaxation play the role of a hot-electron reservoir. Then the relaxation of electrons in one-valley semiconductors becomes faster. Figure 2 shows that hot LO phonons yield faster electrons returning from the L valleys to the central Γ valley. This also contributes to the higher cooling rates.

The evolution of non-equilibrium distributions of LO phonons is shown in figure 3. One can see that the phonon distribution broadens with time. The LO phonon distribution calculated within the two-valley GaAs model significantly differs from that calculated within the one-valley model. The secondary peak on the distribution obtained within the two-valley model is associated with phonon emission both by the electrons in the L valleys and by the lower-energy electrons which have returned from the L valleys.

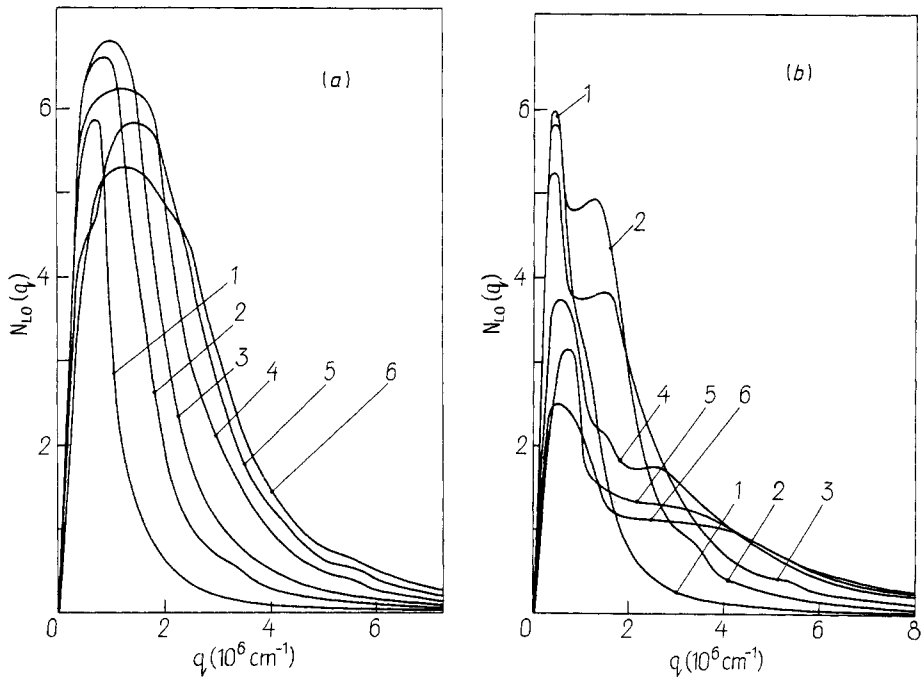

Figure 3. Time evolution of non-equilibrium LO phonon distribution for (*a*) one-valley and (*b*) two-valley GaAs models for various lengths of time after the photoexcitation ($T = 77$ K; $n = 2 \times 10^{18}$ cm^{-3}): curve 1, 0.2 ps; curve 2, 0.6 ps; curve 3, 1 ps; curve 4, 2 ps; curve 5, 3 ps; curve 6, 4 ps.

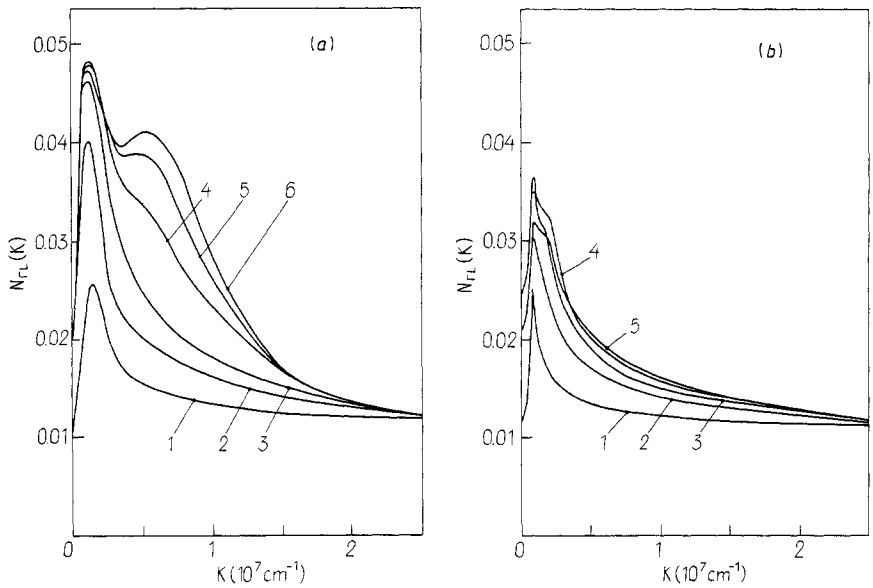

Figure 4. Time evolution of non-equilibrium intervalley phonon distribution (*a*) where the hot LO phonons are taken into account and (*b*) for equilibrium LO phonons. The notation and parameter values are the same as in figure 3.

It is seen from figures 1 and 2 that hot intervalley phonons do not influence considerably the dynamics of electron cooling and intervalley transfer. Some small effects can be seen only in the case when hot LO phonons are not taken into account. Hot-LO-phonon effects are so strong that hot-intervalley-phonon effects cannot manifest themselves against their background.

Figure 4 shows the evolution of non-equilibrium distributions of intervalley phonons. It is seen that the disturbances of the intervalley phonon distributions are more pronounced when hot LO phonons are taken into account. This is due to the higher intensities of electron intervalley scattering under the conditions of hot LO phonons. However, the intervalley phonon disturbances are two orders of magnitude lower than the LO phonon disturbances (figure 3). This is because of the high electron effective mass in the L valleys, resulting in a large q-space volume populated by intervalley phonons and a very small distribution of intervalley phonons. Therefore, more pronounced hot-intervalley-phonon effects are expected in semiconductors with low-mass subsidiary valleys.

In summary, the EMC method for hot-intervalley-phonon problems is proposed. The simulation results have shown that hot intervalley phonons do not affect significantly the electron-cooling and intervalley transfer dynamics in GaAs.

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