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LETTER TO THE EDITOR

Optic-phonon-limited mobility in a polar semiconductor

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Abstract. The effect of coupled-mode LO phonons on the momentum relaxation of electrons is studied within a model that takes the internal thermalization time of the LO-phonon system and the relaxation time of the whole lattice as parameters. Our analysis shows that the LO-phonon-limited electron mobility is markedly reduced at low temperatures due to the formation of finite-lifetime coupled modes in a polar semiconductor.

Considerable interest has recently been focused on the mechanism of the significant enhancement of the electron energy-loss rate (ELR) [1,2] in polar semiconductors, in the temperature region of 15–40 K, over the theoretical prediction of the well known Kogan formula [3] in a two-temperature model. Jain, Jalabert and Das Sarma [4] and Das Sarma, Jain and Jalabert [5] first proposed that coupling of LO phonons to the plasmon excitations of carriers and to the quasiparticle excitations of the electron gas might be responsible for this enhancement. Dharma-Wardana [6] called attention to the necessity of a nonequilibrium treatment of the problem [7]. In a recent paper [8], Lei and Wu pointed out that a model with separate electron and phonon temperatures and the concept of hot-electron energy loss to phonons is meaningful only when the internal thermalization in each subsystem (electron and phonon) is fast in comparison with the relaxation time due to the coupling between them. To simulate the internal thermalization of the LO-phonon system, we introduced a finite imaginary part in the bare phonon-retarded and advanced Green functions: $D^{r(a)}(q, \Omega) = (\Omega - \Omega_q \pm i/\tau_{pp})^{-1}$. τ_{pp} essentially represents the internal thermalization time of the LO-phonon system. The equilibration over the whole phonon system (lattice) takes a longer time τ_p than that needed for thermalizing individual phonons or certain subsets of the phonon modes, e.g. LO phonons, therefore $\tau_p > \tau_{pp}$. With these two relaxation times as parameters, we obtained the electron energy-loss rate by means of the Feynman diagrammatic technique for the Keldysh closed-time-path Green functions, taking account of contributions from all orders of the electron–phonon interaction (so called coupled mode) as suggested by Das Sarma and co-workers [3,4] and including the hot-phonon effect. The predicted energy-loss rate shows a significant enhancement at low temperatures over the prediction of the Kogan formula, in agreement with the experimental trends. By assuming that the anharmonic coupling between LO and acoustic phonons is the only channel for the emitted LO phonons to dissipate their energy to the lattice, Cao, Ting and Singh [9] were recently able to derive a similar but not identical ELR formula using a non-equilibrium Green

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function technique without introducing the phenomenological relaxation times. Their result is also able to account for the low-temperature enhancement of hot-electron ELR.

In addition to ELR enhancement, the finite lifetime LO phonons and their coupled mode with electrons also affect other transport properties of a polar semiconductor. The purpose of this letter is to analyse this coupled-mode effect on the electron mobility in polar systems.

Within the framework of the balance-equation theory of Lei and Ting [10], we can easily extend the discussion of [8] to the case of a drifting electron system under the steady-state high-field transport. We consider a model system which is composed of an interacting electron part (H_e), a LO-phonon part ($H_p = \sum_q H_p(q)$), and a heat bath H_B representing the rest of the lattice vibrations and their coupling with LO phonons. The total Hamiltonian is $H = H_e + H_p + H_{ei} + H_{ep} + H_B$, with H_{ei} and H_{ep} representing the electron–impurity and electron–LO-phonon interactions respectively. In the balance-equation theory, the electron–impurity and electron–phonon couplings are assumed to be effective from time $t = 0$, together with the electric field. The initial state is chosen such that the relative electron system is in a thermal equilibrium state at the electron temperature T_e and the LO-phonon system is in a quasiequilibrium state with a mode-dependent temperature T_q.

$$\hat{\rho}_0 = \frac{1}{Z}\exp(-H_e/T_e)\exp\left(-\sum_q H_p(q)/T_q\right). \tag{1}$$

The statistical averages of the rate of change of the electron total momentum, $\dot{\boldsymbol{P}} = -\mathrm{i}[\boldsymbol{P}, H]$, and the rate of change of the electron energy, $\dot{H}_e = -\mathrm{i}[H_e, H]$, leads to, in a steady-transport state with an average drift velocity $\boldsymbol{v}_d$, the force and energy balance equations of the form

$$N e\boldsymbol{E} + \boldsymbol{f}_i + \boldsymbol{f}_p = 0 \tag{2}$$

$$\boldsymbol{v}_d \cdot (\boldsymbol{f}_i + \boldsymbol{f}_p) + w = 0. \tag{3}$$

Here $\boldsymbol{f}_i$, the frictional force due to impurities , calculated to the lowest order in the scattering potential, has the same form as given in [10]. The frictional force due to LO phonons, $\boldsymbol{f}_p$, and the electron energy-loss rate to the LO-phonon system, w, are given by:

$$\boldsymbol{f}_p = \lim_{t\to\infty} \mathrm{Tr}[\hat{\rho}(t)\boldsymbol{F}_p] \tag{4}$$

$$w = \lim_{t\to\infty} \mathrm{Tr}[\hat{\rho}(t)W] \tag{5}$$

with the force operator $\boldsymbol{F}_p$ and the energy transfer operator W defined by

$$\boldsymbol{F}_p = -\mathrm{i}\sum_{k,q} M_q \boldsymbol{q}(b_q + b_{-q}^{\dagger})\mathrm{e}^{\mathrm{i}q\cdot R} c_{k+q}^{\dagger} c_k \tag{6}$$

$$W = \mathrm{i}\sum_{k,q} M_q \Omega_q (b_q - b_{-q}^{\dagger})\mathrm{e}^{\mathrm{i}q\cdot R} c_{k+q}^{\dagger} c_k. \tag{7}$$

Here $\hat{\rho}(t)$ is the density matrix satisfying the Liouville equation $\mathrm{i}\,\mathrm{d}\hat{\rho}(t)/\mathrm{d}t = [H, \hat{\rho}(t)]$ and the initial condition $\hat{\rho}(t_0) = \hat{\rho}_0$ and $\boldsymbol{R}$ denotes the time-dependent centre-of-mass coordinate.

Calculating $\boldsymbol{f}_p$ and w with the help of the Feynman diagrammatic technique for the Keldysh closed-time-path Green function, which is valid for this multi-temperature $\hat{\rho}_0$ in the balance-equation theory [11], taking account of contributions from all orders of quasiparticle (electron–hole) excitation of electron gas which are coupled to LO phonons through H_{ep} (coupled mode), and treating the hot-phonon effect with a single relaxation time τ_p which

is the time needed for the whole lattice vibration to equilibrate at lattice temperature T, we have, for the LO-phonon induced frictional force f_p and electron energy-loss rate w,

$$f_p = \sum_q \int \frac{d\Omega}{2\pi} \frac{-q}{\tau_p \operatorname{sgn}(\Omega) + \tau(q, \Omega - \omega_q)} \mathcal{R}(q, \Omega, \omega_q) \left[n\left(\frac{\Omega}{T}\right) - n\left(\frac{\Omega - \omega_q}{T_e}\right) \right] \tag{8}$$

$$w = \sum_q \int \frac{d\Omega}{2\pi} \frac{\Omega}{\tau_p \operatorname{sgn}(\Omega) + \tau(q, \Omega - \omega_q)} \mathcal{R}(q, \Omega, \omega_q) \left[n\left(\frac{\Omega}{T}\right) - n\left(\frac{\Omega - \omega_q}{T_e}\right) \right] \tag{9}$$

where

$$\mathcal{R}(q, \Omega, \omega_q) = \frac{-4\Omega\Omega_0/\tau_{pp}}{[\Omega^2 - \Omega_0^2 - 1/\tau_{pp}^2 + \Omega_0/\tau_1(q, \Omega - \omega_q)]^2 + [2\Omega/\tau_{pp} + \Omega_0/\tau(q, \Omega - \omega_q)]^2} \tag{10}$$

is an effective spectrum function,

$$1/\tau(q, \Omega) \equiv -2M_q^2 \Pi_2(q, \Omega) \tag{11}$$

is a wavevector- and frequency-dependent inverse scattering time, reflecting the coupling strength between electrons and phonons, and

$$1/\tau_1(q, \Omega) \equiv -2M_q^2 \Pi_1(q, \Omega). \tag{12}$$

Here $\Pi(q, \Omega) \equiv \Pi_1(q, \Omega) + i\Pi_2(q, \Omega)$ stands for the electron-retarded density–density correlation function at the electron temperature T_e, $n(x) = 1/(e^x - 1)$ is the Bose distribution function and $\omega_q \equiv q \cdot v_d$ is the Doppler shift.

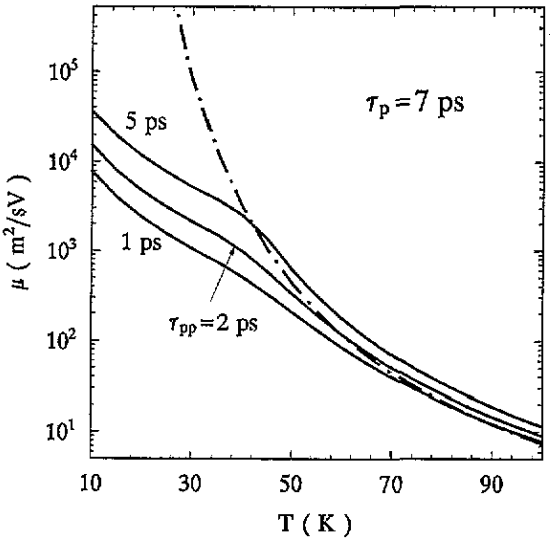

Figure 1. LO-phonon limited linear mobility μ versus the lattice temperature T for bulk GaAs. The solid curves are obtained from (10) and (13) with $\tau_p = 7$ ps and $\tau_{pp} = 1$, 2 and 5 ps respectively. The broken line is the electron mobility of bare LO phonon with $\tau_p = 7$ ps.

With the expressions (8) and (9) for f_p and w, we can solve balance equations (2) and (3) to obtain the drift velocity v_d and the electron temperature T_e. In the weak-current limit

the energy balance requires $T_e = T$ and the linear mobility limited by LO phonons is given by

$$\mu^{-1} = -\frac{1}{eNT}\sum_q \int_0^\infty \frac{d\Omega}{\pi}\,\frac{q_z^2}{\tau_p + \tau(q,\Omega)}\,\mathcal{R}(q,\Omega,0)\,n'(\Omega/T). \tag{13}$$

The LO-phonon limited mobility, calculated from (13) is shown in figure 1 as a function of the lattice temperature at $\tau_p = 7$ ps, $\tau_{pp} = 1$, 2, and 5 ps respectively for a bulk GaAs with carrier density $N_e = 1.5 \times 10^{23}$ m^{-3}, effective mass $m = 0.07m_e$, where m_e is the free electron mass and the LO-phonon energy $\Omega_q = \Omega_0 = 35.4$ meV. The broken curve in the figure is the LO-phonon limited linear mobility, obtained from the conventional mobility formula [10]

$$\mu^{-1} = -\frac{1}{eNT}\sum_q \frac{q_z^2}{\tau_p + \tau(q,\Omega_0)}\,n'(\Omega_0/T) \tag{14}$$

with $\tau_p = 7$ ps. Inclusion of finite-lifetime coupled modes markedly reduces the linear mobility at low temperatures.

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