MONTE CARLO MODELING OF THE DYNAMIC SCREENING EFFECTS ON ULTRAFAST RELAXATION OF PHOTO-EXCITED CARRIERS IN GaAs

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Abstract

The relaxation of photo-excited carriers in GaAs is investigated at 300K using an Ensemble Monte Carlo approach. The screening of the carrier-carrier(c-c) interaction is treated dynamically using a momentum and frequency dependent dielectric function in the Random Phase Approximation and in the Plasmon Pole Approximation. Calculated effective carrier temperatures agree with experimental data for time delays longer than 200fs.

I. INTRODUCTION

Femtosecond lasers allow the study of thermalization and initial relaxation of photo-excited carriers in bulk semiconductors [1, 2] as well as in quantum well structures[3]. Experimental investigations are paralleled by theoretical calculations, mostly Monte Carlo(MC) simulations[1, 2, 4]. Recently polarization related phenomena have also been introduced in an MC model[5], and such model is expected to give more information about the early moments following semiconductor laser excitation. MC simulations with the screening of the c-c interaction treated statically deviate from experimental data during the first 100-500fs after laser excitation, because static screening underestimates c-c scattering rates[1]. On the other hand, Molecular Dynamics(MD) provides a better agreement with the experiment[2] because MD realizes dynamic screening. However, MD requires an extensive CPU time. In this paper, we report on an alternative model for treating dynamic screening of the c-c interaction in MC simulations. The model takes into account the wave-vector and frequency dependence of the dielectric function. Simulations are performed for two different implementations. The first uses the Random Phase Approximation(RPA) to the dielectric function as in the analytical calculations of Meyer and Bartoli[6]. The second approach implements the Plasmon Pole Approximation(PPA) to the dielectric function, recently used by Collet[7] in analytical calculations. The model is applied to carrier relaxation in p-type and i-type GaAs. A laser of 2eV photon energy and 50fs duration is assumed. Two excitation densities of $2 \times 10^{18} cm^{-3}$ and $2.5 \times 10^{16} cm^{-3}$ are simulated, so that c-c and carrier-phonon processes could be observed. Results show a good agreement between the proposed dynamic approach and the experiment for time delays longer than 200fs.

II. COMPUTATIONAL MODEL

The Monte Carlo model for the electrons includes non-parabolic Γ, L and X valleys. The MC program for electrons considers elastic acoustic phonon scattering, the intervalley deformation potential, the screened polar-optical phonon, dynamically screened electron-electron(e-e) and electron-hole(e-h) scattering. The MC program for holes is based on a 3-band model where the heavy and light hole bands are warped, while the split-off band is spherical parabolic. Scattering mechanisms included are elastic acoustic phonon, optical phonon scattering, self-consistent screened polar optical phonon and screened hole-hole scattering.

An alternative formulation of the c-c interaction is implemented, where use is made of a wavevector and frequency dependent dielectric function in the interaction potential. Following the approach of Meyer and Bartoli[6], the interaction potential can be written as:

$$U(\mathbf{q}) = \frac{e^2}{q^2 \epsilon_o \epsilon(q, \omega = \mathbf{q}.\mathbf{v_{cm}})} \tag{1}$$

where $\epsilon(q,\omega)$ is the dielectric function, $\mathbf{q}$ is the relative wavevector, and $\mathbf{v_{cm}}$ is the velocity of the center of mass. The general expression of the RPA is used in the determination of the free-carrier contributions to the dielectric function. Making use of the above interaction potential, the e-h scattering rates are given by:

$$\Gamma_{e-h}(\mathbf{k_h}) = \frac{2p\mu e^4}{2\pi\hbar^3 {\epsilon_o}^2 g} \sum_{k_h} f_{\mathbf{k_h}} \int_o^g \frac{dq}{q^3 |\epsilon(q,\omega)|^2} \tag{2}$$

where e is the electron charge, p is the hole density, μ is the reduced mass of the interacting particles, and $\mathbf{g}$ is a relative wavevector defined as:

$$\mathbf{g} = 2\mu(\frac{\mathbf{k_e}}{m_e} - \frac{\mathbf{k_h}}{m_h}) \tag{3}$$

where $\mathbf{k_e}(\mathbf{k_h})$ is the electron(hole) wavevector, and $m_e(m_h)$ is the electron(hole) mass. In the e-e interaction, p is replaced by n, and electron wave vector and mass rather than hole wavevector and mass are used in $\mathbf{g}$.

The scattering rates are calculated in the Monte Carlo program as follow. First the components of the center of mass velocity of the interacting particles and the components of the relative wavevector are found. In order to determine $\mathbf{q}$, the knowledge of both the initial and final carrier states are required, which is a problem as scattering has not taken place yet. An approximate value can be found by using virtual scattering processes: for a given electron, we choose at random an ensemble of target particles to scatter with, determine the resulting virtual next state and change in wavevectors for each collision. However, the states of the scattering charge carriers are not updated. Thereafter, it becomes possible to determine the components of $\mathbf{q}$ and to calculate the frequency. The next step is the determination of the total dielectric function, where the free carrier contributions are obtained by numerically integrating the corresponding expressions. After repeating this process with an ensemble of target carriers, an average of the c-c scattering rate for the given electron is found. The average c-c scattering rates obtained in the current calculation were about 3 to 7 times higher than the values obtained in the self-consistent static approach of reference [4]. Ideally, the c-c scattering rates should be calculated every time a scattering process takes place. However, the computation time can be reduced by using a three-dimensional scattering table in k-space, where a given scattering rate is stored in a corresponding k-cell to be accessed whenever necessary. For an iteration step of 2.5fs with the scattering table updated every iteration for the first 200fs, one picosecond simulation of 5000 particles took about 11 hours on the IBM3090.

Recently Collet[7] used the PPA dielectric function. This is a simpler analytical approximation, which results in saving of CPU time, as the dielectric function is free of integrations. The scattering rates are still determined using eq.2, and following the procedure presented above. This implementation requires about 3 times less CPU time when compared to the RPA approach.

III. RESULTS

The cooling of photo-excited carriers in p-GaAs was investigated at 300K. The assumed 2.0eV laser photon energy excites carriers from the heavy, light and split-off bands in the ratio 0.46:0.32:0.22, in accordance with recently published data[1]. Figure 1 shows the time evolution of the electron

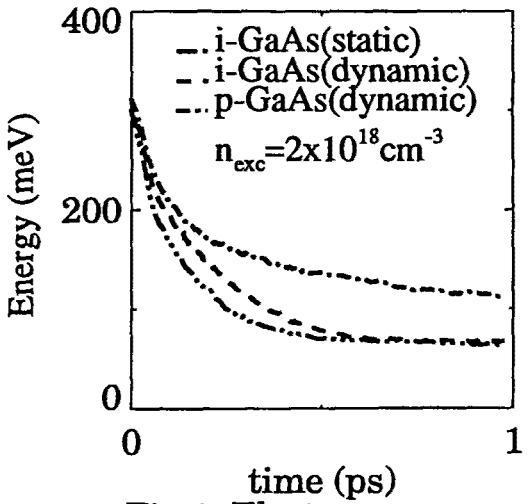

Fig.1. Electron energy

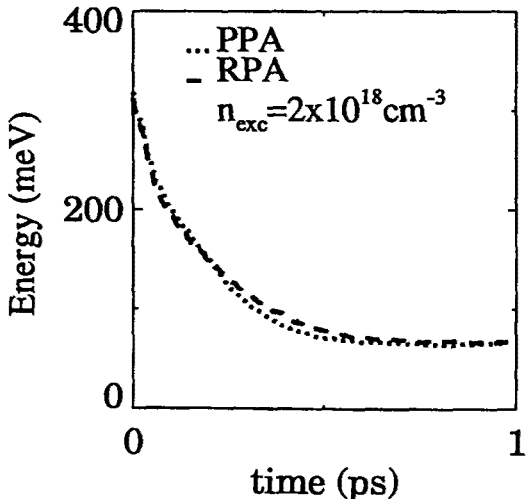

Fig.2. RPA and PPA results

energy, where the origin of the time axis corresponds to the peak of the exciting laser. The figure shows that dynamic screening of the c-c interaction results in faster cooling of the electrons when compared to the time-dependent static model of reference [4]. The faster cooling during the first 500 femtoseconds is mostly due to electron energy loss to holes. Accordingly, holes heat up, but the gained energy is rapidly dissipated through non-polar and polar phonon emission. The faster cooling in p-GaAs demonstrates that added hole concentration due to doping results in additional electron energy loss to holes. In the dynamic case, electrons redistribute energy and momentum among themselves and lose energy to the holes at a faster rate when compared to the static approach. Figure 2 compares the results of the RPA and PPA implementations of the dynamic screening of the c-c interaction. It can be seen that the PPA approximates well the RPA results. The two cases are within 10% of each other.

Figure 3 shows the theoretical effective carrier temperatures extracted from the slope of the near exponential tail of the luminescence intensity for the RPA, the PPA, the static screening model, and the experimental data[1] in i-GaAs, for $n_{exc} = 2 \times 10^{18} cm^{-3}$. The calculated electron temperature is within 10% of the experimental values for time delays longer than 300fs in i-GaAs, and within 10% at 200fs in p-GaAs. It can be seen that the static screening model always predicts electron temperatures higher than the experiment and the present model for time delays shorter than 500fs. However, the dynamic screening models still predict electron temperatures that are higher than experimental data at time delays shorter than 200fs. This is partly due to the approximations used in the calculation of the dielectric functions. Additionally, this model does not include the full details of the energy band structure, ignores higher order quantum corrections in the scattering rate calculations, and polarization and quantum coherence which become important at short time scales.

The simulation was repeated at the lower excitation and doping density of $2.5 \times 10^{16} cm^{-3}$ to ex-

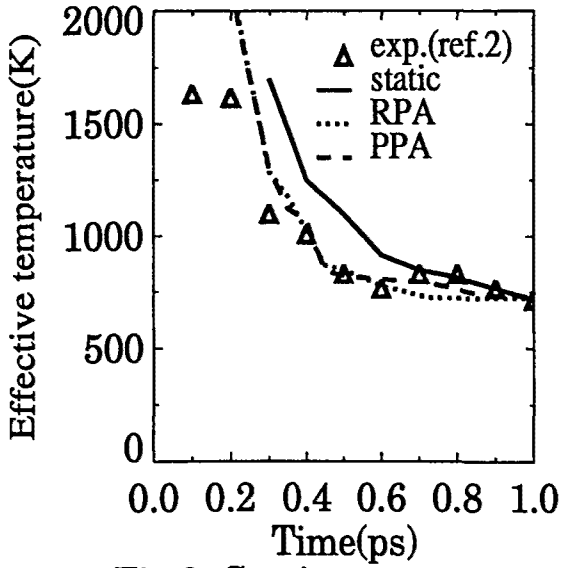

Fig.3. Carrier temperature

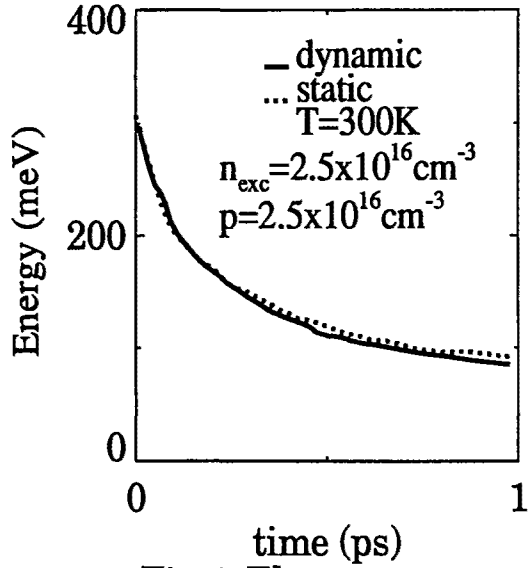

Fig.4. Electron energy

amine the role of c-c and c-phonon processes for both dynamic and static screening. It can be seen in Fig.4 that the average energy is not strongly affected by the screening model used in calculating c-c scattering rates, because, at low carrier densities, the e-phonon interactions are the main energy loss channels.

IV. CONCLUSION

An expression for dynamically screened c-c scattering that takes into account the wavevector and frequency dependence of the dielectric function in the RPA and in the PPA was developed and implemented in an MC program. The relaxation of photo-excited carriers in GaAs was examined using these two screening models, in addition to static screening. The obtained carrier effective temperatures are in good agreement with the experiment for time delays longer than 200fs in the dynamic cases, compared to 500fs in the static case.

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