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Electron-phonon coupling and transient dynamics of hot carriers: from interpretation of photoemission experiments to transport simulations in devices.

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ABSTRACT

The progress in DFT-based description of the electron-phonon scattering allowed to describe the relaxation dynamics of hot or photoexcited electrons in several materials, in very good agreement with time-resolved spectroscopy experiments. As hot carriers also start to attract attention in the context of emerging concepts for energy conversion, here we present our first results related to the coupling of ab initio data with device-oriented Monte Carlo simulation methods. We show that DFT-based description of the electron-phonon intervalley scattering in GaAs, coupled with the stochastic Monte Carlo method, allows to describe the energy transfer from electrons to phonons in transient regime, in good agreement with previous time-resolved photoemission experiments.

Keywords: electron-phonon coupling, semiconductor, photoexcited electrons, Monte Carlo simulations

1. INTRODUCTION

Methods based on density functional theory (DFT) allow today to describe electron-phonon scattering rates from first principles.^{1,2} It was shown that electron transport characteristics of many 3D and 2D semiconductors are well described within the approaches which couple DFT with the Boltzmann Transport Equation (BTE).³ At the same time, the progress in DFT-based description of the electron-phonon scattering also allowed to describe the relaxation dynamics of hot or photoexcited electrons in several materials, in very good agreement with time-resolved spectroscopy experiments.^{4,5} For example, in 4,6, the two-photon photoemission experiments were able to capture both the initial momentum randomization of the photoexcited electrons due to electron-phonon scattering and the energy transfer from electrons to phonons, for electrons photoexcited into the conduction band of GaAs. Both relaxation mechanisms were well described by the DFT-based calculations.^{4,6}

In some cases, however, the theoretical approaches which couple DFT description of materials with the *static* BTE turn out to be insufficient. Instead, one has to describe the evolution in time of photoexcited, nonthermal carrier distributions.⁷⁻¹² Indeed, time-resolved spectroscopy techniques, such as time- and angle-resolved photoemission spectroscopy as well as phase-resolved transient absorption spectroscopy, provide the possibility to monitor *transient* material characteristics which are due to photoexcited carrier distributions evolving on femtosecond and attosecond time scales.^{6,13-16} In a similar way, future generations of energy converters might involve high energy carriers, therefore requiring reliable theoretical approaches to describe the *transient* transport properties of devices.^{17,18} Among the numerical methods available for describing the time evolution of carrier distributions, the particle Monte Carlo method for solving the BTE provides reliable, numerically stable results

at low numerical cost.¹⁹ This approach makes it possible to capture carrier distributions far from equilibrium, and to take into account complex diffusion mechanisms with highly anisotropic behavior.

In this work, we discuss the coupling of device-oriented the stochastic Monte Carlo (MC) approach^{20–22} with the *ab initio* description of the electron-phonon coupling,^{23,24} in the case of GaAs. It must be noted that some of the specific problems encountered when the effective electron-phonon coupling constants calculated with DFT-based methods are coupled with MC approaches were discussed e.g. in Ref. 25 for silicon, and, recently, in Refs. 26, 27 for GaAs. In the present work, we focus specifically on the energy transfer from electrons to phonons in transient regime, which is governed by the intervalley electron-phonon scattering, as was shown e.g. in Ref. 4.

The paper is organized as follows. First, we will present briefly the theoretical framework and technical details of our DFT and MC calculations. Then, we will present the results of the MC simulation of the energy transfer rate from the photoexcited electrons to phonons, coupled to DFT-based intervalley scattering parameters. We will show that DFT-based description of the electron-phonon intervalley scattering in GaAs, coupled with the stochastic Monte Carlo method, allows to describe the energy transfer from electrons to phonons in transient regime, in good agreement with previous time-resolved photoemission experiments.

2. THEORETICAL FRAMEWORK AND COMPUTATIONAL DETAILS

The total electron-phonon scattering rate, or self-energy, is implemented, e.g., in the EPIq code²³ and defined in numerous other works:^{4, 28–30}

$$\Gamma_{n,\mathbf{k}} = \Gamma_{em} + \Gamma_{abs} \quad (1)$$

where

$$\begin{aligned} \Gamma_{em} &= \frac{2\pi}{\hbar} \sum_{m\nu} \int \frac{d\mathbf{q}}{\Omega_{BZ}} |g_{m\nu}(\mathbf{k}, \mathbf{q})|^2 (N_{\mathbf{q},\nu} + 1 - f_{m,\mathbf{k}+\mathbf{q}}) \delta(\varepsilon_{n,\mathbf{k}} - \varepsilon_{m,\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu}) \\ \Gamma_{abs} &= \frac{2\pi}{\hbar} \sum_{m\nu} \int \frac{d\mathbf{q}}{\Omega_{BZ}} |g_{m\nu}(\mathbf{k}, \mathbf{q})|^2 (N_{\mathbf{q},\nu} + f_{m,\mathbf{k}+\mathbf{q}}) \delta(\varepsilon_{n,\mathbf{k}} - \varepsilon_{m,\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu}) \end{aligned} \quad (2)$$

Here, all emission and absorption processes allowed by energy and momentum conservation are taken into account. $g_{m\nu}(\mathbf{k}, \mathbf{q})$ stand for the electron-phonon matrix elements between electronic states with m and n band numbers, coupled *via* the phonon mode ν . $N_{\mathbf{q},\nu}$ stand for phonon population numbers (Bose-Einstein distribution), $f_{n,\mathbf{k}}$ is the electron Fermi-Dirac distribution function, $\varepsilon_{n,\mathbf{k}}$ are electron eigenenergies and $\omega_{\mathbf{q}\nu}$ are phonon frequencies. The total electron-phonon scattering rate expresses the probability for an excited electron to change its initial momentum, i.e. to be scattered elsewhere in the Brillouin zone.^{4, 6}

The density of final electronic states *FDOS* represents the phase space available for scattering from a given initial electronic state, it is determined by the energy and momentum conservation rules and by the temperature *via* the phonon occupation numbers (i.e. *via* Bose-Einstein coefficients):

$$FDOS_{n,\mathbf{k}} = \frac{2\pi}{\hbar} \sum_{m\nu} \int \frac{d\mathbf{q}}{\Omega_{BZ}} [(N_{\mathbf{q},\nu} + 1 - f_{m,\mathbf{k}+\mathbf{q}}) \delta(\varepsilon_{n,\mathbf{k}} - \varepsilon_{m,\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu}) + (N_{\mathbf{q},\nu} + f_{m,\mathbf{k}+\mathbf{q}}) \delta(\varepsilon_{n,\mathbf{k}} - \varepsilon_{m,\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu})] \quad (3)$$

The rate of energy transfer from electrons to phonons, reads:^{4, 28, 31}

$$\begin{aligned} \frac{\delta E}{\delta t} &= \Gamma_{em} \omega_{em} - \Gamma_{abs} \omega_{abs} = \\ &= \frac{2\pi}{\hbar} \sum_{m\nu} \int \frac{d\mathbf{q}}{\Omega_{BZ}} \omega_{\mathbf{q}\nu} |g_{m\nu}(\mathbf{k}, \mathbf{q})|^2 (N_{\mathbf{q},\nu} + 1 - f_{m,\mathbf{k}+\mathbf{q}}) \delta(\varepsilon_{n,\mathbf{k}} - \varepsilon_{m,\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}\nu}) - \\ &\quad - \frac{2\pi}{\hbar} \sum_{m\nu} \int \frac{d\mathbf{q}}{\Omega_{BZ}} \omega_{\mathbf{q}\nu} |g_{m\nu}(\mathbf{k}, \mathbf{q})|^2 (N_{\mathbf{q},\nu} + f_{m,\mathbf{k}+\mathbf{q}}) \delta(\varepsilon_{n,\mathbf{k}} - \varepsilon_{m,\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}\nu}) \end{aligned} \quad (4)$$

	Scattering channel	$\Gamma - L, L - \Gamma$	$\Gamma - X, X - \Gamma$	$L - L$	$X - X$	$X - L, L - X$
MC from 36	D^{eff} , eV/Å	10	10	10	7	5
	ω_{eff} , meV	27.8	29.9	29.0	29.9	29.3
DFT-based, this work	D^{eff} , eV/Å	4	4	4	4	4
	ω_{eff} , meV	19	19	19	19	19

Table 1. Effective deformation potentials and phonon frequencies for intervalley scattering in GaAs: MC parameters from Ref. 36 and *ab initio* DFT-based parameters determined in this work.

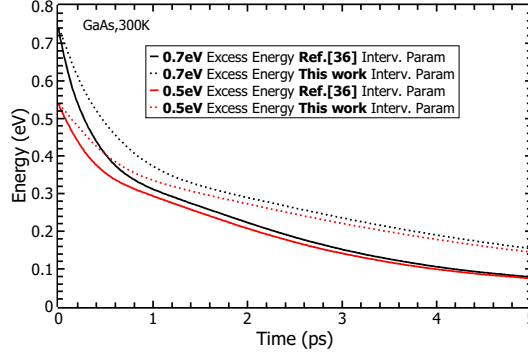


Figure 1. MC simulation of the evolution with time of the average energy of out-of-equilibrium carrier distributions excited initially at 0.5 eV and 0.7 eV above the conduction band minimum.

In this work, we have used the method of calculation of the electron-phonon matrix elements based on the density functional perturbation theory (DFPT)^{32,33} and interpolation in the Wannier representation^{29,34} using the EPIq code.^{23,24,34} All technical details for the DFT-based description of GaAs can be found in 24.

The effective electron-phonon parameters which are necessary to couple the DFT-based data with MC approach, can be obtained from the quantities of eqns. 2 and 3, calculated for specific scattering channel, i.e. for specific phonon modes and/or for specific parts of the Brillouin zone:²

$$|g_{n,\mathbf{k}}^{eff}| = \sqrt{\Gamma_{n,\mathbf{k}}/FDOS_{n,\mathbf{k}}} \quad (5)$$

The electron-phonon deformation potentials are related to the electron-phonon matrix elements as follows:³⁵

$$D^{eff} = \frac{\sqrt{2\rho\Omega\omega_{eff}}}{\hbar} |g^{eff}| \quad (6)$$

Here, ρ is the mass density of the crystal, Ω is the crystal volume, ω_{eff} is phonon frequency.

The deformation potentials defined in eq. 6 which are commonly used in MC solvers are empirical parameters adjusted to reproduce the characteristics of the velocity vs. electric field in the stationary regime. The set of parameters defined in Ref. 36 which were used previously in our MC approach and the ones derived from DFT in this work are listed in Table 1.

3. RESULTS

Although the electron-phonon matrix elements calculated with DFT methods depend on both the electronic and phonon states, the averaging procedure of eq. 5 which included all phonon modes and was limited to intervalley processes (i.e. phonons with $|\mathbf{q}| > 0.25\frac{2\pi}{a}$, where a is lattice parameter) allowed us to conclude that, for the dominant intervalley channels in GaAs, the dependence of the effective electron-phonon matrix elements on the initial electronic state was weak. Finally, our DFT calculations allowed us to choose the constant value of $D_{eff}^{dft} = 4$ eV/Å as representative of the strength of the electron-phonon intervalley coupling in GaAs. One can notice from table 1 that the average strength of the intervalley scattering and the effective phonon frequencies

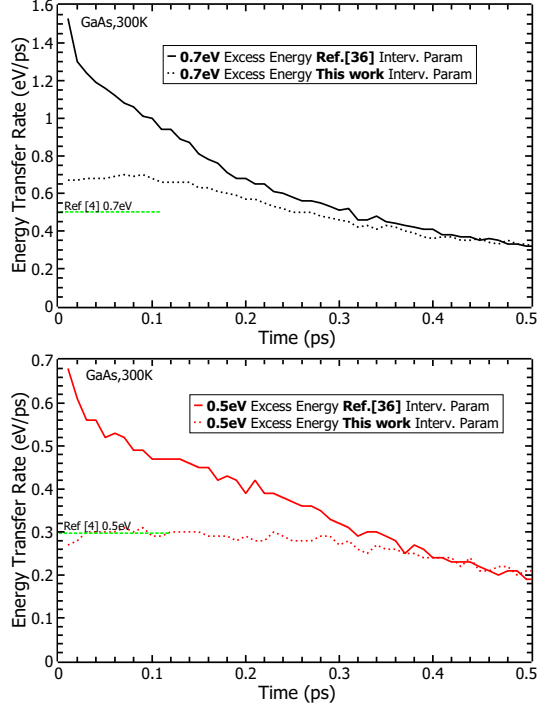


Figure 2. MC simulation of the evolution with time of the energy transfer rate from electrons to phonons, for the out-of-equilibrium carrier distributions excited initially at 0.7 eV (upper panel) and 0.5 eV (lower panel) above the conduction band minimum. The energy transfer rate curves were obtained from the average energy curves shown in Fig. 1. The values of the energy transfer rate from photoexcited electrons to phonons in GaAs, measured in Ref. 4 using time-resolved photoemission are indicated by the green lines.

determined with DFT differ strongly from the values used initially in MC simulation of Ref. 36. This difference is expected to have a strong impact on the transient regime at high carrier energy.

The results of the time-dependent MC simulation of the evolution with time of the average energy of out-of-equilibrium carrier distributions excited initially at 0.5 eV and 0.7 eV above the conduction band minimum are plotted in Fig. 1. The initial electronic distributions were modeled by Gaussian functions centered around 0.5 eV and 0.7 eV excess energies. We compare the MC results obtained with the intervalley scattering constants presented in table 1: the ones of Ref. 36 (solid curves) and the ones determined in this work on the basis of DFT description (dashed curves). As one can see in Fig. 1, as expected, the change in the intervalley scattering constant and in effective frequencies reduces strongly the energy transfer rate from electrons to phonons, due to the dominant role of the intervalley scattering in the energy transfer from photoexcited electrons to phonons.⁴ Also as expected, the energy transfer rate is found to reduce with time, as the electron distribution approaches equilibrium.

In Fig. 2, we show the evolution with time of the energy transfer rate from electrons to phonons, for the same out-of-equilibrium carrier distributions as in Fig. 1. The energy transfer rate curves were obtained from the average energy curves shown in Fig. 1. As one can see in Fig. 2, at early times, the change in the intervalley scattering constant strength changes strongly the energy transfer rate from electrons to phonons.⁴ Interestingly, as one can see in Fig. 2, for time values greater than 0.4 ps, the energy transfer rate is not affected by the drastic change in the intervalley scattering parameters. Finally, as shown in Fig. 2, our MC results using D_{eff}^{dft} are found in good agreement with the experimental energy transfer rate from photoexcited electrons to phonons, which was measured in Ref. 4 using time-resolved photoemission.

4. CONCLUSION

In conclusion, we have presented the results of a successful coupling of the stochastic MC simulation with DFT-based description of the intervalley electron-phonon coupling in GaAs. We find that the change in the intervalley scattering constant strength changes strongly the energy transfer rate from electrons to phonons for times smaller than 0.4 ps, and that the MC results using DFT values are found in good agreement with the experimental energy transfer rates from photoexcited electrons to phonons, which were measured with time-resolved photoemission. Moreover, we find that, for the rate of energy transfer from electrons to phonons, the steady state is not affected by the change in the intervalley scattering description, in contrast to transient state.

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The DFT calculations were performed using the Quantum ESPRESSO,³³ EPIq²³ and Wannier90³⁷ packages.

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