Fullband particle-based simulation of high-field transient transport in III-V semiconductors.

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ABSTRACT

Motivated by the recent experimental measurements of Tera-Hertz radiation [1], this work presents the transient analysis of photogenerated electron-hole pairs in GaAs and InP *pin* diodes using a full-band particle-based simulator.

Excellent agreement is found between the experimental and simulated results of the transient acceleration and velocity overshoot effects in GaAs and InP *pin* diodes due the femto-second optical excitation of carriers.

Keywords: Tera-Hertz radiation, high-field transport, Monte Carlo simulation.

1 INTRODUCTION

Ultra-fast optical excitation can be used as a probe to study the nonlinear behavior of high-field electronic conduction, which can be an important design consideration in modern high-speed semiconductor devices. Recent experimental measurements, reported in [1], have provided insight into the microscopic mechnanisms governing highly nonequilibrium transport in GaAs and InP. Using a full-band particle-based simulator previously discribed in [2], the transient behavior of photogenerated electron-hole pairs in GaAs and InP *pin* diodes is modeled. The simulations of the transient acceleration and velocity overshoot effects after femto-second optical excitation of carriers successfully reproduces the experimental measurements.

Within the framework of the experiment, radiation fields due to electrons and holes cannot be distinguished, and the contribution due to holes is often neglected. However, the simulation shows that the hole contribution is quite significant. Hole velocity overshoot effects are also presented, and are found to be due to the change in effective mass in the heavy hole valence band.

This work is organized as follows, a brief discussion of the experimental and simulation setup is presented in the next section, than a comparison of the results and a discussion is presented, and finally a conclusion is given in the last section.

2 TERA-HERTZ RADIATION

2.1 Experiment

In the experminetal setup a mode-locked Ti:Sapphire laser with a pulse duration of 12fs, a central photon frequency of 1.49 eV, and a bandwidth of 120meV, is used to optically excite electron-hole pairs in a GaAs and InP *pin* diode with an intrisic region 500nm long. Each pump of the laser creates a low density $(5 \times 10^{-14} cm^{-3})$ of carriers, as a result Coulomb scattering due to the phot0-generated carriers as well as screening effects can be neglected. The measured THz electric field amplitude is proportional to the first time derivative of the diode current density. The time derivative of the current is determined experimentally from the acceleration of charges due to the externally applied electric field and scattering, the dielectric response of the crystal lattice due to free carrier displacement, and the current drop due to carriers leaving the intrinsic region. The free carrier contribution to the THz signal is calculted by correcting the amplitude and phase spectra with the dielectric response function of the semiconductor. In this way the experimental measurements can be directly compared with the simulation results, which only show the free carrier response.

2.2 Simulation

A full-band particle-based simulation tool previously described in [2] is used to model the above described experiment. The full-band description of the dispersion relation is important to descibe the charge transport at high electric fields (up to 130 kV/cm). The simulation tool uses an empirical pseudo-potential method to describe the full-band structure of both electrons and holes in GaAs and InP. The full band phonon spectra is also calculated using a valence shell model. In particular, both the longitudinal acoustic and optical phonons have been included for the deformation potential interaction, and the polar optical interaction is treated with the full dispersion of the longitudinal optical phonons. Impact ionization scattering has also been included using the empirical method described in [3]. Calibration of the steady-state velocity-field characteristics for both GaAs and InP have been compared with values reported in literature [3] and show good agreement, as can be seen for InP in Fig. 1. The technique used for the steady-state simulations is the so-called Cellular Monte Carlo (CMC) method which originated with name Cellular Autamata. The transient simulations were run with a hybrid Ensemble Monte Carlo (EMC)/CMC technique. Within this approach EMC scattering tables are used in the high energy regions of the Brillouin zone.

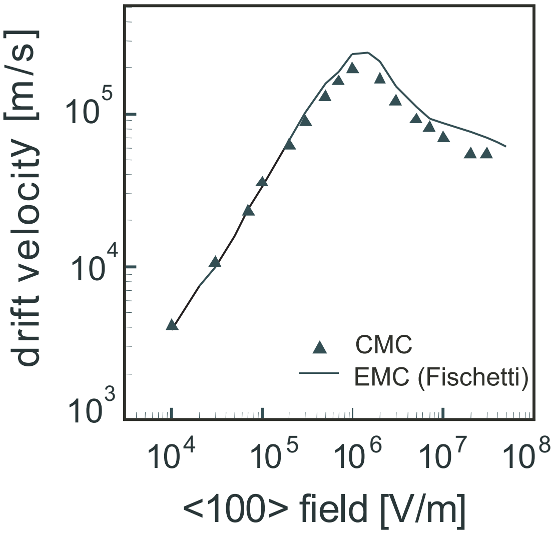

Figure 1: Steady-state electron velocity as a function of electric field for InP at 300K. The CMC is the Cellular Monte Carlo method and used in these simulations, refered to as the Cellular Automata (CA) method in literature.

Carriers are only simulated in the intrinisc region of the *pin* diode since the diffusive transport which takes place for carriers that leave the intrinsic region is very slow, and any contribution to the THz signal is negligible. The intrinisic region of the GaAs and InP are simulated with a 500x100 homogeneous grid in real space with a cell side dimension of 1nm. A constant electric field is applied across the device and the photoexcitation process is simulated by injecting electron-hole pairs into the intrinsic region. The number of injected particles is determined using an empirical model for the generation rate [4],

$$G(t) = I_0[\cosh(\frac{2.634t}{t_p})]^{-1}, \quad (1)$$

where t_p is the half-width of the pulse, and I_0 is the incident intensity determined by the experimental measurement of the total density of injected carriers. The time dependent electron and hole densities are calculated by integrating the generation rate, the total number of electron-hole pairs simulated is 100,000. The change in concentration at each time step, for both types of carriers is then given by the equation,

$$\delta n(t) = \frac{2n_{inj}}{\pi}(\tan^{-1}(e^{w(t-t0+\delta t)}) - \tan^{-1}(e^{w(t-t0)})), \quad (2)$$

where $w = 2.634/t_p$, n_{inj} is the total density of injected carriers, δt is the time step set to $0.2fs$, and t_0 represents the time at which the pulse is turned on. The influence of the dipole radiation on the internal field has been neglected due to the low carrier densities. The energy of the carriers is determined by the optical pulse frequency, and electrons are assigned to the lowest conduction band and holes are assigned to the highest valence band, which corresponds to the heavy hole band. The real space positions are determined using the absorption coefficient for interband transitions in bulk semiconductors.

The current density as a function of time in the *pin* diode is calculted using the equation [5],

$$J(t) = J_e(t) + J_h(t) = \frac{Q_e}{Vol}\sum_{i}^{N_e} v_i(t) + \frac{Q_h}{Vol}\sum_{j}^{N_h} v_j(t), \quad (3)$$

where Q_e and Q_h are the super-particle charge for electrons and holes respectivily, Vol is the volume of the intrinsic region, N_e and N_h are the number of electrons and holes in the sample, and $v(t)$ is the corresponding velocity. The velocity can than be calculted as,

$$v_{e,h}(t) = \frac{J_{e,h}(t)}{en(t), ep(t)} \quad (4)$$

where e, h referes to electrons or holes and $n(t)$,$p(t)$ is electron and hole concentration, respectively. The acceleration is then determined by taking the first derivative and the displacement is calculted by integration.

3 RESULTS AND DISCUSSION

Simulations are run for several electric field values in both GaAs and InP, and comparisons with experiment show excellent agreement. The acceleration of electrons and holes in InP for a field of 90kV/cm is shown in Fig. 2.

The hole contribution to the radiation field in the nonequilibrium regime is generally neglected due to the large effective mass in the heavy hole band. In our simulation results, which allows for the direct examination of the influence of holes, we find that the holes significantly contribute to the transient acceleration. In fact, the peak acceleration of hole can be as high as 1/4 of the electron acceleration. Another interesting phenomena found in the transient response of holes is a pronounced velocity overshoot. It is well known that, the mechanism for electron velocity overshoot is due to intervalley

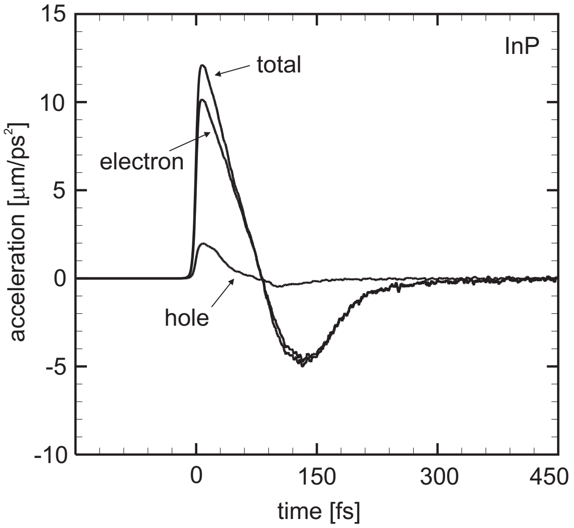

Figure 2: Charge acceleration in InP at 300K for an applied electric field of 90 kV/cm.

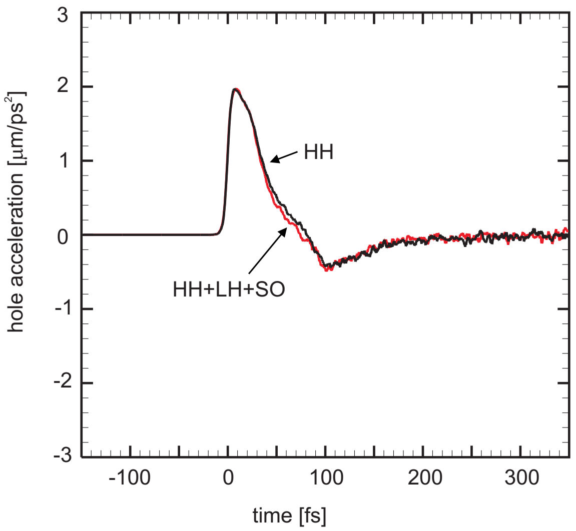

Figure 3: Comparison of hole acceleration in InP simulations with only one heavy hole (HH) band and with heavy hole, light hole and spin split off bands (HH+LH+SO). No significant change in the results is found. The negative acceleration is due to the changing effective mass along the heavy hole band. An externally field of 90kV/cm was applied.

transfer from the Γ-valley to the L-valley. As electrons scatter into the L-valley their mobility decreases due to the heavier effective mass. No such mechanism exists in the valence bands since the carriers originate in the heavy hole band. Instead, the velocity overshoot for holes is due to the change in effective mass in the heavy hole band.

Comparisons of the maximum drift velocities in GaAs for several applied field values are shown in Fig. 4. The peak velocity of electrons is lower than the experimental measurements, and better agreement is found when the velocity is calculated with the entire signal, included electrons and holes. The time required to reach the maximum drift velocity in GaAs for an applied electric field of 30 kV/cm is 172fs and 53fs for 130 kV/cm, which is comparable to the measured values of 200fs and 55fs, respectively.

The displacement is calculted from the double integral of the acceleration. At significantly high electric fields the displacement at the maximum peak velocity is expected to be approximately the drift distance necessary for electrons to reach an energy corresponding to the Γ-L valley splitting, which is 330meV in GaAs and 660meV in InP. The simulation results show comparable values for high fields, but are significantly lower than the experimental results for fields less than 100kV/cm.

The simulations of InP were run using the full CMC for the dynamics algorithm. The total simulated time is 600 fs and took approximately 1.5-2 hours of CPU time. Due to memory restrictions, the GaAs simulations used the hybrid CMC/EMC algorithm, with the EMC implemented in the regions of the bands where the electron and hole energes are above 3eV and the CMC elsewhere as described in [2]. The time required to simulate 600 fs was approximately the same (1.5-2 hours).

4 CONCLUSIONS

In this study we have successfully modeled velocity overshoot effects in GaAs and InP due the transient acceleration of photogenerated carriers for fields as high as 130 kV/cm. The simulations successfully reproduced the experimental measurements of the THz radiation caused by the acceleration of charged particles. The relative influence of electrons and holes on the experimental results has also been assessed. Holes have been found to contribute significantly to the overall transient response. Velocity overshoot effects due to holes have also been shown, due to the change in effective mass along the heavy hole band.

Acknowledgments

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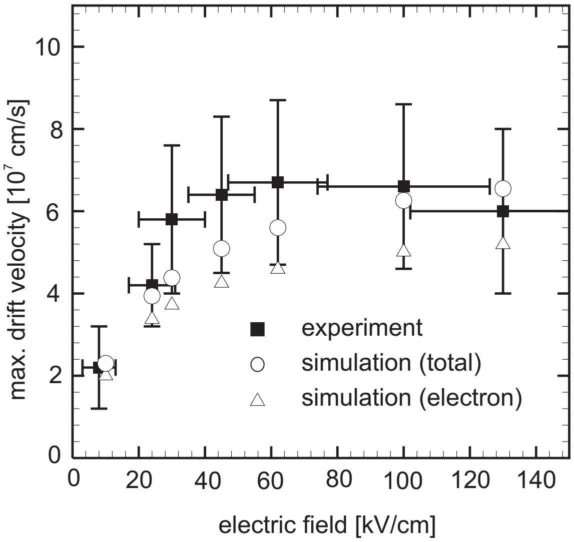

Figure 4: Simulated peak velocity versus electric field compared with experiment for GaAs at 300K. The peak velocity calculted with electrons and holes is in better agreement with experiment values, than for electrons alone.

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