Fullband particle-based simulation of optical excitation in Silicon *pin* diodes

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ABSTRACT

In this study, a fullband particle-based simulator is used to model optical excitation in silicon. This work is motivated by previous simulations of transient transport in III-V material as well as recent experimental measurements of optically excited Si *pin* diodes. The simulation results show evidence of velocity overshoot at high fields ($\geq$100 kV/cm) which is not present in the experiment. Further simulations show that the influence of lattice temperature may be responsible for the discrepancy.

Keywords: Optical excitation, Silicon, Fullband particle-based simulator.

1 INTRODUCTION

In this study, a fullband particle-based simulator [1] [2] is used to model photo-generated electron-hole pairs in Si to investigate charge transport at high electric fields and ultra-short time scales. Previous fullband optical excitation studies were conducted in III-V *pin* diodes and showed excellent agreement with experimental measurements of velocity overshoot behavior [3]. This analysis combined with recent experimental measurements of optically excited Si *pin* diodes has motivated this work.

The simulation of electron-hole excitation in indirect materials is more complicated than in the previous work due to the phonon assited absorption process. All six phonon modes are represented as a fullband spectra and a search must be made over all conduction, valence and phonon bands to find all possible three particle states that satisfy the conservation laws. A table of states is constructed and during runtime electrons and holes are generated in the intrinsic region of the *pin* diode based on the ratio of the emission to absorption of the phonons. The peak laser frequency used in the experiment is very large (approximately 1.6 eV) so that the number of possible final states in the simulation exceeds 500,000. The spectral width of the laser is currently neglected because of the increased number of final states.

The simulations only show electron and hole velocity overshoot for fields above 100 kV/cm, while in the experimental work no overshoot is observed at any fields. The temporal transition to steady-state transport is also found to be faster than in the experiment. Simulations with increased lattice temperatures show a decrease in the velocity overshoot suggesting that the discrepancy may be due in part to self-heating in the experimental work. Further work needs to be done to investigate the causes of the velocity overshoot in the simulations.

In the following section the fullband particle-based simulation tool is briefly described. The approach used to model the phonon assisted optical excitation is then discussed. Finally, the simulation results are presented and comparisons with experimental work is discussed.

2 FULLBAND SIMULATOR

Simulations are performed with a fullband particle-based code which has been previously described in detail [4]. The band structure is calculated with an empirical pseudo-potential method [5] and the full band phonon spectra is calculated using the valence shell model and includes the spin orbit interaction. Deformation potential scattering rates are calculated using the longitudinal optical and all acoustic phonon modes and impact ionization scattering is included using the empirical method as described in [6]. The calibration of the steady-state velocity and energy characteristics of bulk Si have been shown in [7] and show good agreement with values reported in literature [6].

The fullband simulation is crucial in these experiments due to the high excitation energies. The possible electron states are shown in Fig. 1 for a peak laser frequency corresponding to 1.6 eV. As can be seen no simple analytic approximation can be used to represent these conduction band states, and the valence band states are even more complex.

3 PHONON ASSISTED OPTICAL EXCITATION

To calculate the electron and hole momentum and energy after excitation, the emission and absorption of all six phonon modes is considered. During the initialization of the simulation a search is made over the appropriate bands in the discretized Brillouin zone and the entire phonon spectra. In these simulations 2 con-

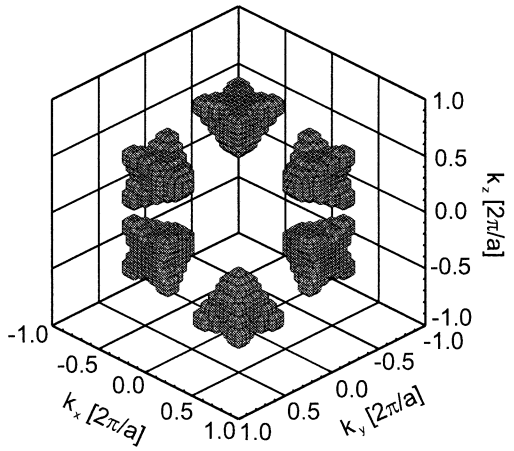

Figure 1: Conduction band equienergetic surfaces (0.5 eV) corresponding to the maximum electron energy that can participate in the optical excitation process.

duction bands and 3 valence bands are included in the transition process. A table is then constructed of all electron-hole-phonon processes that satisfy energy and momentum conservation. In order to conserve computation resources, only a fraction of the total number of electron-hole pairs that are to be injected are stored in the table. In this work the number of final states that are stored are 200,000 (out of 800,000 possible) and the total number of simulated electron-holes pairs is 100,000. During run time a phonon emission or absorption state is selected from this list based on the ratio N_q/N_q+1. This method of including all possible phonon assisted final states gives an accurate description of the indirect exicitation process while ensuring that momentuam and energy are conserved.

The photo-excitation process is simulated by injecting electron-hole pairs at a rate calculated with an empirical generation rate [8] as described in [3], which is dependent on the total carrier injection density and the laser pulse half-width. The timestep used for injection is 0.2 fs and the excitation pulse has a duration of 10 fs. The energy of the photo-generated carriers is computed with the optical pulse frequency of the laser, corresponding to 1.6 eV. In this work, the spectral broadening of the laser is neglected. The bandwidth is large (210 meV) but the influence should be decreased due to the high excess carriers energies and the influence of the phonons. The influence of the laser spectrum is further discussed in the following section.

4 RESULTS

The simulated *pin* diode is represented by a 500 nm intrinsic region discretized by a 500x100 homogeneous grid in real space. The slow diffusive transport in the doped regions should not influence the radiation signal so that the simulation regime is limited to the central intrinsic zone of the *pin* diode. A constant field is applied to the structure. The maximum concentration created by the optical excitation is low, $(1 \times 10^{16} cm^{-3})$, and since the applied field is so high ($\geq$ 100 kV/cm) the affect of the dipole radiation on the internal fields is insignificant. An uniform spatial distribution of injected carriers is assumed due of the relatively small absorption coefficient of Si [9].

The carrier acceleration is calculated with the time derivative of the current density which is governed by the externally applied electric field, scattering events, and the current drop due to carriers leaving the intrinsic region. The transient acceleration and velocity is shown in Fig. 2 for an external field of 100 kV/cm and 340 kV/cm. As can be seen, velocity overshoot is apparent for fields above 100 kV/cm. Below 100 kV/cm the initial energy of the excited electrons and holes is approximately equal to or less than the steady-state values so the large momentuam relaxation time prevents velocity overshoot [10]. Figure 3 shows the ensemble energy of electrons and holes as a function of time for applied fields of 100 kV/cm and 340 kV/cm at 300K. For an electric field of 100 kV/cm the energy changes very little and is consistent with the relative lack of velocity overshoot. The energy distribution of electrons and holes at different times near the time at which the velocity overshoot occurs is shown in Fig. 4 for an applied field of 340 kV/cm. The side valley energy positions in Si are interchanged as compared to GaAs, giving rise to electron transfer into the X-valleys for carriers in the high energies tails. This phenomena is currently being investigated to determine its influences on the behavior transient velocity.

In the experimental measurements no velocity overshoot is observed at any applied bias. One explanation may be a difference in lattice temperature between the experiment and the simulation. Although the experiments were run at room temperature, self-heating due to the laser may have increased the lattice temperature. In order to examine the influence that temperature has on the overshoot simulations were run at 400 K for an applied field of 340 kV/cm. The results are shown in Fig. 5 for electrons and holes and the impact on the overshoot is to decrease the peak value for both types of carriers by approximately 6×10^6 cm/s. Although this is a significant amount, it is not enough to explain the lack of overshoot in the experiment. The change in simulation temperature only affected the scattering rates and the influence on the bandstructure was not considered.

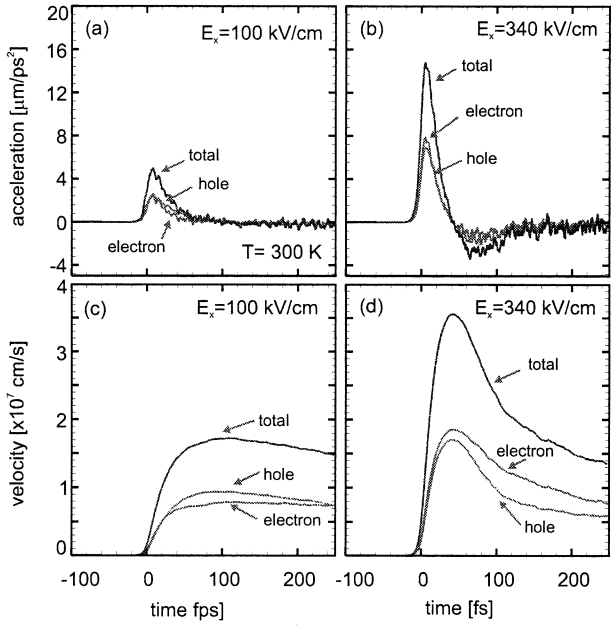

Figure 2: Simulated transient behavior of electron and holes in a Si *pin* diode structure. (a) and (b) show the acceleration as a function of time and (c) and (d) give the corresponding velocity. The velocity overshoot is very pronounced for fields above 100 kV/cm.

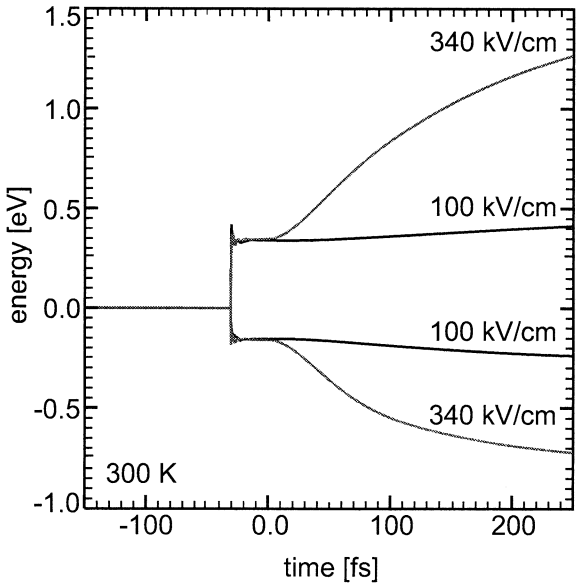

Figure 3: Average velocity of electrons and holes as a function of time for fields of 100 kV/cm and 340 kV/cm at 300K. Hole energy is defined as negative.

Further simulations need to be run to determine if the change in bandgap and phonon structure with temperature will further decrease the maximum velocity.

These simulation were all performed for a delta function excitation energy of 1.6 eV and the laser structure was neglected, but in reality the energy spectra has bandwidth of approximately 200 meV. To examine the influence this has on the results, simulations were run for an excitation energy equal to 1.7 eV with the resulting transient velocity is shown in Fig. 5 for a field of 340 kV/cm. This also has the effect of decreasing the peak overshoot velocity by approximately 2×10^6 cm/s for both electrons and slightly less for holes for this field. The reduction in peak velocity overshoot is due to the increase in carrier energy which acts to reduce the momentum relaxation time.

5 FUTURE WORK

The simulation results show a very obvious velocity overshoot which is not reproduced in the experimental measurements. The cause of the discrepancies could be due to a range of issues which are currently being investigated. One possible source of experimental error is that due to the indirect bandgap, a direct measurement of the electric field inside the intrinsic region of the *pin* diodes is not possible. Instead, the field values are estimated from the external bias and the width of the intrinsic zone of the samples. Furthermore, an absolute calibration of the experimentally determined velocities turns out to be difficult due to the low signal to noise ratio of the data. Temperature effects could play a large role, both through the electron-hole excitation energy, bandstructure effects and issues related to hot phonons. Impact ionization also plays an important role in the transient transport behavior since the high electric fields in this work give rise to carriers with very high energies. A more accurate model for impact ionizations is currently being implemented and the inflence of this mechanism on the velocity overshoot behavior will be examined.

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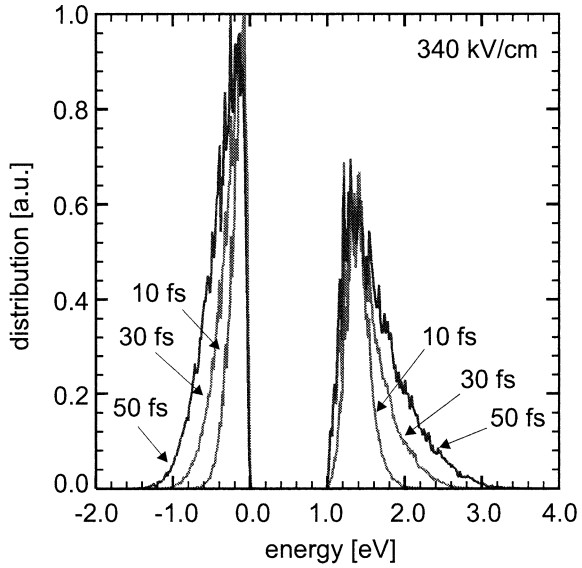

Figure 4: Distribution of electron and hole energy at at three different times for an applied field of 340 kV/cm.

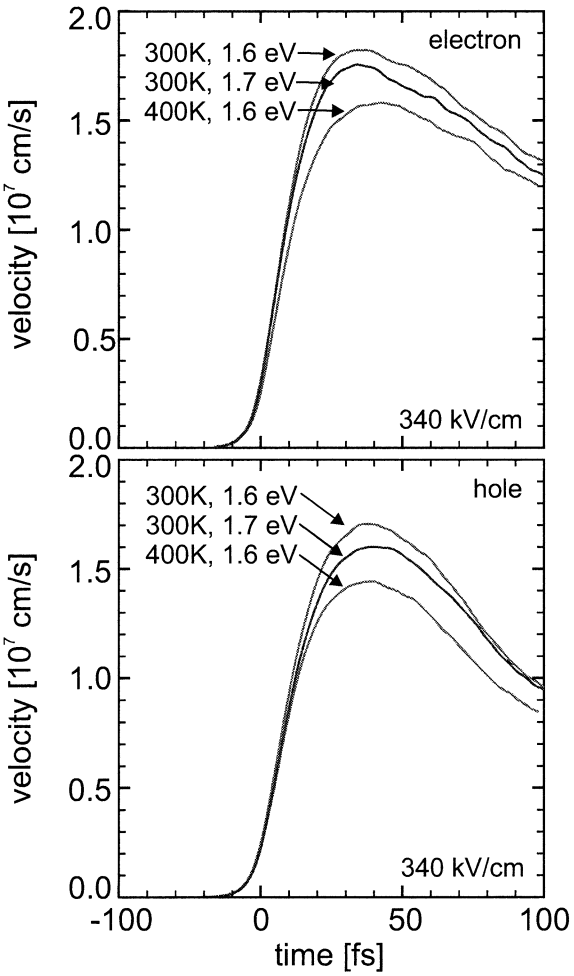

Figure 5: Comparison of velocity overshoot behavior for electrons and holes for an applied field of 340 kV/cm.

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