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Ensemble Monte Carlo Calculation of the Hole Initiated Impact Ionization Rate in Bulk GaAs and Silicon Using a k- Dependent, Numerical Transition Rate Formulation

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Abstract. The hole initiated impact ionization rate in bulk silicon and GaAs is calculated using a numerical formulation of the impact ionization transition rate incorporated into an ensemble Monte Carlo simulation. The transition rate is calculated from Fermi's golden rule using a two-body screened Coulomb interaction including a wavevector dependent dielectric function. It is found that the effective threshold for hole initiated ionization is relatively soft in both materials, that the split-off band dominates the ionization process in GaAs, and that no clear dominance by any one band is observed in silicon, though the rate out of the light hole band is greatest.

1. Introduction

The study of interband impact ionization is of great importance to understanding the operation of most semiconductor devices. In many structures, such as field effect transistors and most bipolar transistors, impact ionization can lead to deletérious effects greatly reducing the overall performance of these devices. In other structures, such as avalanche photodiodes, APDs, and IMPATT diodes the control of impact ionization is essential in producing an optimized device. Subsequently, the design and simulation of many important semiconductor structures requires an accurate description of impact ionization.

The early theories of impact ionization [1,2] provided a means of understanding the underlying physics of the process, but have limited usefulness for predicting the ionization rate in a device structure. Major strides in improving the theory of impact ionization were first taken by Shichijo and Hess [3] by incorporating the full details of the energy bandstructure into the calculation of the ionization rate. However, their method and those of others [4] used a simplified formula for the ionization transition rate, the Keldysh formula [5]. Though the Keldysh formula has been commonly used it has several major limitations. Among these are its failure to include any wavevector dependence of the ionization rate, its reliance on two fitting parameters, and its derivation based on parabolic energy bands.

Recently, there has been great progress in constructing an accurate theory of the impact ionization transition rate which overcomes the limitations of the Keldysh formula [6-16]. In most of these theories the transition rate is numerically evaluated enabling the inclusion of the full details of the bandstructure through a direct calculation of the transition rate without any parametrization. These theories have enabled a much greater understanding of the physics of impact ionization. To the authors' knowledge, the numerical theories have all concentrated on electron initiated ionization and no work has been done on hole initiated impact ionization. It is the purpose of this paper to present the first calculations of the hole initiated impact ionization rate in bulk silicon and GaAs using a numerical formulation of the transition rate.

2. Model description

The calculations are performed using an ensemble Monte Carlo simulator which includes the full details of the valence bands and the phonon scattering mechanisms. The model incorporates two advanced features beyond that typically used [3,4]. The first improvement is the inclusion of a completely numerical technique for calculating the phonon scattering rates, i.e., acoustic, nonpolar and polar optical, which accounts for the anisotropy and warping of the energy bands [17]. The second modification is the inclusion of a fully numerical treatment of the ionization transition rate including a wavevector dependent dielectric function. The dielectric function is determined using the model dielectric function of Levine and Louie [18]. The background carrier concentration is assumed to be 5.0×10^{16} cm^{-3}.

The transition rate is evaluated following the approach of Wang et al. [7,8] used previously for electron initiated ionization. The hole initiated ionization rate is determined for the heavy, light and split-off valence bands at each mesh point within a finely spaced, 1419 point, *k*-space grid spanning the reduced zone of the first Brillouin zone and is incorporated into the Monte Carlo simulator. By performing an additional averaging over energy, further information about the ionization transition rate can be gleaned. It is found that the energy dependent transition rates are comparable among all three valence bands at low energy in silicon. At higher energy, the transition rate within the split-off band is only slightly larger than the corresponding rate within the light hole band, but the rates within both of these bands are very much larger than that within the heavy hole band. In contrast, in GaAs, the energy dependent ionization rate within the split-off band is substantially larger than that in either the light or heavy hole bands. The rate within the heavy hole band in GaAs is particularly low.

3. Calculated results

The calculated hole initiated ionization rate as a function of inverse electric field along the (100) direction in bulk silicon is plotted in Figure 1. Experimental measurements [19-21] which comprise a representative set of data are plotted in Figure 1 as well. As can be seen from the figure, the calculations lie within the range of the experimental measurements and are in particularly good agreement with Overstraeten's results [19]. It is further found that most of the ionization events (between 60% and 50 % of the total) in silicon originate from within the light hole band at all of the applied fields considered. At higher electric field strengths, the contribution from the split-off band increases significantly, to ~35%, while that from the heavy hole band decreases , to ~10%.

The calculated hole impact ionization rate in bulk GaAs along the (100) direction as a function of inverse electric field is plotted in Figure 2 along with the experimental measurements of Bulman et al. [22]. Again fair agreement between the calculations and the experimental results are obtained. In GaAs, owing to the much higher transition rate within the split-off band, the vast majority of hole initiated events, from ~60% at 250 kV/cm to ~80% at 500 kV/cm, originate from within the split-off band. Less than 5% of the ionization events originate from within the heavy hole band at all electric fields in GaAs.

The nature of the effective threshold energy can be ascertained by calculating the quantum yield. The quantum yield is plotted as a function of hole injection energy in both GaAs and silicon in Figure 3. As can be seen from Figure 3, 100% hole ionization occurs at ~5 and ~4 eV in silicon and GaAs respectively. For both materials notice that the quantum yield is appreciably less than 1 at energies less than 5 and 4 eV respectively indicating that the

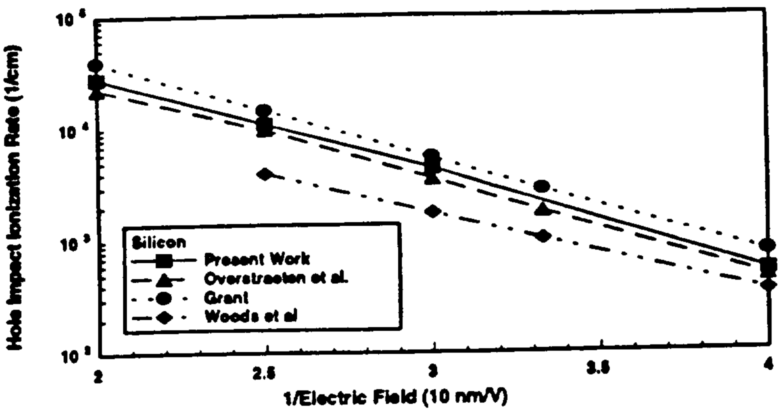

Figure 1: Hole impact ionization rate in silicon as a function of inverse electric field.

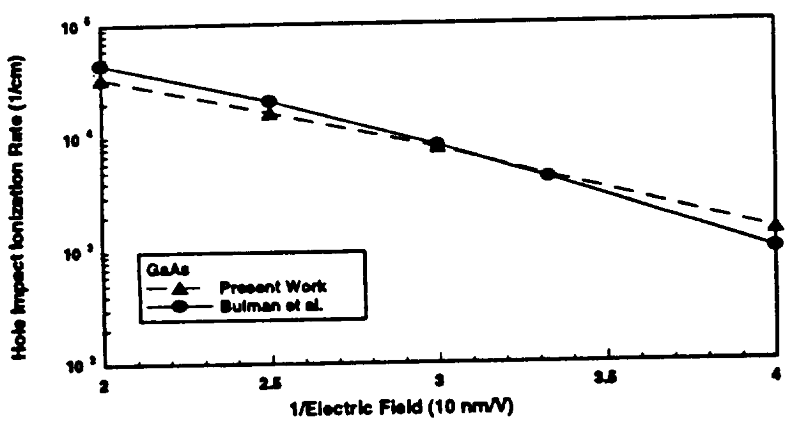

Figure 2: Hole impact ionization rate in GaAs as a function of inverse electric field.

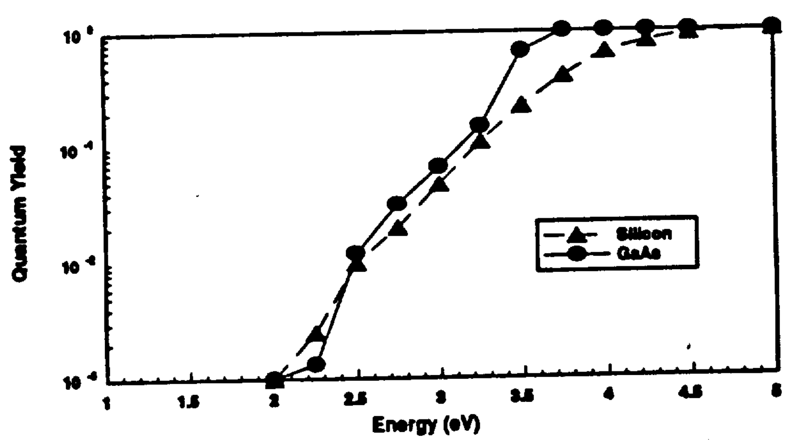

Figure 3: Quantum yield for both Silicon and GaAs.

holes do not necessarily ionize at these energies. This result implies that the effective hole ionization thresholds in both silicon and GaAs are relatively soft. Additionally, owing to the fact that the quantum yield saturates sooner in GaAs than in silicon, the threshold is apparently somewhat harder in GaAs than in silicon.

4. Conclusions

In this paper, the first calculations of hole initiated impact ionization in bulk GaAs and silicon using a complete numerical formulation of the transition rate have been presented. It is found that the effective hole ionization threshold energies in both materials are relatively soft. Comparison of the quantum yield data for holes to that for electron initiated ionization [23] shows that the threshold energy is relatively soft for both carrier species in these materials. Interestingly, the electron ionization threshold in GaAs is also somewhat harder than the electron ionization threshold in silicon as was determined in references 7 and 8. It is further found that the vast majority of ionization events originate from within the split-off valence band in GaAs while no band clearly dominates the ionization process in silicon.

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