Monte Carlo investigation of minority electron transport in silicon

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Abstract

The transport of minority electrons of room temperature silicon has been investigated, using an Ensemble Monte Carlo (EMC) approach. Theoretical expressions for electron-hole scattering which take into account the ellipsoidal nature of the conduction band valleys have been incorporated into the EMC model. Minority electron mobility calculations compared favorably with experimental results of Tang and coworkers [2,3]. A 45% decrease in the zero field mobility was observed at 100V/cm. Transient calculations showed that the electron-hole interacations decrease electron energy, reduce electron steady state velocity, and decrease the transfer rate of electrons to the cold valleys for $p=10^{18}cm^{-3}$ and an electric field of 10kV/cm.

Introduction

Minority electron transport is an important parameter in many semiconductor devices, such as, npn bipolar transistors and HBT's to name a few. Knowledge of the transport characteristics and the mechanisms which effect it is important for proper design and simulation of semiconductor devices. Experiments have shown that minority electrons have transport properties which are much different from majority electrons in bulk semiconductors. These properties have also been shown to be dependent on the carrier concentration, electric field, temperature and material properties [1-5]. For example, Tang and coworkers [2,3] reported a considerable reduction in the zero field mobility of minority electrons in room temperature silicon when the drift field was 100V/cm. Morohashi and coworkers observed the same reduction at temperatures from 77k to 300k with electric fields between 25V/cm and 700V/cm. They attributed this reduction to the electron-hole drag effect which results in a net momentum transfer between the majority and minority carriers. In this paper we examine the effect of electron-hole scattering on the transient response and mobility of minority electrons injected into p-doped silicon. Simulations are performed using a lattice temperature of 300k, a doping concentration of $10^{18}cm^{-3}$ and an electric field of 10kV/cm for the transient calculations and a doping concentration of $4.5\times10^{16}cm^{-3}$ for mobility calculations. Field are applied along the <001> crystallography direction.

Monte Carlo Model

The EMC model for electrons includes all of the ellipsoidal six x-valleys with elastic intravalley acoustic phonon, f- and g-type inelastic intervalley optical phonon scattering, ionized impurity scattering, and electron-hole scattering. Ionized impurity scattering rates are calculated using Ridley's formulation [6]. The physical parameters are the same as those used by Brunetti and coworker [8]. The scattering rate of an electron and hole initially in state ($\mathbf{k}_e$,$\mathbf{k}_h$) to all possible final states ($\mathbf{k}'_e$,$\mathbf{k}'_h$) is given by (bold letters indicate vector quantities)

$$\lambda_{eh}(\mathbf{k}_e, \mathbf{k}_h) = \frac{\mathrm{p m_o e^4}}{2\pi \mathrm{N}\hbar^3 \varepsilon^2} \frac{(\mathrm{m_o}/\mu_d)^{1/2} \mathrm{g}^\star}{\beta^{\star 2}(\mathrm{g}^{\star 2} + \beta^{\star 2})} \tag{1}$$

In equation (1), $\mathrm{g}^\star$ is the transformed relative wave vector, p is the hole concentration, μ_d is the reduced mass, e is the electron charge, $\mathrm{m_o}$ is the free electron mass, ε is the dielectric constant, $\hbar$ is the Plank constant, N is the number of particles, and $\beta^\star = \beta(\mu_d/\mathrm{m_o})^{1/2}$, where β is the magnitude of the inverse screening length.

The Monte Carlo model for holes uses a single heavy hole band as described by Ottaviani and coworker [9] which includes the warping and non-parabolic effects of the degenerate valance band using the method proposed by Reggiani and coworkers [10]. During transient calculations, two values of the parameter β in equation (8) of [10] is used to account for the increasing hole energy as a function of time. A threshold energy was established such that holes below this threshold energy had a lower value of β than holes above it. Scattering mechanisms included in the hole MC model are acoustic phonon scattering, optical phonon scattering, and ionized impurity scattering using Ridley's formulation. Degeneracy has been included using the method proposed by Lugli and Ferry [7]. The physical parameters used are given in [11].

Coupling between the electron EMC and hole MC programs is accomplished through the e-h interaction. The e-h scattering rate, which is dependent upon the evolving distribution functions of both carriers, is calculated self-consistently every 0.1ps during transient calculations and 1.0ps during mobility calculations. Simulations were performed with an electron concentration of $10^{14}\mathrm{cm}^{-3}$. Due to this low electron concentration the effects of electron-electron scattering on the electron distribution and the effects of electron-hole scattering on the majority hole distribution is ignored. Both carriers are given an initial Maxwellian distribution and are assumed to be in equilibrium with the lattice when the electric field is switched on.

Results

Figure 1 shows a comparison between the experimental minority electron mobility and EMC calculations as a function of electric field. Solid circles represent experimental values [2,3], clear circles represent EMC results, and clear boxes represent calculated majority electron mobility. Figure 1 shows, at zero applied field, minority and majority mobilities are equal but under the influence of an applied field the minority mobility decreases rapidly.

At zero applied field, both carriers have an vanishing drift velocity and the average momentum exchange between carriers is zero during electron-hole interactions. Hence, the dominant scattering mechanism will be impurity scattering resulting in a minority electron mobility comparable to that of majority electrons at a doping concentration of $4.5\times10^{16}\mathrm{cm}^{-3}$. Under the influence of an electric field, the electrons and holes will drift in opposite directions and there will be a momentum exchange between electrons and holes as a result of the opposite average drift velocities. This results in a rapid decrease in the mobility of minority electrons. Experiments by Tang and coworker [2,3] reported a 48% decrease in the mobility at 100V/cm. Our calculations showed a similar result. This sharp reduction in mobility is consistent with the e-h drag effect. As the field increases, the

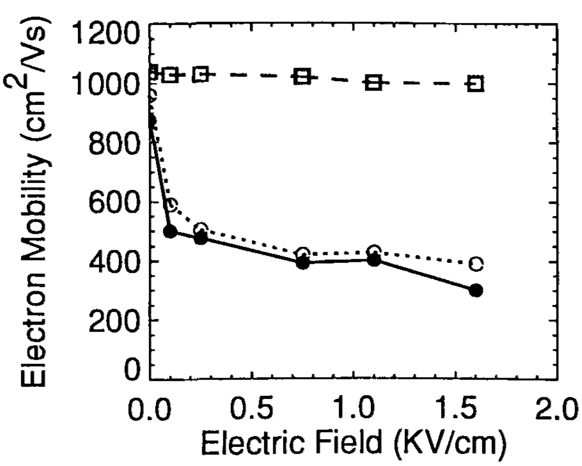

Figure 1: Minority electron mobility in silicon p=4.5×10^{16}cm^{-3}. ● experimental values, o EMC calculations, □ majority electron calculations.

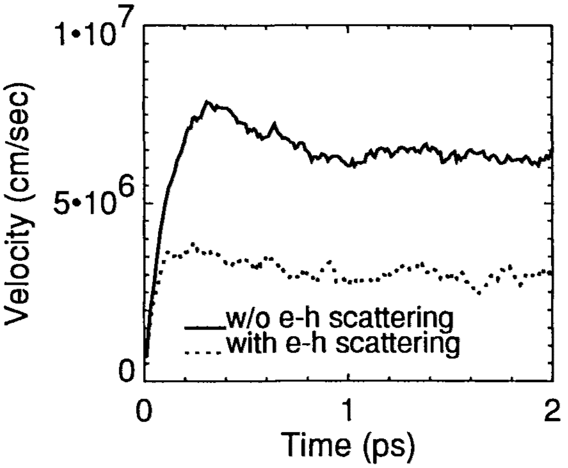

Figure 2: Minority electron drift velocity in silicon p=10^{18}cm^{-3}.

velocity of both carriers also increases. This results in a larger exchange of momentum from the electrons to the holes, but due to the Coulombic nature of the e-h interaction the scattering cross section decreases. The effects of the larger momentum transfer and the smaller scattering cross section results in an saturation of the drag effect. This is shown in figure 1, where the mobility decreases at a much slower rate as the field is increased. Our EMC calculations are in good agreement with experimental results. In order to examine the effect of electron-hole interactions on the transient transport, calculations were performed with a doping concentration of 10^{18}cm^{-3} under the influence of an electric field of 10kV/cm. Figure 2 shows a 52% decrease in the electron steady state velocity when the electron-hole interactions are included. The reason for this large decrease in velocity is due to both the energy loss by the electrons to the hole plasma and the momentum exchange between carriers. As seen in figure 3, both the hot and cold valleys lose energy to the hole plasma. This energy loss leads to a decrease in the valley population transition rates, as figure 4 shows.

Conclusion

We have investigated the effects of electron-hole interactions on the minority electron mobility and minority electron transient response. We observed a rapid decrease in zero field minority electron mobility under the influence of an electric field. This result demonstrates the drag effect of the hole plasma on the minority electrons. Transient calculations showed that the electron-hole interactions decrease electron energy, reduce steady state electron drift velocity, and decrease the transfer rate of electrons to the cold valleys.

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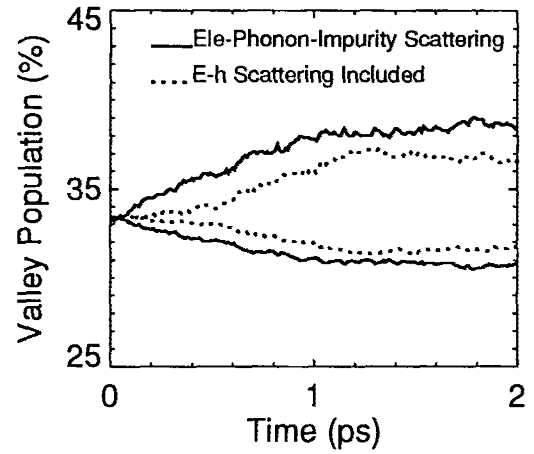

Figure 3: Transient electron energy
Upper lines represent hot valley electron energy and lower lines cold valley energy.

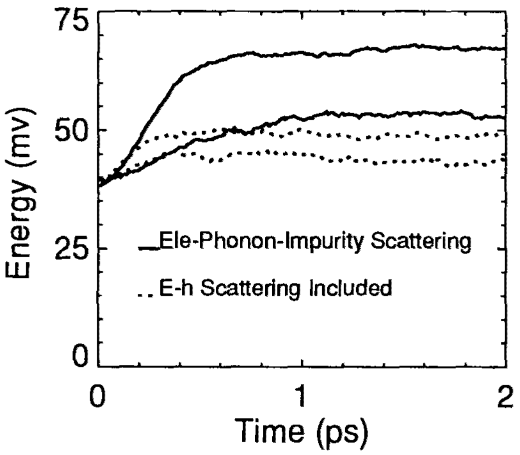

Figure 4: Transient valley population
Upper lines represent cold valley population and lower lines hot valley population.

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