Electron-Hole Scattering Effects in Silicon

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Abstract

The role of electron-hole scattering on the low field mobility of electrons in *p*-doped silicon is examined using an Ensemble Monte Carlo approach. The transport model includes both electron and hole dynamics with coupling between the electron and hole systems through coulombic electron-hole interactions. The electron-hole scattering rate is calculated using the elliptical nature of the conduction band valleys and non-parabolicity of the valence band. Minority electron low-field drift mobilities are calculated at acceptor concentrations of $4.5\times10^{16}\mathrm{cm}^{-3}$ and $3.8\times10^{18}\mathrm{cm}^{-3}$ at 300K. Calculations are in excellent agreement with experimental values.

I. Introduction

Experimental investigations of minority electron transport in silicon report a considerable reduction in electron mobility in the presence of an applied electric field[1,2]. This decrease is attributed to the drag effect of electron-hole scattering which is a result of the net momentum transfer from electrons to holes. In this work, Ensemble Monte Carlo techniques are used to examine the low-field mobility of minority electrons in silicon.

Previous microscopic studies of minority electron transport using Monte Carlo techniques have been conducted for GaAs[3,4] and silicon[5,6]. Furuto and coworkers[3] compared experimental drift velocity in *p*-doped GaAs with Monte Carlo calculations. The hole transport model used in their work contained only heavy holes and simulated hole dynamics with a drifted Maxwellian distribution. Their hole model ignores the complex nature of the valance band. Sedra and coworkers[4] used a more accurate hole transport model and performed simulations using a single particle Monte Carlo technique. A shortcoming of both their works and our previous work in silicon[5,6] is the use of the Brooks-Herring impurity scattering model. This model is based on the first Born approximation and is invalid for impurity concentrations above $10^{17}\mathrm{cm}^{-3}$ at room temperature. This was clearly shown in our previous calculations at $3.8\times10^{18}\mathrm{cm}^{-3}$[6] where calculated low field mobility overestimated experimental values[1]. A new impurity scattering model for Monte Carlo calculations was developed, to correct this problem[7].

In this contribution we report low field drift mobility of electrons in room temperature silicon for acceptor concentrations of of $4.5\times10^{16}\mathrm{cm}^{-3}$ and $3.8\times10^{18}\mathrm{cm}^{-3}$ at 300K. Calculations are reported using an improved hole transport model[8] and impurity scattering model[7].

II. Transport Model

The transport model includes the dynamics of both electrons and holes. Modeling of both carriers is required, due to the strong effect of the hole plasma on electron transport. The hole transport model includes warped non-parabolic heavy and light hole bands and a spherical spin-orbit band. The non-parabolic nature of the heavy and light hole bands is represented by an energy dependent effective mass. The scattering mechanisms taken into account are intra and inter-band elastic acoustic and non-polar optical phonon scattering. More details on the hole transport model along with comparisons to experimental values are reported elsewhere[8].

The electron transport model contains all six non-parabolic ellipsoidal x-valleys. Three intervalley g-type phonon scattering between parallel valleys, three intervalley f-type phonon scattering between perpendicular valleys, elastic intervalley acoustic phonon scattering, ionized impurity scattering, and electron-hole scattering. The phonon scattering and material parameters given by Brunetti and coworkers[9] and the intra and inter-valley phonon scattering rates calculated by Jacoboni and Reggiani[10] are used in this work. Since calculations are reported at low fields and doping concentrations greater than $10^{17}\mathrm{cm}^{-3}$, impurity scattering models based on the first Born approximations, such as the Brooks-Herring model, overestimate experimental mobility. For this reason a new impurity scattering model was developed and implemented in our Monte Carlo program[7]. The model and method used to implement electron-hole scattering is discussed in the next section.

III. Electron-Hole Scattering Rate

The interaction between an electron and hole is assumed to be a screened coulomb potential. The probability of an electron and hole making a transition from the initial state $(\mathbf{k}_e, \mathbf{k}_h)$ to a final state $(\mathbf{k}'_e, \mathbf{k}'_h)$ as a result of a Coulombic interaction is given by the Fermi Golden rule for first-order transistions. By summing over all final electron and hole states and determining whether or not the final states are occupied after the scattering mechanism is chosen[10], the scattering rate becomes

$$\mathrm{S_{eh}}(\mathbf{k}_e, \mathbf{k}_h) = \frac{\mathrm{Q^4 m_o p}}{2\pi\hbar^3\epsilon^2\beta^{*2}}\left(\frac{\mathrm{m_o}}{\mu_\mathrm{d}}\right)^{1/2}\int \frac{\mathrm{g}^*}{(\beta^{*2}+\mathrm{g}^{*2})} f_{\mathbf{k}_h} d\mathbf{k}_h \tag{1}$$

where m_o is the free electron mass, p is the hole concentration, μ_d is defined as

$$\mu_\mathrm{d} = (\mu_x\mu_y\mu_z)^{1/3} \tag{2}$$

where

$$\frac{1}{\mu_\mathrm{i}} = \frac{1}{\mathrm{m_h}} + \frac{1}{\mathrm{m_i}} \tag{3}$$

and (i specifies the direction x,y,z)

$$\mathrm{g}^* = \left(\mathrm{g}_x^{*2} + \mathrm{g}_y^{*2} + \mathrm{g}_z^{*2}\right)^{1/2} \tag{4}$$

where

$$\mathrm{g}_i^* = (\mathrm{m_o}\mu_\mathrm{i})^{1/2}\left(\frac{\mathrm{k}_{e_i}}{\mathrm{m_i}} - \frac{\mathrm{k}_{h_i}}{\mathrm{m_h}}\right). \tag{5}$$

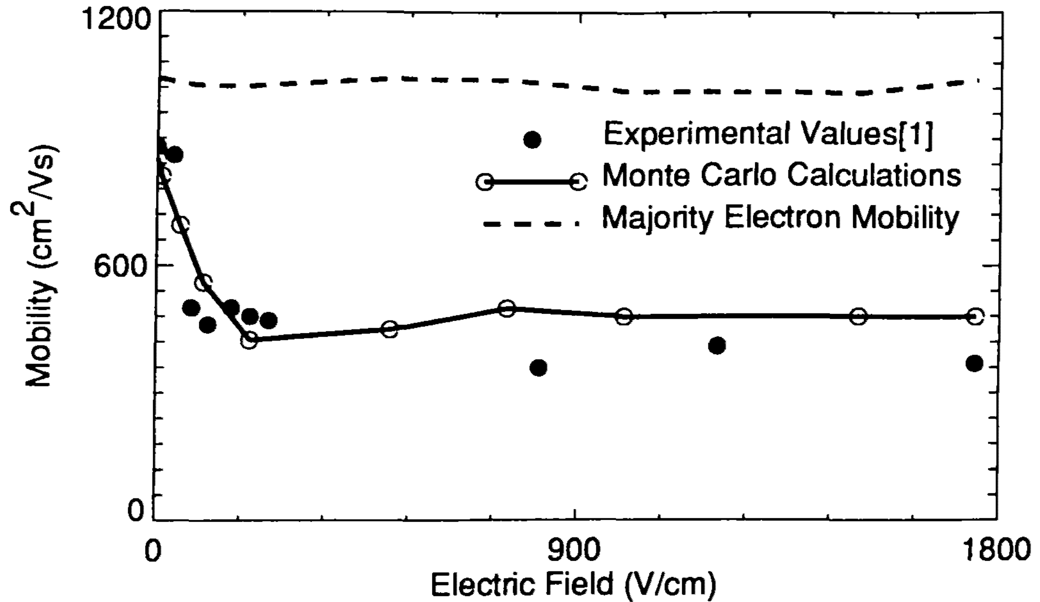

Figure 1: Minority Electron mobility in room temperature silicon as a function of applied electric field for an acceptor concentration of $4.5\times10^{16}cm^{-3}$.

The relative wavevector g is made more complex by the direction dependent electron mass and energy dependent hole mass. In its present form, equation (1) is not suitable for calculating scattering rates in an Ensemble Monte Carlo program, since the hole distribution function is not known before the scattering event is chosen. To overcome this problem, the method proposed by Brunetti and coworkers[9] is used where the term $g^*/(g^{*^2}+\beta^{*^2})$ is replaced by its maximum value of $1/2\beta^*$. By using the maximum value, the resulting scattering rate is the scattering rate for electron-hole scattering plus a self-scattering rate and a rejection method is used.

IV. Results

Figures (1) and (2) show minority electron mobility calculations and experimental data as a function of applied electric field for acceptor concentrations of $4.5\times10^{16}cm^{-3}$ and $3.8\times10^{18}cm^{-3}$, respectively. Majority electron mobility is shown for comparison. As these figures show, there is good agreement between experimental results report by Tang and coworkers[4] and Monte Carlo calculations. The experimental results of Tang and coworkers[4] show a 45% decrease from the zero field mobility at only 100V/cm at both acceptor concentrations while Monte Carlo calculations show a 40% decrease under the same conditions. This dramatic decrease in mobility when an electric field is applied is due to the drag effect of electron-hole scattering. After the initial decrease, mobility essentially stays constant as the electric field is increased. This saturation of the drag effect is due to the inherent Coulombic nature of electron-hole scattering. As the electric field is increased, the velocity of both carriers also increase resulting in a larger exchange of momentum during electron-hole scattering. But, as with any Coulombic interaction, as the velocity increases the scattering cross section decreases. The larger exchange of

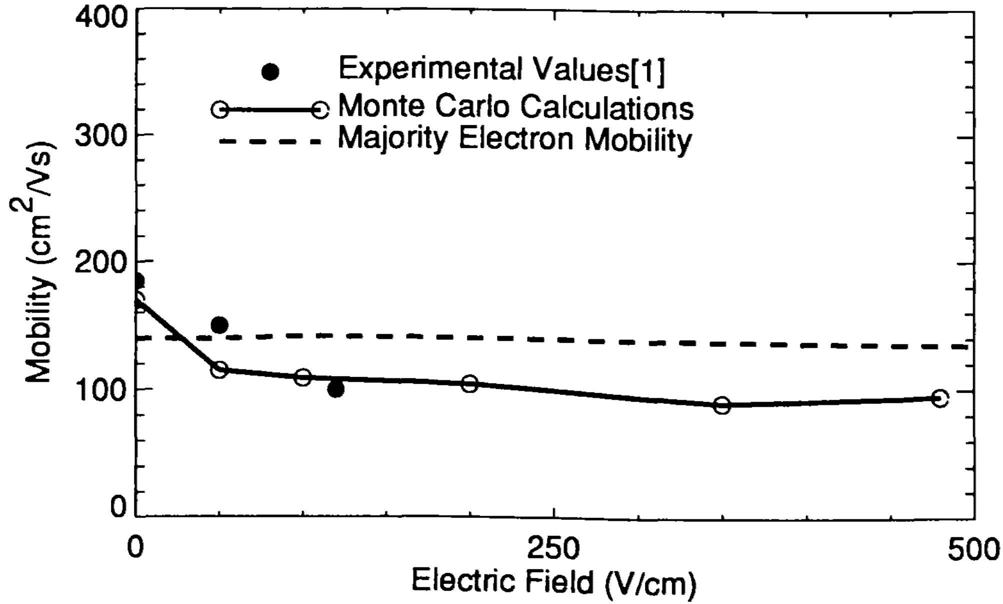

Figure 2: Minority Electron mobility in room temperature silicon as a function of applied electric field for an acceptor concentration of $3.8\times10^{18}\mathrm{cm}^{-3}$.

momentum is countered by a decrease in the frequency of the interactions resulting in a saturation of the drag effect.

V. Conclusion

Minority electron transport in room temperature silicon has been examined using an Ensemble Monte Carlo approach that includes the dynamics of both electrons and holes. A theoretical expression for electron-hole scattering which takes into account the ellipsoidal nature of the conduction band valleys and non-parabolicity of the valence band was developed and implemented. Improved hole transport and impurity scattering models were also implemented. Using the model discussed in sections (II) and (III), calculations are in excellent agreement with experimental results. Both calculated and experimental data show a dramatic decrease from the zero field mobility when the electric field is only 100V/cm. This reduction is attributed to the drag effect of electron-hole scattering.

VI. References

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