Ionized Impurity Scattering Model for Monte Carlo Calculations

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Abstract

An ionized impurity scattering model for Monte Carlo calculations is proposed. This model includes the following four corrections to the simple Brook-Herring model: 1) momentum dependent screening, 2) the second Born term for single impurity scattering, 3) dressing effect of impurities on electron wavevectors, 4) scattering from pairs of impurities. Monte Carlo calculations are performed for majority electrons in silicon at 300K and 77K with donor concentrations from 10^{15}cm^{-3} to 10^{20}cm^{-3}. Calculations show this model provides a substantial improvement to models based on the first Born approximation.

I. Introduction

Monte Carlo techniques have become a popular method to simulate the characteristics of modern semiconductor devices. In these device simulation programs, an ionized impurity scattering model based on the first Born approximation is commonly used[1,2]. For many materials, such as silicon and GaAs, models based on the first Born approximations overestimate mobility for concentrations greater than 10^{16}cm^{-3} at room temperature[3]. With ionized impurity concentrations in many semiconductor devices greater than 10^{16}cm^{-3}, an improved impurity scattering model for Monte Carlo calculations is clearly needed. Recently Kay and Tang[4] proposed an improved model for Monte Carlo calculations. Their model included phase-shift analysis and multiple impurity scattering where they calibrated their model to fit experimental data. Fischetti[5] showed excellent quantitative agreement with experimental data for both n and p doped silicon at 300K by including plasmon scattering to phase-shift analysis and short-range carrier-carrier scattering. Another approach which is becoming more popular when simulating coulombic interactions is Molecular Dynamics. Ferry and workers[6] obtained excellent agreement with experimental results for GaAs at 77K. Molecular Dynamics has the disadvantage of requiring large amounts of CPU time.

In this work we include four corrections to the simple Brooks-Herring impurity scattering model and incorporate these in an Ensemble Monte Carlo program. These corrections include momentum dependent screening, dressing effects on the electron wavevectors, the second Born approximation, and multiple-impurity scattering. Mobility is calculated for majority electrons in silicon at 300K and 77K for impurity concentrations ranging from 10^{15}cm^{-3} to 10^{20}cm^{-3}.

II. Electron Transport Model

The electron transport model contains all six non-parabolic ellipsoidal x valleys. Three intervalley g-type phonons between parallel valleys and three intravalley f-type between perpendicular valleys, elastic acoustic phonon scattering, electron-electron scattering and impurity scattering are considered. The phonon scattering and material parameters given by Brunetti and coworkers[7] and the phonon scattering rates calculated by Jacoboni and Reggiani[8] are used in this work. Electron-electron scattering rates take into account the ellipsoidal nature of the conduction band as developed by Osman and coworkers[9]. The impurity scattering model is discussed in the next section.

III. Electron-Impurity Scattering Model

A review of the procedure used to implement corrections to the basic Brooks-Herring impurity scattering model is given in this section. A more complete description will be published elsewhere[10].

As discussed in the introduction, four corrections to the standard Brooks-Herring impurity scattering model are implemented in our Monte Carlo program. The standard Debye screening length is modified by including a momentum dependent correction using the equation developed by Chung and Ferry[11]. Momentum dependent screening results in a scattering rate which is dependent upon the scattering angle θ. For a screened coulombic potential based on the first Born approximation the scattering rate becomes

$$S(\mathrm{k},\theta) = \Omega(\mathrm{k})\frac{1}{\beta^2(\theta)\left[\frac{\beta^2(\theta)}{2\mathrm{k}^2}+1-\cos\theta\right]^2} \tag{1}$$

where $\Omega(\mathrm{k})$ is the wavevector dependent constant normally seen in the Brooks-Herring scattering rate equation. This scattering rate cannot be calculated in its present form, since the state after scattering is not known prior to the scattering event. This is dealt with in Monte Carlo calculations by using a large correction to the inverse screening length resulting in a scattering rate with internal self-scattering. When impurity scattering is chosen, the scattering angle is selected using a rejection method. Once the scattering angle is known, it is then determined whether impurity or self-scattering terminated the particle's free flight.

The three other corrections are developed following a procedure similar to Moore[12] which is also described by Langer[13] and Rickaysen[14]. The basic procedure is to expand the self energy and define a dressing function as the real part and a width function as the imaginary part of the self-energy terms[15]. In this work, we included the first two terms of the self energy for single impurity scattering which can be thought of as the first and second Born terms and the first term for scattering by a pair of impurities. The dressing effect on the electron wavevectors is included only on the first single impurity term. The dressing effect on electron energy was small compared to other the corrections, this was also observed by Moore[16], and is not included.

When the dressing effect of the impurities on the electron's wavevector is included, the

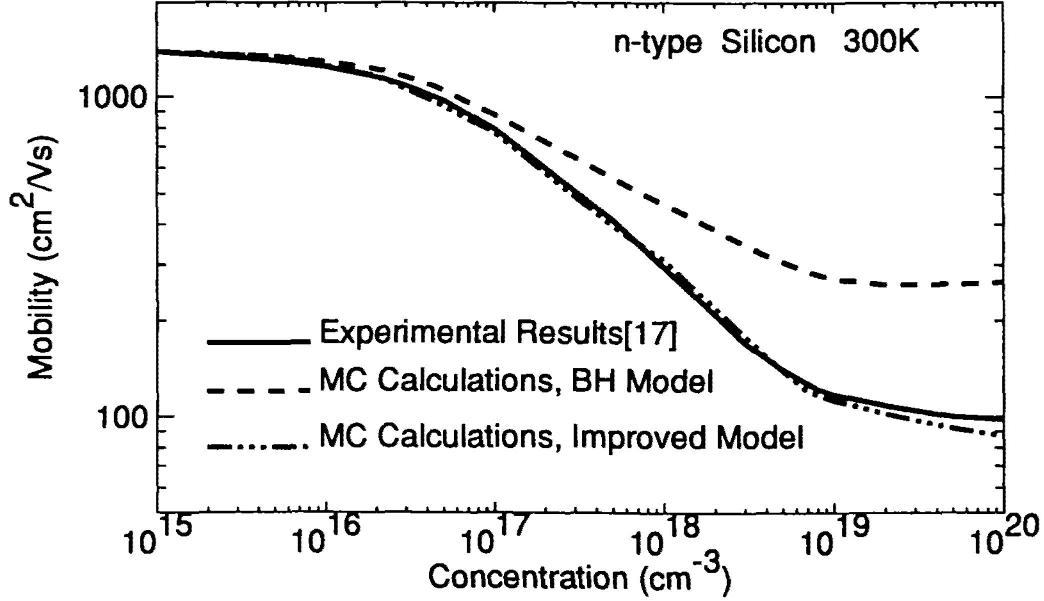

Figure 1: Majority Electron Mobility as a function of ionized impurity concentration for silicon at 300K

scattering rate based on the first Born term becomes

$$S_{dressing}(k) = S_{bh}\left[1 - \frac{nm^2e^4}{8\pi\hbar^4\epsilon^2\beta^3}\frac{(3\beta^2+4k^2)}{\beta^2+4k^2)^2}\right]^{-2} \qquad (2)$$

where S_{bh} is the scattering rate using the Brooks-Herring model, n is the impurity concentration, m is the electron mass, e is electron charge, ϵ is the material constant, and $\hbar$ is Planck's constant. If momentum dependent screening is used, S_{bh} is given by equation (1) and is incorporated in the same manner.

The scattering rate for the second Born term is given by

$$S(k,\theta) = \frac{nm^2e^6}{4\pi^2\hbar^5\epsilon^3\beta^4}\left[\frac{\tan^{-1}\left(\frac{x}{1+y+4x}\right)^{1/2}}{\sin(\theta/2)(1+y+4x)(1+4x)}\right] \qquad (3)$$

where $x = \frac{k^2}{\beta^2}\sin^2(\theta/2)$ and $y = 4k^2/\beta^2$. Equation (3) is integrated numerically over θ to obtain the scattering rate and a rejection method is used to determine the scattering angle θ. As observed by other researchers[16], the correction to mobility by the second Born term is large in region where the first Born term alone is valid $k^2/\beta^2 >> 1$. This is dealt with by setting the scattering rate for the second Born term to zero when the first Born term alone is valid.

The multi-particle transition rate is found by considering only the lowest approximation for scattering from a pair of impurities. This is the same form as developed by Moore[12] and Rickaysen[14]. The resulting scattering rate is quite complex and will not be given

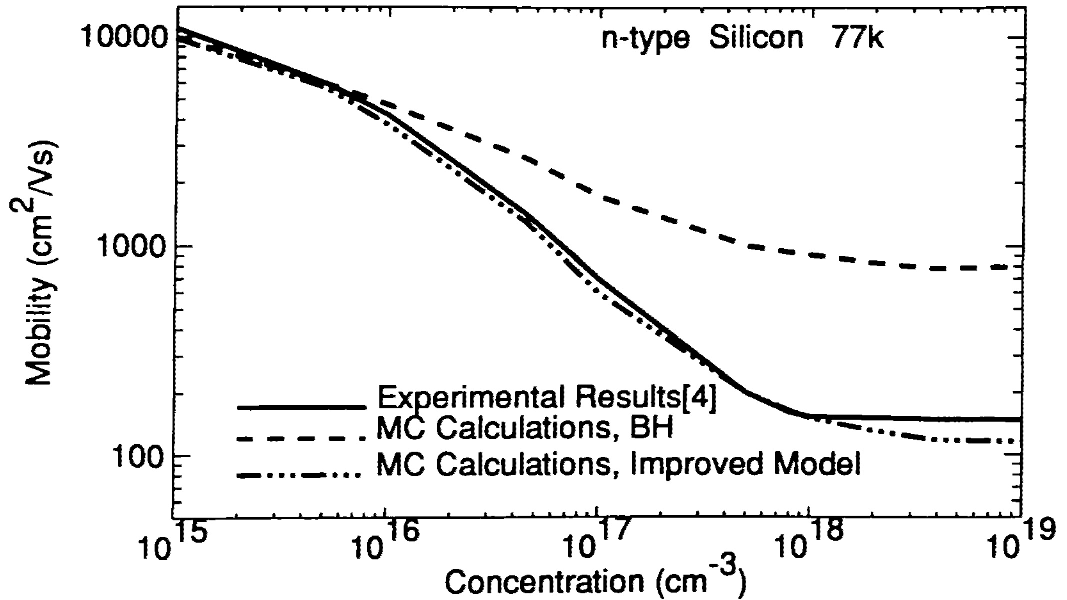

Figure 2: Majority Electron Mobility as a function of ionized impurity concentration for silicon at 300K

here. Multiple impurity scattering is incorporated in the same manner as the second Born term.

IV. Results

Figures 1 and 2 show a comparison of the basic Brooks-Herring model, the model discussed in this paper, and experimental data[17] for silicon at 300K and 77K, respectively. As figure 1 shows, the proposed model clearly improves upon the Brooks-Herring impurity scattering model and compares favorably with experimental data over the range of concentrations considered. Figure 2 shows the discrepancy between the Brook-Herring model and experimental data widens as the temperature is decreased. Again, the proposed model clearly improves upon the Brooks-Herring model.

V. Conclusion

We have proposed an improved impurity scattering model for Monte Carlo calculations. The improved model includes four corrections to the Brooks-Herring impurity scattering model. Results for n-doped silicon at 300K and 77K show our model substantially improves mobility calculations compared to models based on the first Born approximation.

VI. References

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