Soft Sphere Model for Electron Correlation and Scattering in the Atomistic Modelling of Semiconductor Devices

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As MOSFET devices within the deep sub-micron regime are modelled, it is no longer feasible to represent the charged dopants by a continuous charge distribution. In this regime an ensemble of devices, each with different spatial distributions and the number of dopants, must be modelled. However, it is computationally prohibitive to solve for the full Coulomb interaction required for particle simulators, especially for an ensemble of devices. To address this point, the paper focuses on the issue of modelling the dynamics in the presence of discrete carrier–carrier scattering and carrier-fixed impurity scattering which is suitable for efficient simulations of large ensembles of devices.

Keywords: Soft sphere model; Electron correlation; Carrier–carrier scattering; Atomistic modelling; Monte Carlo

1. INTRODUCTION

As the length scales of Si MOSFETs continue to shrink towards the deep sub 0.1 μm regime, semiconductor device modelling must move into the new area of atomistic scale modelling. This is a new area for device modelling; at these scales it is no longer possible to represent the charged impurities by a continuous charge distribution with a definitive doping density, as is assumed in commercial simulators [1], and some of the most advanced Monte Carlo simulators [2]. In the

atomistic regime, the spatial distribution and the actual number of dopants must be treated as discrete random variables. In a full 3D simulation, the number of dopants over an ensemble of devices is assumed to follow a Poisson distribution, and shifts the paradigm of numerical device simulation from modelling a single device to an ensemble of devices. Therefore, the 3-D statistical atomistic simulations become essentially a four-dimensional (4-D) problem where the fourth dimension is the size of the statistical sample [3]. The fluctuations in dopants lead to a number of new predictions for

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devices; among the established predictions we may mention the strong fluctuations in threshold voltage from device to device where macroscopic device parameters, such as doping density and spatial dimensions, are identical [4].

The atomistic regime has been recently modelled by a number of groups [4–9] using a low voltage approximation where the current flow is treated in a Drift Diffusion or generalised Drift Diffusion approximation. Here the current is determined from the current continuity equation *via* a solution of Poisson's equation for the electrostatic potential in the presence of a static discrete impurity distribution. For self-consistency, these atomistic models should also treat the conduction electrons/holes as a discrete spatial distribution (which will fluctuate in number) as in a particle based approach such as in a Monte Carlo simulation [10–12]. However, this is an extremely heavy computational task on the atomistic scale because of the details of the injection and/or extraction of carriers at the contacts. The task is made even more daunting due to the need to frequently recompute the electrostatic forces, especially the short-range forces, in order to obtain statistically reliable results. Although one could in principle resort to a direct calculation of the electrostatic forces felt by the carriers; this would also be extremely computationally demanding. This is the case even when using highly efficient Poisson mesh solvers such as the multigrid technique [13,14], and the correction procedure for short-range forces proposed by Gross *et al.* [12]. The present paper addresses this problem of modelling the dynamics of discrete carrier flow in a semiconductor device by utilising a suitably simple model of the carrier–carrier scattering and/or carrier fixed-impurity scattering; such a model is necessary for efficient simulations of large ensembles of devices. Section 2 of this paper describes in detail the model potential used in our soft sphere collision simulators. Section 3 presents the preliminary results from a Monte Carlo simulator which utilises the soft sphere potential model for carrier–carrier and carrier fixed-impurity scattering.

2. SOFT SPHERE POTENTIAL MODEL

The electrostatic interaction between carriers or carriers and fixed impurities is *via* the long range Coulombic potential, $1/r$ (see Fig. 1). The screened coulomb potential $e^{(-\beta r)}/r$ is shown for comparison, where r is the inter-particle separation. The soft-sphere model replaces the long range

FIGURE 1 Schematic representation of the soft sphere scattering model potential. The solid line indicates the bare Coulomb potential; the dashed line represents the screened Coulomb potential.

FIGURE 2a Carrier–carrier scattering utilising the soft sphere interaction potential in the case when the interaction energy is less than the soft sphere potential barrier (W).

FIGURE 2b Carrier-carrier scattering utilising the soft sphere interaction potential in the case when the interaction energy is greater than the soft sphere potential barrier (W).

Coulomb force with a short range potential in which the potential is zero for the inter-carrier separation $r > 2R_c$. This jumps discontinuously to a constant value, W , for $r \leq 2R_c$ (shown in Fig. 1). R_c and W are to be regarded as adjustable parameters for the model; although physically they might be interpreted as the screening radius and the Coulomb potential at twice the screening radius respectively. In a classical collision model carriers will undergo hard-sphere scattering for energies less than W but will interact with one other *via* the model potential for higher energies. These two regimes are depicted schematically in Figures 2a and 2b respectively. The state after scattering for two particles assumes for simplicity a spherically symmetric bandstructure. Interactions in this manner are most easily calculated by transforming to

the 'centre of momentum' frame of Ref. [15]. Here, the condition separating hard-sphere and soft-sphere collisions is given by: $(1/2)\mu v_{12}^2 \geq W$, where μ is the reduced mass of the system given by $(m_1 m_2 / m_1 + m_2)$ and v_{12} is the relative velocity vector between the two vectors and is given by: $v_{12} = v_1 - v_2$. The masses and velocities of particles 1 and 2 are denoted by m_1, v_1 and m_2, v_2 respectively. Purely for the sake of simplicity, we have chosen to consider motion only in a 2-D plane. For the case when the energy of the two-particle system is less than W , velocities after scattering V'_1 and V'_2 for particles 1 and 2 are given by:

$$V'_1 = V + \left(\frac{m_2}{M}\right) v'_{12} \quad (1)$$

$$V'_2 = V - \left(\frac{m_1}{M}\right) v'_{12} \quad (2)$$

where $V = (m_1/M)V_1 + (m_2/M)V_2$ and $M = m_1 + m_2$. The x and y components of v_{12} given by:

$$v'_{12x} = \frac{v_{12x}(r_{12y}^2 - r_{12x}^2) - 2r_{12x}r_{12y}v_{12y}}{4R_c^2} \quad (3)$$

and

$$v'_{12y} = \frac{v_{12y}(r_{12x}^2 - r_{12y}^2) - 2r_{12x}r_{12y}v_{12x}}{4R_c^2} \quad (4)$$

Note that $\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$ is the relative position vector between the centre of the two particles. However, in the case where the energy is greater than W , Eqs. (1) and (2) are preserved but with Eqs. (3) and (4) replaced by:-

$$v'_{12x} = \frac{\mu r_{12y}^2 v_{12x} - \mu r_{12x} r_{12y} v_{12y} + \sqrt{\mu} r_{12x} \sqrt{4\mu R_c^2 (v_{12y}^2 + v_{12x}^2) + 2\mu r_{12x} r_{12y} v_{12y} v_{12x} - 8WR_c^2}}{4\mu R_c^2} \quad (5)$$

and

$$v'_{12y} = \frac{\mu r_{12x}^2 v_{12y} - \mu r_{12x} r_{12y} v_{12x} + \sqrt{\mu} r_{12y} \sqrt{4\mu R_c^2 (v_{12y}^2 + v_{12x}^2) + 2\mu r_{12x} r_{12y} v_{12y} v_{12x} - 8WR_c^2}}{4\mu R_c^2} \quad (6)$$

These equations result from applying the classical conservation laws, conservation of energy and momentum (angular and linear), before and after the collision, so $(1/2)mV_1 + (1/2)mV_2 - W = (1/2)mV_1' + (1/2)mV_2'$. The resulting equations are most easily achieved from within the centre of mass frame of reference.

It should be noted that the model as presented is restricted to dilute concentrations, since only collision pairs are considered. Although, it is probable that in regions of high carrier concentration three body collisions may be important. Indeed, it is interesting to note that within such collisions it is possible that one carrier may gain a significant amount of energy from the other 2 particles – a situation analogous to Auger Recombination [16]. We may speculate that this provides one explanation for sub threshold impact ionization, where impact ionization has been shown to occur when the applied bias across a device is less than the bandgap energy.

3. RESULTS

Here we present preliminary results from our two-dimensional Monte Carlo simulator for holes, with periodic boundary conditions, within which we have implemented the soft-sphere scattering potential model described above along with all the standard phonon scattering mechanisms. In order to rapidly evaluate the Monte Carlo model with minimal computational effort, we have used a spherically symmetric bandstructure. This is not a limitation of our model and a more realistic bandstructure may be used for full device simulation [17]. The soft sphere model is efficiently implemented within the simulation by introducing a ‘*chaining mesh*’ or ‘*linked list*’ approach [18, 19]. This method was originally developed for the simulation of liquids where hard-sphere like models are common; the length of each cell of the chaining mesh is R_c . The use of this method, when the number of particles is greater than a few tens, can reduce the time required to locate the

positions of neighbouring particles by an order of magnitude or more. Unfortunately, such methods can only be used when the force is short ranged such as in the soft-sphere potential model.

Figures 3a and 3b show typical carrier spatial configurations without and with soft-sphere collisions respectively. We can see that in Figure 3b the particles tend to be a distance of $2R_c$ away from their nearest neighbour as we would expect due to the soft-sphere collision. This is in contrast to simulations with point-like particles (Fig. 3a) where the carriers may become arbitrarily close. This can be seen by examining the

FIGURE 3a A typical spatial correlation distribution for a carrier ensemble with point like collisions.

FIGURE 3b A typical spatial correlation for a carrier ensemble with soft sphere collisions.

pair distribution $g(r)$:

$$g(r) = \rho^{-2} \left\langle \sum_i \sum_{j \neq i} \delta(\mathbf{r}_i) \delta(\mathbf{r}_j - \mathbf{r}) \right\rangle \quad (7)$$

The inter-particle force will lead to current crowding in confining geometries; where there will be a high energetic cost for one particle overtaking another. This will be most important for low energy carriers as they will be unlikely to be able to overcome the barrier due to the soft sphere potential, W . Thus the electron–electron

correlation will have strong implications for carrier injection into and out of the channel, whereas the movement of highly energetic carriers is likely to be relatively unaffected. We can see this by considering $g(r)$ for carriers in thermal equilibrium, and highly energetic carriers as shown in Figures 4a and 4b respectively. We can see clearly that for the energetic carriers there is more penetration of carriers to within a distance of $2R_c$ or less, as we would expect.

4. CONCLUSIONS

We have discussed the problem of simulating atomistic scale devices using particles where only a few discrete carriers are present. In this regime it is important to consider the strong coulombic inter-particle forces, which lead to electron correlation, over an ensemble of devices to obtain statistically valid results. We have presented an efficient soft-sphere potential model, which facilitates the modelling of an ensemble of atomistic devices using conventional particle techniques. This would otherwise be computationally prohibitive. The important aspects of electron–electron correlation, such as current crowding at the contacts and the energy cost of overtaking in confined channels, have been discussed. Additionally we have provided one possible explanation for sub bandgap impact ionization.

Acknowledgements

J. R. Watling would like to EPSERC for funding under grant number GR/L53755. The authors, grateful acknowledge the assistance of Richard Wilkins for careful reading of this manuscript.

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FIGURE 4a The pair distribution function $g(r)$, for particles, in thermal equilibrium at $T = 300$ K, interacting via our soft-sphere potential model.

FIGURE 4b The pair distribution function $g(r)$, for energetic particles, interacting via our soft-sphere potential model.

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