

Extended Models of Coulomb Scattering for the Monte Carlo Simulation of Nanoscale Silicon MOSFETs

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Submitted to the Faculty of Engineering, Department of Electronics
and Electrical Engineering, University of Glasgow in fulfilment of the
requirements for the degree of Doctor of Philosophy

November 2009

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Abstract

The International Technology Roadmap for Semiconductors (ITRS) specifies that MOSFET logic devices are to be scaled to sub-10nm dimensions by the year 2020, with 32nm bulk devices ready for production and double-gate FinFET devices demonstrated down to 5nm channel lengths. Future device generations are expected to have lower channel doping in order to reduce variability in devices due to the discrete nature of the channel dopants. Accompanying the reduced channel doping is a corresponding increase in the screening length, which is even now comparable with the channel length. Under such conditions, Coulomb scattering mechanisms become increasingly complex as the scattering potential interacts with a larger proportion of the device.

Ionized impurity scattering within the channel is known to be an important Coulombic scattering mechanism within MOSFETs. Those channel impurities located close to the heavily doped source and drain or both, will induce a polarisation charge within the source and drain. These polarisation charge effects are shown in this work to increase the net screening of the channel impurities, due to the inclusion of remote screening effects, and significantly decrease the scattering rate associated with ionized impurity scattering. Remote screening can potentially reduce the control by ionized channel impurities over channel transport properties, leading to an increased sub-threshold current.

A potential model has been obtained that is based on an exact solution of Poisson's equation for an ionized impurity located close to one or both of these highly doped contact regions. The model shows that remote screening effects are evident within a few channel screening lengths of the highly doped contact regions. The resultant scattering model developed from this potential, which is based on the Born approximation, is implemented within a Monte Carlo simulator and is applied to MOSFET device simulation.

The newly developed ionized impurity scattering model, which allows for remote screening, is applied in the simulation of two representative MOSFET devices: the first device being a bulk MOSFET device developed for the 32nm technology generation; the second device is an Ultra-Thin-Body Double Gate (UTB DG) MOSFET developed for the forthcoming 22nm technology generation. Thorough investigative simulations show that for both the bulk MOSFET and the UTB DG MOSFET, that remote screening of channel impurities in these devices is not a controlling effect. These results prove that the current model for ionized impurity scattering employed in Monte Carlo simulations is sufficient to model devices scaled to at least the 22nm technology node, predicted to be in production in the year 2012.

Acknowledgements

There are many people that I would like to thank for helping me to complete this thesis, which I am sure without their help would never have reached an end! Starting with Jeremy Watling who seemed reasonably happy to read through the many drafts of chapters I produced, carefully pointing out errors, typos and discussing with me the points in my work which needed reinforcing. Despite our many heated discussions during my PhD studies, I am now very sure that Jeremy's guidance did really get me to the end of this work and I truly appreciate this.

I would also like to thank John Barker who provided me with this project to study which I found interesting and often extremely challenging, the very reasons I signed up for the PhD in the first place! I wish John all the best in his retirement (which I am sure he looked forward to if only to avoid having to read my thesis!) and I hope that this work achieves all he wanted from the project in the first place.

Thanks also go to Craig Alexander who was very happy to let me use his Monte Carlo simulation program and then answering the many questions I had about it. I also appreciate the help and support of Karol Kalna who was prepared to answer to my often long and winding questions, and of course to regularly beating me at the badminton and squash matches we often played (I have yet to win a game). Really, thanks to everyone in the Device Modelling Group at the University of Glasgow for all your help over the years, including: Asen Asenov for his endless encouragement; Scott Roy for his supportive advice (and straight answers!); Andrew Brown, Gareth Roy and Campbell Millar for their help with everything drift-diffusion and MOSFET related; and finally also to Fiona Baxter who always seemed interested and enthusiastic about my progress!

All my friends in work and at home I should really also thank for the many times I was bummed and had a good old moan about my PhD. Although I swear I doubt that any of them have actually any idea what I was really doing, or for that matter any interest! Thanks also to my Mum who really, really tried to understand what I was doing if only so that she could tell people what I did when they asked, and to the very well received home-cooked dinners!

Publications and Conferences

E. A. Towie, J. R. Barker and J. R. Watling, "Inhomogeneous Electron-Impurity Scattering in High Degeneracy, Nanometre Scale Silicon MOSFETs," Condensed Matter and Materials Physics 2007: University of Leicester, UK, Apr. 12-13, 2007.

J. R. Barker, E. A. Towie, and J. R. Watling, "Inhomogeneous Electron-Impurity Scattering in High Degeneracy, nanometre Scale Silicon MOSFETs including image charge effects: new models," 12th International Workshop on Computational Electronics: Oct. 8-10, 2007.

J. R. Barker, E. A. Towie, and J. R. Watling, "The influence of polarisation and image charges on electron- impurity scattering in high degeneracy, nanometre scale silicon wrap-round gate MOSFETs", 2008, International Symposium on Advanced Nanodevices and Nanotechnology, Waikoloa, Hawaii, USA, Dec. 2-7, 2007.

J. R. Barker, E. A. Towie, and J. R. Watling, "The influence of polarisation and image charges on electron- impurity scattering in high degeneracy, nanometre scale silicon wrap-round gate MOSFETs," Journal of Physics: Conference Series, vol. 109, 012009, 2008

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Chapter 1 Introduction

The International Technology Roadmap for Semiconductors (ITRS) [1] is a set of manufacturing guidelines which are used by industry to ensure that modern devices are both profitable to manufacture and are efficient in use. The roadmap covers all aspects of production from process technology to final device performance and also highlights the areas where research and development (R&D) are required. In this work the interest within the ITRS is concerned with the digital logic devices roadmap which discusses the scaling and performance of CMOS devices, that is the MOSFET.

The current generation of MOSFETs are based on the bulk or planar devices with a physical gate length of 32nm and are quite advanced with high- κ /metal-gate stacks and strained channels [2-4]. High- κ insulators have been introduced to combat the scaling of the gate oxide, which when using the traditional SiO₂ would otherwise only be a few atomic layers thick [5, 6]. The reintroduction of metal gates (poly-Si gates had been used for almost the previous two decades of scaling due to the increased control over the device and minimal production cost) reduces the negative impact of the high- κ dielectric [7-10]. Channel performance can be improved through the use of strain which increases the carrier mobility [11-13] and there is also an interest in moving to a (110) silicon crystal orientation [9, 14].

The roadmap projects that the MOSFET device can be scaled to a physical gate length of 8.1nm by the year 2022. The bulk device is predicted to be scaled to a physical channel length of 14nm by 2016, therefore to achieve the end of roadmap device scaling requires a different device structure that reduces Short-Channel Effects (SCEs) (see the textbook by Taur [15] for more detail on SCEs) and completes the required performance levels specified by the ITRS.

A device which offers greater scaling than the bulk device has been led by IBM and is the Silicon-On-Insulator (SOI) MOSFET. It remains mostly unchanged from the bulk device in terms of the layout of the gate, channel and source/drain with the difference being that the silicon substrate is much shallower and is placed on an insulator. The SOI MOSFET device offers a performance gain of 20-35% over the bulk MOSFET and is particularly suitable for low-power applications [16]. It too utilises the technological improvements developed for use in the bulk device of high- κ /metal gate and channel strain as seen in the latest generations [17-19]. Although this device provides greater scaling, the roadmap predicts a physical channel length of 10.7nm by 2019, it is not considered to be the device structure to take MOSFET devices to sub-10nm dimensions.

1.1 Coulomb Scattering

The device which is described in the ITRS as the “ultimate MOSFET device” due to its scalability to the end of the roadmap is the Double-Gate (DG) or FinFET device [1]. The DG device is a particularly favourable device for the roadmap as it greatly reduces the deleterious short-channel effects (SCEs) whilst maximising drive current [20]. This device can also be easily integrated into the existing conventional planar manufacturing process [21]. DG devices have been demonstrated down to 5nm physical channel lengths [12, 22, 23] where fully functional SRAM cells have been recently produced using the DG FinFET structure [24].

It is well understood that each new scaling generation in the coming years provides new challenges and will require that new device structures be utilised. This of course means that the device simulators must also be extended and improved to model the complex processes that are involved. A particular effect evident in devices that has been under extensive research is that of Coulomb scattering which is an increasingly deleterious effect on device performance as the dimensions are reduced below typical screening lengths [25].

The focus of this work is to develop an advanced Coulomb scattering model that describes the interaction of channel ionized impurities with their corresponding polarisation charges induced in the source and drain regions. In the following section a brief review of the major Coulomb scattering processes under study in current generation MOSFETS is undertaken. Following this, the aims and objectives of this research will be stated and an outline of the structure of this work will be presented.

1.1 Coulomb Scattering

This form of scattering is based on the Coulomb potential, given by equation (1.1) [26], for a point charge with a charge Ze (e is the electronic charge and Z is the number of free charges) located at $\mathbf{r}_1$ in a medium of permittivity $\epsilon_r \epsilon_0$. This form of the potential is often called the bare Coulomb potential as it does not include the interaction of the other carriers in the definition of the potential.

$$V(\mathbf{r}) = \frac{Ze}{4\pi\epsilon_r\epsilon_0} \frac{1}{|\mathbf{r} - \mathbf{r}_1|} \quad (1.1)$$

It is clear from the definition of this potential that there will be a singularity when $\mathbf{r} = \mathbf{r}_1$ and that the potential will drop off slowly. Inclusion of the surrounding charge density allows the screening potential of the other carriers to be considered in this potential and is often termed the screened Coulomb potential. This form of the Coulomb potential can be written as

1.1 Coulomb Scattering

$$V(\mathbf{r}) = \frac{Ze}{4\pi\epsilon_r\epsilon_0} \frac{\exp(-|\mathbf{r} - \mathbf{r}_I|/\lambda)}{|\mathbf{r} - \mathbf{r}_I|} \quad (1.2)$$

where λ is the static screening length which is typically given by the Debye-Hückel form, written here for a non-degenerate system as

$$\lambda = \sqrt{\frac{\epsilon_r\epsilon_0 k_B T}{e^2 n}} \quad (1.3)$$

where k_B is Boltzmann's constant, T is the lattice temperature in Kelvin and n is the free electron density. The screened Coulomb potential retains the infinitely high peak of a point charge when $\mathbf{r} = \mathbf{r}_I$ but the introduction of the static screening length, λ , reduces the range over which the potential is noticed. This is more clearly demonstrated in Figure 1.1 where the two potential models are plotted for arbitrary units.

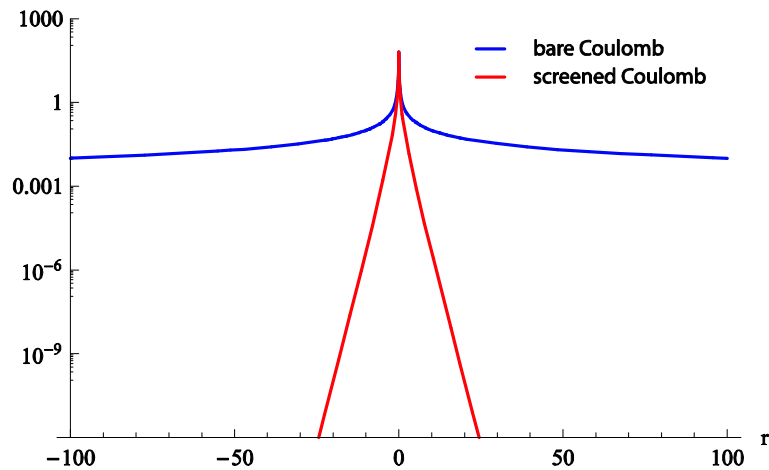


Figure 1.1: Plot of the bare and screened Coulomb potentials for a point charge located at $\mathbf{r}_I = 0$.

Coulomb scattering in MOSFET simulation commonly describes the effect on device performance of carrier interactions with ionized impurities and the other carriers. Ionized impurity (II) scattering has the more dominant effect in controlling the carrier transport in doped silicon, in particular the mobility of carriers [27-29]. This mechanism is by far the most important Coulomb scattering mechanism due to the unavoidable nature of impurity scattering in MOSFET devices. It arises from the doping of the silicon semiconductor material with either donor or acceptor atoms. Doping is used to modify and improve the electrical properties of silicon such as to improve the threshold voltage by doping the channel or improving drive current by heavily doping the source/drain wells.

1.1 Coulomb Scattering

Carrier-carrier (e-e) scattering is dominant at high carrier concentrations, above $\sim 10^{17} - 10^{18} \text{ cm}^{-3}$ in silicon and redistributes the carrier momentum among the ensemble [30]. The e-e scattering mechanism is broken into two separate regimes: the interaction of two carriers with each other, binary e-e scattering [31, 32]; the interaction of a carrier with an oscillating carrier collective, that is plasmon scattering [33, 34]. The distinction between the two regimes, the long-range or plasmon interaction and the short-range or e-e interaction is typically defined by the screening length. E-e interactions at a distance greater than the screening length apart are described in terms of plasmon scattering and those closer are described by the short-range interaction. This distinction follows the natural division of e-e interactions where plasma oscillations are manifest over distances greater than screening length, and at distances less than the screening length the interactions behave more like interacting individual particles [35].

These interactions are two of the many different forms of Coulombic scattering that are modelled in MOSFET devices. A depiction of the various Coulomb scattering processes that have been studied for the simulation of MOSFET devices is given in Figure 1.2.

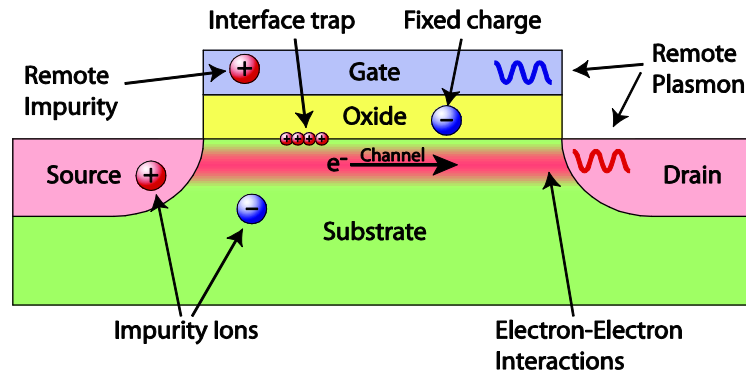


Figure 1.2: Various Coulomb scattering processes found in modern MOSFET devices.

In this figure the majority of Coulombic scattering processes are remote, that is the charged scattering centre is located some distance from the carrier which it scatters. There has been a large increase in the number of researchers studying remote Coulomb scattering recently as the shrinking device dimensions enhance the remote effects.

Remote charge scattering from ionized impurities located in the gate region of poly-silicon gate (remote impurities) devices [36-38] is a strong scattering mechanism in oxide layers less than 3nm thick [39]. This scattering mechanism has been reduced by the introduction of the high- κ materials in the oxide layer which provide a thicker oxide layer for an equivalent silicon dioxide capacitance and a reduced Coulomb potential strength through an increased permittivity, $\epsilon_r \epsilon_0$.

1.2 Aims and Objectives

The introduction of high- κ materials may have reduced poly-Si charge scattering but it has introduced further remote Coulomb scattering due to trapped charges in the gate stack (fixed charges) [40]. The effect of these trapped charges is quite significant on effective device mobility and alters the drive current [41, 42]. Trapped charges are formed during the production of these devices and there is the possibility that future process techniques may reduce the number of trapped charges in the oxide layers.

The introduction of metal gates to MOSFET devices with high- κ dielectrics has been demonstrated to increase device performance and also improves the screening of the remote interactions [7]. Despite this, a recent and extensive study of such devices still found that remote coulomb scattering still causes significant mobility degradation [8].

Remote e-e scattering has also been presented to have a negative impact on device performance for devices with thin oxides and channel length less than 40nm [43]. The high density carrier gasses or plasmons that are present in the heavily doped source, drain and poly-silicon gate regions interact with carriers in the channel region and degrade channel mobility. Interactions of channel carriers with the plasmons in the source and drain regions will reshape the carrier distribution in the channel, moving carriers towards the high energy tail of the distribution [44].

The interaction of the channel carriers with gate plasmons, also referred to as Coulomb drag has been studied [45] and quantitative agreement has been shown experimentally [46]. This remote interaction is strong in poly-silicon gate devices but with the increased screening of a metal gate, the remote Coulomb interaction is minimised [7].

1.2 Aims and Objectives

The effect of the closeness of the source and drain highly-doped regions on channel ionized impurity scattering has not been studied previously and is the focus of this work. The induced polarisation charges in the source and drain will increase the screening of the channel impurities (hence remote screening) and will impact the transport of carriers through the channel. This newly studied effect is entitled remote screening of channel impurities and the effect will increase as the channel length is reduced in future generations.

The aim of this work is to produce the new remotely screened scattering model that can be utilised efficiently in the Monte Carlo simulation of MOSFET devices to describe the interaction of channel ionized impurity with the source and/or drain. This new scattering model must be able to cooperate with the existing ionized impurity model. Using the newly developed scattering model,

1.3 Thesis Outline

Monte Carlo simulations of two example MOSFET devices will be simulated to examine the effect on current and next generation devices.

1.3 Thesis Outline

This thesis will be laid out in the following structure:

Chapter 2 will discuss the most common methods of ionized impurity scattering within Monte Carlo simulations in a literature review. This will include some discussion of existing extensions (or advancements) to the basic model which have been previously studied. The distinctions of each model will be highlighted and the relative advantages of each will be discussed.

Chapter 3 presents a brief introduction to the Monte Carlo simulation methodology used within this work. Starting by covering the fundamentals of the Monte Carlo approach, this includes the Boltzmann Transport Equation (BTE) and the self-scattering procedure, the chapter then moves on to the scattering models and the numerical procedure. Calibration results of the Monte Carlo simulator are also presented to demonstrate the accuracy of the used approach with experimental data.

Chapter 4 calculates the scattering (or interaction) potential for the remotely screened ionized impurity model. The resultant potential is then verified against a fully self-consistent, numerical Poisson solution to ensure the calculation is correct. As will be discussed in this chapter, a simplified model is obtained which is shown to be almost identical to the full model.

Chapter 5 utilises the scattering potential to calculate and analyse a complete scattering model suitable for Monte Carlo simulation. A thorough study is also completed to demonstrate that a further simplification to the scattering model can be made which increases the computational efficiency with negligible loss of accuracy. A new numerical approach to the simulation of ionized impurity scattering is also introduced which greatly reduces simulation time without negative impact on the scattering model.

Chapter 6 completes Monte Carlo simulation of MOSFET devices with the newly developed remote screening model for channel ionized impurities. A typical current generation bulk MOSFET device is simulated along with a future generation double-gate structure to examine the effects of remote screening on the channel performance. In accompaniment to the numerical device simulation, an estimated analysis of the analytical channel mobilities is also calculated for the devices to confirm the simulation results.

1.3 Thesis Outline

Finally in Chapter 7 the conclusions of this work are summarised and suggestions for future work are discussed.

Chapter 2 Literature Review

2.1 Introduction

The focus of this PhD work is on ionized impurity (II) scattering in Monte Carlo (MC) simulation, where in a later chapter, an advanced correction to the Brooks-Herring (BH) model will be developed. There are many methods and techniques used to model the scattering of carriers by ionized impurities, of which the most common and important techniques shall be reviewed here.

The first approach to impurity scattering model developed, the Conwell-Weisskopf (CW) model, will be discussed in Section 2.2. This model utilises the Rutherford ion scattering approach, combined with an empirical cut-off to remove the divergent nature of the Coulomb potential approach. Although this approach is not used here in MC simulations of room-temperature MOSFET devices, it is a significant model and is essential to include in a review of impurity scattering.

The BH model is perhaps the most commonly referenced model with regard to II modelling and as such has had the most development in terms of extensions. This approach differs from the CW model in the definition of the scattering potential, where the BH model includes the screening effect of the surrounding carriers. In section 2.3 this model will be reviewed.

The CW and BH models propose different methods of dealing with the divergence of the Coulomb potential, of which both have strong disadvantages at differing points in MOSFET device simulation. Ridley's Third-Body Exclusion (TBE) model combines these two approaches to remove the disadvantages and obtain a model suitable for device simulation. This model is successfully applied to MC simulations within the simulator used in this work and is reviewed in section 2.4 along with a discussion on the need for such an approach.

With modern devices being scaled to sub-50nm dimensions, the number of actual dopants and their position within the channel region has a large effect on device performance. The discrete nature of dopants in modern nanoscaled devices can be modelled using an *ab initio* atomistic approach within both Drift-Diffusion (DD) and MC simulations. Section 2.5 will briefly review this approach of atomistic impurity scattering where dopant atoms are treated as discrete charges in the electrostatic solution of the device. Although this approach does not use a typical scattering rate representation, it is an important method for modelling the effect of ionized impurities in MC simulation.

2.1 Introduction

For reference, the method used here to obtain scattering rates for MC is based on application of Fermi's Golden Rule to obtain a scattering probability rate, $P(\mathbf{k}, \mathbf{k}')$, for a carrier from a state $\mathbf{k}$ to a state $\mathbf{k}'$. Fermi's Golden Rule for an elastic collision, such as the interactions involved in II scattering, is given by [30]

$$P(\mathbf{k}, \mathbf{k}') = \frac{2\pi}{\hbar} |\mathbf{H}_{\mathbf{k}\mathbf{k}}|^2 \delta(E(\mathbf{k}') - E(\mathbf{k})) \quad (2.1)$$

where $|\mathbf{H}_{\mathbf{k}\mathbf{k}}|^2$ is the square of scattering matrix element and the Dirac delta function, $\delta(\cdot)$, ensures that energy is conserved in the interaction. The scattering matrix element is obtained from the Fourier Transform of the scattering potential, U_s , and can be written as

$$\mathbf{H}_{\mathbf{k}\mathbf{k}} = \frac{1}{\Omega} \int d^3\mathbf{r} \exp(-i\mathbf{q} \cdot \mathbf{r}) U_s(\mathbf{r}) \quad (2.2)$$

where $\mathbf{q} = \mathbf{k}' - \mathbf{k}$ denotes the transfer of momentum between the carriers and Ω is the unit volume. The scattering rate which can be used within the MC simulation can be found by summing the scattering probability rate over all possible final states, defined as equation (2.3), where the scattering rate is a function of the magnitude of the state $\mathbf{k}$.

$$\Gamma(\mathbf{k}) = \sum_{\mathbf{k}'} P(\mathbf{k}, \mathbf{k}') \quad (2.3)$$

This can easily be converted to an integral for a 3-dimensional system using the following definition

$$\sum_{\mathbf{k}'} P(\mathbf{k}, \mathbf{k}') \equiv N_k \int d^3\mathbf{k}' P(\mathbf{k}, \mathbf{k}') \quad \text{with } N_k = \frac{\Omega}{(2\pi)^3} \quad (2.4)$$

In the calculation of the scattering rate, both the incoming and outgoing carrier wave vector, $\mathbf{k}$ and $\mathbf{k}'$ respectively, are expanded in the spherical coordinate system, $\mathbf{k} = \{k, \theta_k, \varphi_k\}$ and $\mathbf{k}' = \{k', \theta_{k'}, \varphi_{k'}\}$. By allowing the reference frame of the outgoing wave vector to be aligned with the incoming wave vector (that is by allowing $\theta_k = 0$), the angles of the incoming wave vector are cancelled. As a result of this expansion, often the scattering rate equations are written as function of a vector variable $\mathbf{k}$ yet utilise a scalar magnitude k on the RHS.

2.2 Conwell-Weisskopf

The CW approach to ionized impurity scattering is based in the Rutherford formula for scattering by a charged ion [47]. This approach treats the ionized impurity as a single point charge which is entirely independent from all other ions. The scattering electron is assumed to have a well-defined trajectory. The model utilises the classic Coulomb point charge which models a single impurity atom in a perfect crystal lattice [47, 48]. The scattering potential for the CW model, based on the bare Coulomb potential, is given by equation (2.5).

$$U_s(\mathbf{r}) = eV(\mathbf{r}) = \frac{Ze^2}{4\pi\epsilon_{Si}\epsilon_0} \frac{1}{r} \quad (2.5)$$

Completing the Fourier transform and Born approximation of the scattering potential, the following scattering matrix element is obtained

$$|\mathbf{H}_{\mathbf{k}'\mathbf{k}}|^2 = \left(\frac{Ze^2}{4\pi\epsilon_{Si}\epsilon_0} \right)^2 \frac{1}{\Omega^2} \left(\frac{4\pi}{\mathbf{q}^2} \right)^2 \quad (2.6)$$

Here the number of impurity charge units is given by Z , the static permittivity of silicon is $\epsilon_{Si}\epsilon_0$ and the momentum transfer wave-vector for an elastic collision (assuming that $E(\mathbf{k}) = E(\mathbf{k}')$) is specified as $\mathbf{q}^2 = 2\mathbf{k}'^2(1 - \cos\theta)$. Evaluating this using spherical co-ordinates for parabolic, spherical bands with Fermi's Golden Rule, equation (2.1), gives the following scattering rate

$$\Gamma_{CW} = \left(\frac{Ze^2}{4\pi\epsilon_{Si}\epsilon_0} \right)^2 N_I \frac{2^3\pi m^*}{\hbar^3} k \int_0^\pi \frac{\sin\theta}{\mathbf{q}^2} d\theta \quad (2.7)$$

where N_I is the impurity density. The remaining integral in equation (2.7) diverges for $\theta \rightarrow 0$. This is a known problem with the bare Coulomb potential, in that the potential has an infinite range over which it is felt.

Using Rutherford scattering, the scattering electron is treated as a classical particle which interacts with the impurity according to the impact parameter, b . This impact parameter describes the interaction of the electron with the impurity via the scattered angle of the electron. It is defined as the perpendicular distance between the scattered electron and impurity ion and is depicted in Figure 2.1.

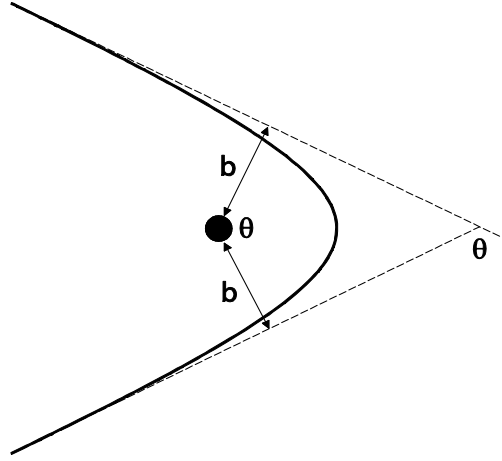


Figure 2.1: Definition of the impact parameter, b , from Rutherford scattering.

Conwell and Weisskopf solved the problem of the diverging scattering rate by introducing a limit on the potential that defines a cut-off distance for the impact parameter, given by equation (2.8). The limit that was introduced is based on the assumption that the scattering event is a two-body event, an electron scattering with a single impurity.

$$b = \left(\frac{Ze^2}{4\pi\epsilon_{\text{Si}}\epsilon_0} \right) \frac{m^*}{\hbar^2 k^2} \cot\left(\frac{\theta}{2}\right) \quad (2.8)$$

To ensure that the electron scatters from only the closest impurity, the impact parameter is cut-off at half the average inter-ion separation distance. Here the definition of the average inter-impurity ion distance for a uniform distribution is given as $a = N_I^{-1/3}$ [48]. The impact parameter and average inter-ion separation distance are plotted in Figure 2.2 (a) and (b) respectively.

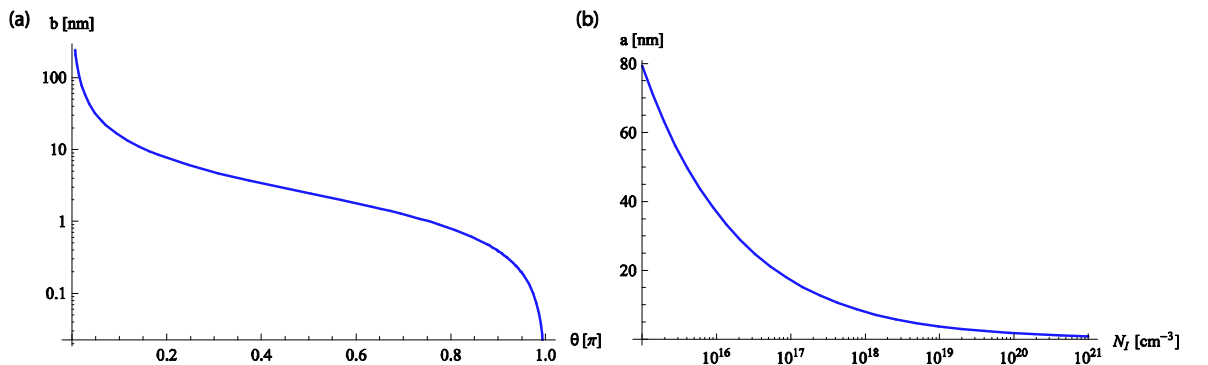


Figure 2.2: (a) Semi-log plot of the impact parameter for an electron of energy $E = 25\text{meV}$ and (b) the plot of the average inter-ion separation using $a = N_I^{-1/3}$.

2.3 Brooks-Herring

Defining half the average inter-ion distance as the maximum impact parameter in equation (2.8), e.g. $b_{\max} = \frac{1}{2} N_I^{-1/3}$, and solving for the angle, the definition for the minimum scattering angle can be obtained as

$$\theta_{\min} = 2 \tan^{-1} \left(\left(\frac{Ze^2}{4\pi\epsilon_{Si}\epsilon_0} \right) \frac{m^*}{\hbar^2 k^2} \frac{1}{b_{\max}} \right) \quad (2.9)$$

Using equation (2.9), $\theta_{\min}$, as the lower limit of the integral in equation (2.7) allows the integral to be completing yielding the CW scattering rate.

$$\Gamma_{CW} = \left(\frac{Ze^2}{4\pi\epsilon_{Si}\epsilon_0} \right)^2 N_I \frac{\pi}{2^{3/2} m^{*1/2} E^{3/2}} \cot^2 \left(\frac{\theta_{\min}}{2} \right) \quad (2.10)$$

The CW model finds a solution to the problem of the divergent scattering model due to the diverging scattering potential, although it has been often criticised for the artificial manner of using half the average inter-ion separation. It has also been noted that the choice of exactly half the separation distance is rather arbitrary and other methods have been suggested. These have included the spherical symmetry on the distribution of impurity ions [49] and even a probabilistic method [50, 51] such as equation (2.11).

$$a = \left(\frac{4}{3} \pi N_I \right)^{-1/3} \Gamma \left(\frac{4}{3} \right) \approx (2\pi N_I)^{-1/3} \quad (2.11)$$

The major limitation of the CW approach is that it fails to take into account the effect of the mobile charge surrounding the impurity on the scattering potential. This space charge would effectively screen the potential forcing a quicker drop off at large distances from the ionized impurity. This failure in the model will cause an over-estimation of the scattering rate when the mobile charge is much less than impurity density, as in the depletion-region of a p-n junction [52].

2.3 Brooks-Herring

The BH model for ionized impurity scattering uses the Coulomb potential to model a single ionized impurity but also includes the effect of screening from the space charge surrounding the impurity. The screening effect is generally calculated as a length scale which describes the distance the potential will take to respond to a change in the charge density and can be found from the linearized form of the Poisson equation. The Poisson equation for a point charge is given as

2.3 Brooks-Herring

equation (2.12), here Ze is the charge on the impurity located at $\mathbf{r}_1$ and the charge density in the system is $\rho(\mathbf{r}) = e(p(\mathbf{r}) - n(\mathbf{r}) - N_A^-(\mathbf{r}) + N_D^+(\mathbf{r}))$.

$$\nabla^2 V(\mathbf{r}) = -\frac{\rho(\mathbf{r})}{\epsilon_{Si}\epsilon_0} - \frac{Ze^2}{2\pi\epsilon_{Si}\epsilon_0}\delta(\mathbf{r}-\mathbf{r}_1) \quad (2.12)$$

Linearization of this equation through the Thomas-Fermi method [53] and assuming a small perturbation in the neutral space-charge, the Poisson equation can be written as

$$\nabla^2 V(\mathbf{r}) = \epsilon_{Si}\epsilon_0 k_C^2 V(\mathbf{r}) - \frac{Ze}{2\pi\epsilon_{Si}\epsilon_0}\delta(\mathbf{r}-\mathbf{r}_1) \quad (2.13)$$

where $\lambda_C = k_C^{-1}$ and

$$k_C^2 = \frac{e^2 n}{\epsilon_{Si}\epsilon_0 k_B T} \frac{\mathfrak{F}_{-\frac{1}{2}}(\eta)}{\mathfrak{F}_{\frac{1}{2}}(\eta)} \quad (2.14)$$

This solution uses Fermi-Dirac statistics for the carrier densities and the degenerate Debye-Hückel form of the inverse screening length, k_C , where $\eta = E_F/k_B T$ and $\mathfrak{F}_j$ is the Fermi-Dirac integral of order j [54]. Typical values for the degenerate screening length given by equation (2.14) are shown in Figure 2.3.

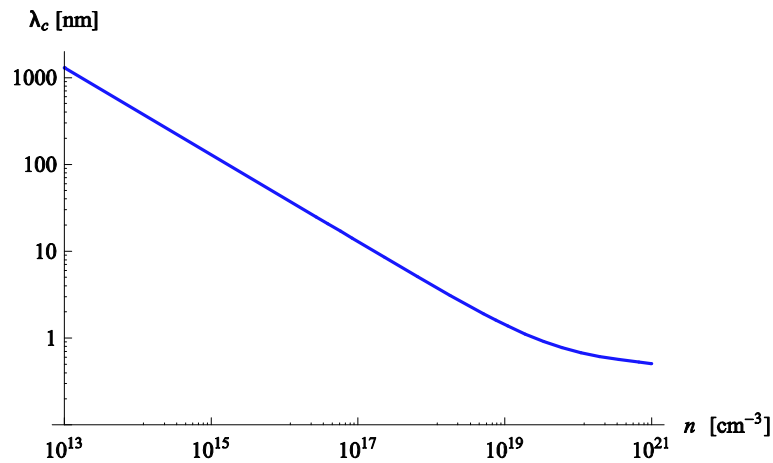


Figure 2.3: Plot of the degenerate Debye-Hückel screening length.

The potential solution to equation (2.13) can then be found using appropriate boundary conditions as the screened Coulomb model, given as the energy in equation (2.15). After completion of the

2.3 Brooks-Herring

Fourier transform and taking the Born approximation, the scattering matrix element can be derived as equation (2.16).

$$U_s(\mathbf{r}) = eV(\mathbf{r}) = \frac{Ze^2}{4\pi\epsilon_{si}\epsilon_0} \frac{\exp(-k_C\mathbf{r})}{\mathbf{r}} \quad (2.15)$$

$$|\mathbf{H}_{\mathbf{k}'\mathbf{k}}|^2 = \left(\frac{Ze^2}{4\pi\epsilon_{si}\epsilon_0} \right)^2 \frac{1}{\Omega^2} \left(\frac{4\pi}{\mathbf{q}^2 + k_C^2} \right)^2 \quad (2.16)$$

Comparing this equation with the scattering matrix element from the CW approach in the previous section, equation (2.6), we can see that the screening length removes the singularity as $\mathbf{q} \rightarrow 0$. Clearly, the CW scattering matrix element can be found by setting the inverse screening length to zero, that is $k_C = 0$.

The scattering rate can be calculated using equation (2.16) in Fermi's Golden Rule and summing over all final states. Here $E_{k_C} = \hbar^2 k_C^2 / 2m^*$ and the scattering rate has been multiplied by the number density of impurities per unit volume, $N_I \Omega$.

$$\Gamma_{BH} = \left(\frac{Ze^2}{4\pi\epsilon_{si}\epsilon_0} \right)^2 N_I \frac{2^{3/2} \pi}{m^{*1/2} E_{k_C}^2} \frac{E^{1/2}}{1 + 4E/E_{k_C}} \quad (2.17)$$

The BH approach is generally more widely accepted [48] as it has removed the divergence of the scattering rate with low-angle scattering. This is true as long as there is enough mobile charge available to screen the Coulomb potential within a reasonable distance [55]. In conditions where there are very few carriers to screen the potential, the BH model returns to the similar divergent nature found in the unscreened model. There has been many corrections and improvements made to the BH model, many of which are detailed in the review by Chattopadhyay & Queisser [48].

2.3.1 Momentum-Dependent Screening

The standard BH approach uses a static screening model which in this chapter is the degenerate Debye-Hückel model of equation (2.14) model which is momentum independent. It has been suggested by some authors [56, 57] that this model for screening is not sufficiently accurate at high doping densities and is being over-estimated. To correct this a momentum-dependent screening correction has been developed which can be applied to the BH case [58, 59].

2.3 Brooks-Herring

Momentum dependent screening can be calculated from the dielectric function assuming that the impurity potential is time-independent and thus the frequency is zero [56]. The wave-vector dependent dielectric function for degenerate statistics can then be written as

$$\varepsilon(\mathbf{q}, 0) \equiv \varepsilon(\mathbf{q}, 0) = 1 + \frac{k_C^2}{\mathbf{q}} F(\xi, \eta) \quad (2.18)$$

$$F(\xi, \eta) = \frac{1}{\mathfrak{F}_{-\frac{1}{2}}(\eta)} \frac{1}{\xi \sqrt{\pi}} \int_0^\infty \frac{x}{1 + \exp(x^2 - \eta)} \ln \left| \frac{x + \xi}{x - \xi} \right| dx \quad (2.19)$$

Here k_C^2 is the inverse screening length given by equation (2.14), $\mathbf{q}^2 = 2\mathbf{k}^2(1 - \cos\theta)$ is the momentum transfer of the scattering and $\mathfrak{F}_j(\eta)$ is Fermi integral of order j . The values ξ , x and η are related to the momentum transfer wave vector, carrier momentum and Fermi level respectively.

$$\xi^2 = \frac{\hbar^2 \mathbf{q}^2}{8m^* k_B T} \quad (2.20)$$

$$x^2 = \frac{\hbar^2 \mathbf{k}^2}{2m^* k_B T} \quad (2.21)$$

$$\eta = \frac{E_F}{k_B T} \quad (2.22)$$

The momentum dependent screening correction factor has been plotted in part (a) of Figure 2.4. The plot demonstrates the correction to the screening at large momentum transfer and the return to the static screening model at $F(0, \eta) = 1$. Within degenerate conditions ($\eta > 0$) the screening correction is reduced as is expected from a higher screening density.

2.3 Brooks-Herring

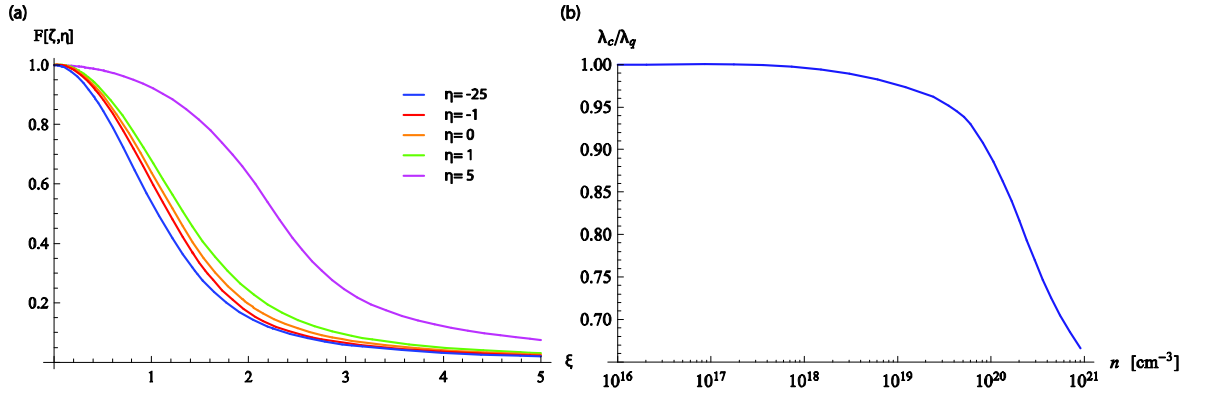


Figure 2.4: (a) The momentum dependent screening factor, $F(\xi, \eta)$, over several values of the reduced Fermi energy, η , and (b) the ratio of momentum dependent screening to Debye-Hückel screening.

The corrected impurity potential is calculated by applying the dielectric function of equation (2.18) to the Fourier Transform of equation (2.5), the CW scattering interaction potential.

$$V_{mom}(\mathbf{q}) = \frac{V(\mathbf{q})}{\epsilon(\mathbf{q}, 0)} = \left(\frac{Ze^2}{4\pi\epsilon_{si}\epsilon_0} \right) \frac{1}{\Omega} \frac{4\pi}{\mathbf{q}^2 + k_C^2 F(\xi, \eta)} \quad (2.23)$$

The scattering rate can then be calculated using Fermi's Golden Rule with the square of the above matrix element, equation (2.23). Noting that the integral in equation (2.19) must be completed numerically which restricts the θ integral from being completed, the scattering rate can be written as

$$\Gamma_{mom}(\mathbf{k}) = \left(\frac{Ze^2}{4\pi\epsilon_{si}\epsilon_0} \right)^2 N_I \frac{8\pi m^* k}{\hbar^3} \int_0^\pi \frac{\sin \theta}{(\mathbf{q}^2 + k_C^2 F(\xi, \eta))^2} d\theta \quad (2.24)$$

Momentum dependent screening is expected to decrease the inverse screening length at large $\mathbf{q}$ values. This will occur at high carrier densities and cause an increase in the scattering rate corresponding to the reduction in magnitude of the screening.

The momentum dependent correction is demonstrated with respect to the static screening model in plot (b) of Figure 2.4. Here the carriers are assumed to have the room temperature average thermal energy, $E = \frac{3}{2}k_B T$ at 300K. The scattering angle defining the momentum transfer wave-vector, $\mathbf{q}$, is selected through the corresponding peak angular scattering probability. The peak angular scattering probability is found by obtaining the maximum of the integrand in equation (2.24).

2.4 Third-Body Exclusion

The effect of the correction is negligible below $\sim 10^{17} \text{ cm}^{-3}$ where most ionized impurity scattering is small-angle forward scattering and hence $\mathbf{q}(\theta \rightarrow 0) \approx 0$. At higher densities, where high-angle scattering is dominant, the momentum dependent correction can reduce the screening by up to 30%.

In the limit of $\lim_{q \rightarrow 0} \xi \rightarrow 0$, the momentum dependent scattering model given by equation (2.24) will return to the BH model. In other words, when the carrier densities are very low the scattering model will return to the screened BH approach. At the opposite limit, $\lim_{q \rightarrow \infty} \xi \rightarrow \infty$, when carrier densities are very high, the scattering model will behave like the unscreened CW approach.

2.4 Third-Body Exclusion

The problem of divergent scattering rates with ionized impurity scattering is a difficult problem to solve. The two well-known methods by CW and BH use different solutions to reduce the range of the Coulomb potential. Of these two methods the BH approach has been more widely accepted as it includes the screening of the impurity potential by mobile charge in the system. It allows the Coulomb potential to be curtailed at a distance defined by the screening length. This method is generally very successful when there is sufficient mobile charge in the system to screen the impurity potential. If there is a lack of mobile charge carriers available to screen the potential, the model will return to the divergent nature.

In the CW model the Coulomb potential is strictly cut-off at half the average inter-ion separation distance, assuming a uniform impurity distribution. This method guarantees that the divergent nature of the Coulomb potential is contained and ensures that the scattering event is solely a two-body process. Ridley has developed a model which reconciles the two approaches used by CW and BH, entitled the TBE model. By introduction of a function that gives the probability of another ionized impurity being closer to the scattering carrier, the BH model can be modified to incorporate the CW cut-off [55, 60].

This model provides the CW and BH models as limiting cases such that if the screening length is less than half the average inter-ion separation the screened potential is used otherwise it returns the unscreened, cut-off model used by CW. Figure 2.5 plots the three scattering models against the mobile electron concentration and the cross-over from the BH to CW approaches is clear in the TBE model. In this figure, the electron energy is assumed to be $E = 25 \text{ meV}$ and the background impurity concentration is fixed at $N_I = 10^{18} \text{ cm}^{-3}$.

2.4 Third-Body Exclusion

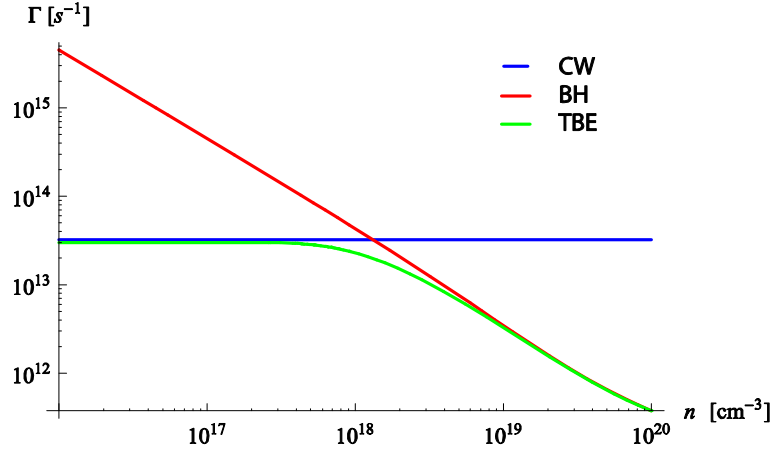


Figure 2.5: Cross-over of TBE scattering model from the CW to the BH approaches.

The probability that no other ion is closer to the scattering electron is a function of the impact parameter, b , and is given as [55]

$$P(b) = \exp(-\pi a b^2 N_I) \quad (2.25)$$

where a is half the average inter-ion separation given by equation (2.11) and N_I is the density of ionized impurities. The impact parameter is then defined from the differential scattering cross-section for the BH model as

$$\begin{aligned} \pi b^2 &= 2\pi \int_{\theta}^{\pi} \sigma(\theta_b) \sin \theta_b d\theta_b \\ &= \left(\frac{Ze^2}{4\pi\epsilon_{Si}\epsilon_0} \right)^2 \frac{2^3 \pi m^{*2}}{\hbar^4} \frac{1}{4k^2 + k_C^2} \frac{1 + \cos \theta}{2k^2 (1 - \cos \theta) + k_C^2} \end{aligned} \quad (2.26)$$

To obtain the Ridley TBE model, the probability function is applied to the differential scattering cross-section to obtain [60]

$$\sigma_R(\theta) = \sigma(\theta) P(b) \quad (2.27)$$

The scattering rate is calculated by integrating the Ridley differential cross-section, σ_R , over θ and multiplying by the impurity density and the group velocity, $\mathbf{v}(\mathbf{k}) = \hbar \mathbf{k} / m^*$.

$$\Gamma_R = \mathbf{v}(\mathbf{k}) N_I \int_0^{\pi} \sigma_R(\theta) d\theta \quad (2.28)$$

2.5 Atomistic Impurity

Completing the integral and after some manipulation, the final scattering rate can be expressed as

$$\Gamma_R = \frac{\mathbf{v}(\mathbf{k})}{a} \left[1 - \exp \left(-\frac{a}{\mathbf{v}(\mathbf{k})} \Gamma_{BH} \right) \right] \quad (2.29)$$

In this expression Γ_{BH} is given by equation (2.17), the BH scattering rate and $a = (2\pi N_I)^{-1/3}$ is the average inter-ion separation distance.

The Ridley TBE model combines the approach of the more widely accepted screened approach used by BH with the CW cut-off method of removing the divergence. This model for ionized impurity scattering can be applied consistently to all conditions in a MC simulation without worry of it producing excessively large scattering rates when there is few mobile carriers to screen the electrons. It is an advantageous II scattering model as it can be applied to all simulation conditions but it is not as accurate a II model as the BH approach and will underestimate the effect of II scattering in MOSFET devices [61].

The TBE model has traditionally been the approach for II scattering in the MC code used in this work but it is not an ideal approach. As a result, in Chapter 5 a more advanced II model is developed and utilised which retains the accuracy of the BH approach whilst reducing the divergent scattering rate nature inherent to BH.

2.5 Atomistic Impurity

Although the atomistic impurity approach to scattering from ionized impurities is distinct to the research within this thesis, it is important to discuss the method used. A brief overview of the technique will be covered here and further detail of the method and effect on device performance is referred to the original authors [62-64].

As device dimensions are scaled to well below $0.1\mu m$, the effect of impurity centres within the device become much more important [63]. There will be relatively few dopant ions needed to obtain the required doping level. Hence, it is necessary to look at the effect of the discrete nature of these dopants on device performance and carrier transport [65].

Typical MC impurity scattering methods utilise an approach based on Fermi's Golden rule where ionized impurities are included via a continuous background doping level. Atomistic impurity scattering takes a different approach to the normal method used within such MC simulations. In atomistic scattering the discrete impurity charge is included directly into the mesh-based solution

2.6 Conclusion

of the non-linear Poisson solution for the electrostatic potential. This electrostatic solution is then used in an Ensemble Monte Carlo (EMC) simulator where conventional II scattering is removed from the scattering tables [66]. Hence, by incorporating the dopant potential into the electrostatic solution of the system, the effect of the dopant on carrier transport can be examined in detail within the MC simulation [67].

The atomistic impurity scattering approach is a classical approach to the problem in that the scattering of the carriers from the II is modelled through the classical transport of MC particles. In other words, rather than using a quantum mechanical description of II scattering utilising a scattering rate, the atomistic approach scatters particles through the electrostatic field of the ionized impurity directly. Therefore as particles are scattered from the electric fields present using Newton's laws of motion, the classical component of MC simulation, the atomistic approach is a classical solution to the problem.

This approach highlights the effect that discrete impurities have on the electrostatics and current drive of the device. Threshold voltage and drain currents vary with exact dopant number and position within the channel and is unavoidable as MOSFET sizes are scaled to decanano dimensions [62, 64, 68].

2.6 Conclusion

This chapter has completed a review of the three major II scattering models used within MC simulations. Starting with the CW model which is considered to be the first approach developed to model II scattering in semiconductors. The CW model is developed from the bare Coulomb potential that neglects the screening effect of the mobile charge. To control the divergence of the bare Coulomb potential it uses an empirical cut-off on the impact parameter such that any scattering event with an impact parameter larger than half the inter-ion separation is neglected. This approach is successful in controlling the divergence but can be quite inaccurate in device conditions when the mobile carrier density can be several orders of magnitude smaller than the impurity density. This reason limits the use of the CW approach to simulation of bulk semiconductors where the mobile charge cannot deviate far from the background impurity density.

The BH model includes the screening effect of the mobile charge on II scattering and is more suitable to a wide variety of device simulations. The use of the mobile charge density to cut-off the potential is a more physical approach to the problem than that utilised in the CW model and provides a better measure of carrier mobility in conditions where carrier density is far from the impurity density. Unfortunately, the BH scattering model suffers a problem of divergent scattering

2.6 Conclusion

rates when the carrier density is several orders of magnitude smaller than the impurity density. As the magnitude of the scattering rate has a direct effect on MC simulation by increasing the physical number of scattering events per unit time, a divergent scattering rate renders simulation unfeasible.

The CW and BH models each use a different approach to controlling the Coulomb potential which have advantages in different circumstances. The TBE model combines these approaches to provide a model which doesn't diverge but also includes the important mobile charge screening effect. This model is particularly advantageous in MC simulations as it can be used consistently in all device conditions but will underestimate the effect of II scattering when the mobile charge density is much smaller than the II density. The importance of including the screening effect of mobile carriers whilst controlling the divergent nature of II scattering forces the use of this non-ideal approach. As mentioned earlier in this chapter, a better model based on the BH approach which reduces the divergent nature is developed in Chapter 5 and applied in this work.

In reviewing the major techniques for II scattering, it is also important to include the approach of atomistic impurity scattering. This is not a typical scattering model utilising Fermi's Golden Rule, instead it resolves discrete ionized impurities in the electrostatic solution to allow simulation of the effect of position and number on device performance. It can be considered a classical approach to the problem by modelling the II scattering through the electrostatic fields which transport the particles using Newton's laws of motion. This approach allows device variability of IIs at the atomic scale to be modelled which is increasingly important as device dimensions shrink.

Chapter 3 Monte Carlo Simulation

3.1 Introduction

The Monte Carlo (MC) simulation methodology is ideal to study the effects of complex scattering mechanisms in MOSFET devices and is the simulation methodology used in this PhD thesis. The MC method is a stochastic technique to solve large and complex mathematical problems, and is applied here for semiconductor device simulation by means of a particle method to solve the Boltzmann Transport Equation (BTE).

The MC simulation program used in this research has been developed to simulate electron transport in nMOSFET devices. It is a fully self-consistent 3D approach coupled to a non-linear Poisson solver and is capable of solving various MOSFET device structures such as the bulk, silicon-over-insulator and double-gate structures. Calibration of the simulator is completed against experimental data for the properties of silicon such as the energy- and velocity-field characteristics and the bulk, concentration-dependent mobility. There is also device calibration in terms of the universal or inversion mobility which has to be matched with experimental data. Once this calibration has been completed, a wide variety of silicon MOSFET structures can be simulated.

This chapter will begin with a brief review of MC fundamentals in section 3.2, including a discussion on the BTE, the band structure and the process of carrier scattering. Following this, the scattering mechanisms employed in the MC simulation used here will be presented and discussed in section 3.3. The method with which devices are solved numerically with the MC procedure is covered in section 3.4. Finally, the calibration of the simulation with experimental data will be demonstrated in section 3.5.

3.2 Monte Carlo Fundamentals

3.2.1 Boltzmann Transport Equation

The BTE is a complex integro-differential equation that describes the semi-classical transport of carriers in a volume of phase space. The BTE is semi-classical as it describes the carrier transport using the classical equations of motion with Newton's laws, but describes the scattering of the carriers through quantum mechanical terms.

3.2 Monte Carlo Fundamentals

The solution to the BTE is the distribution function, $f(\mathbf{r}, \mathbf{k}, t)$, which gives the probability of finding a carrier at a time t in the 6-dimensional phase space. Essentially the BTE is a bookkeeping equation for the distribution function recording the flow of carriers in and out of position and momentum space. The BTE must also ensure that particle continuity is conserved, for instance if there is a greater in-flow than out-flow in a volume in phase space or carrier scattering directs many carriers to a volume, the distribution function must change to conserve the particle number.

Once the distribution has been found, many important properties of devices can be obtained. These include the charge density, the carrier density, the mean carrier velocity and the mean carrier energy. These quantities can be found from the distribution function by integrating over all $\mathbf{k}$ states, such as the carrier density in equation (3.1) or the average kinetic energy density in equation (3.2).

$$n(\mathbf{r}, t) = \frac{N_k}{\Omega} \int_{\mathbf{k}} f(\mathbf{r}, \mathbf{k}, t) d^3\mathbf{k} \quad (3.1)$$

$$W(\mathbf{r}, t) = \frac{N_k}{\Omega} \int_{\mathbf{k}} E(\mathbf{k}) f(\mathbf{r}, \mathbf{k}, t) d^3\mathbf{k} \quad (3.2)$$

For equilibrium systems the distribution function is often expressed by the Fermi distribution for degenerate systems or the Maxwell-Boltzmann distribution for non-degenerate systems. For such equilibrium conditions the distribution function can be calculated from the Fermi energy and the lattice temperature. It is also possible to define the displaced or drifted distribution function which represents a non-equilibrium distribution function and is considered only a good approximation for low-field conditions [30].

The BTE can be derived from the quantum mechanical Liouville-Von Neumann transport equation under a number of simplifying assumptions [69, 70]. It is also possible to define the BTE using an elemental procedure in terms of carrier in- and out-flows of a small volume in phase space over a short time period [30]. It is worth noting that the Drift-Diffusion (DD) and hydrodynamic approaches can be derived from moments of the BTE.

The general form for the semi-classical BTE is given by equation (3.3) below [30, 71, 72]

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f + \dot{\mathbf{k}} \cdot \nabla_{\mathbf{k}} f = \left. \frac{\partial f}{\partial t} \right|_{coll} \quad (3.3)$$

3.2 Monte Carlo Fundamentals

where f is the distribution function that is to be solved, $\mathbf{v}$ denotes the change in position of the carriers (the carrier group velocity) and $\hbar \dot{\mathbf{k}}$ the change in crystal momentum of the carriers subject to the externally applied fields. The 2nd and 3rd terms on the LHS of the BTE refer to the time rate of change of the distribution function from the movement of the carriers in position space and from the movement of carriers in $\mathbf{k}$ space respectively, ensuring particle continuity. These terms essentially represent the carrier dynamics which obey the classical equations of motion given by equations (3.4) and (3.5) where the Hamiltonian can be written as $H(\mathbf{r}, \mathbf{k}) = E(\mathbf{k}) + eV(\mathbf{r})$ [32].

$$\mathbf{v} = \frac{d\mathbf{r}}{dt} = \frac{1}{\hbar} \nabla_{\mathbf{k}} H = \frac{1}{\hbar} \frac{\partial E(\mathbf{k})}{\partial \mathbf{k}} \quad (3.4)$$

$$\hbar \dot{\mathbf{k}} = \frac{d\mathbf{k}}{dt} = -\frac{1}{\hbar} \nabla_{\mathbf{r}} H = -\frac{1}{\hbar} e \frac{\partial V(\mathbf{r})}{\partial \mathbf{r}} = -\frac{1}{\hbar} e \mathbf{E}(\mathbf{r}) \quad (3.5)$$

Incidentally, the electric field is determined by Poisson's equation

$$\nabla^2 V = -\nabla E = -\frac{e}{\epsilon_{Si} \epsilon_0} (p - n + N_D^+ - N_A^-) \quad (3.6)$$

where $\epsilon_{Si} \epsilon_0$ is the dielectric constant for silicon, V is the electrostatic potential, e is the electronic charge, p the mobile hole density, n the mobile electron density and N_D^+, N_A^- the ionized donor and acceptor density.

The term on the RHS of the BTE, equation (3.3), refers to the time rate of change of the distribution function from collisions of the carriers in phase space. This scattering term on the RHS of the BTE equation can be expressed for a degenerate system as

$$\begin{aligned} \left. \frac{\partial f}{\partial t} \right|_{coll} = & \int_{\mathbf{k}'} f(\mathbf{r}, \mathbf{k}', t) (1 - f(\mathbf{r}, \mathbf{k}, t)) P(\mathbf{k}', \mathbf{k}) d^3 \mathbf{k}' \\ & - \int_{\mathbf{k}'} f(\mathbf{r}, \mathbf{k}, t) (1 - f(\mathbf{r}, \mathbf{k}', t)) P(\mathbf{k}, \mathbf{k}') d^3 \mathbf{k}' \end{aligned} \quad (3.7)$$

where $P(\mathbf{k}, \mathbf{k}')$ is the probability of scattering from a state $\mathbf{k}$ to a state $\mathbf{k}'$, $f(\mathbf{r}, \mathbf{k}, t)$ gives the probability of finding a carrier at state $\mathbf{k}$ and $(1 - f(\mathbf{r}, \mathbf{k}', t))$ gives the probability of state $\mathbf{k}'$ being empty. For the MC approach used in this work this equation can be simplified assuming a non-degenerate system such that $f(\mathbf{r}, \mathbf{k}, t) \ll 1$ allowing the terms $(1 - f(..))$ to be removed.

3.2 Monte Carlo Fundamentals

The BTE is a linear equation (for a non-degenerate system) which is not easily solved and although analytical solutions have been found, these are generally limited to small regions of interest by the approximations involved to obtain the solution. Numerical approaches to solving this equation are more commonly applied and have been far more successfully, offering solutions which can be applied to many device conditions. Numerical solutions to the BTE include an iterative approach which solves the whole distribution function at each iteration [30, 71]. This approach was adopted early in the development of such numerical approaches and is suitable for low-field conditions. Another more advanced approach is the expansion of the BTE using spherical harmonics and has been readily applied to MOSFET simulation [30, 73].

The approach used in this work is also an early approach but has been very successful in device simulation and is the most popular solution. The numerical method used is of course the particle based MC methodology and is quite different from the other numerical approaches in that it models the transport of particles directly. The MC method allows the physics of carrier transport to be modelled and yields results for devices that are close to experimental data [71, 74-76]. The numerical MC simulation methodology will be discussed in more detail later in the chapter.

It is important to briefly discuss the three major approximations employed in the BTE equation. A more detailed examination of the approximations involved than that given here can be found in references [30, 69].

The most important approximation made in the BTE is that of the single particle description of the ensemble of particles in a real system. The distribution function in the full problem describes the probability of state of a large number of carriers. Assuming that carrier-carrier interactions are weak, true for dilute concentrations, the ensemble carrier distribution function can be reduced to a single carrier distribution. Although in silicon MOSFETs the carrier concentrations are not always weak the carrier-carrier interactions can be included separately via the scattering term on the RHS. The single particle description remains valid in this case as carrier-carrier interactions affect the distribution function by redistribution of carrier momentum which can be equally well described in the single particle description. It should be noted that the influence of long-range carrier-carrier interactions (electron-plasmon interactions) on the system is included indirectly through the electric field term, governed by Poisson's equation (3.6), provided that the mesh spacing and timestep intervals are carefully chosen [77, 78].

The second approximation, mentioned earlier in this section, is the treatment of the carriers as classical particles which obey Newton's laws. This is clear from the definition of the distribution function which defines both the position and momentum of a given particle. This assumption will hold as long as the electric field is slowly varying over a length comparable to the average carrier

3.2 Monte Carlo Fundamentals

wavelength. Using the thermal de Broglie wavelength equation, the wavelength of an average thermal carrier is $\lambda_B = h / \sqrt{2m^*k_B T} \approx 13nm$ at room temperature (300K).

The third approximation relates to scattering and states that scattering events are assumed to be instantaneous and localised in space. In other words, the carrier does not change position or gain energy from the electric field during the collision. This approximation can be considered valid as long as the mean time between collisions, τ , is greater than $\tau \gg \hbar/k_B T$. This can be related to the mean distance between collisions using the relation $l = v\tau$ and multiplying both sides by the average carrier velocity. This then states that the mean distance between collisions must be greater than the average thermal wavelength, λ_B .

3.2.2 Band Structure

The electrons in a perfect crystal can be modelled by Bloch states, including the periodic crystal potential, with the wave function [71]

$$\Psi_{nk}(\mathbf{r}) = u_{nk}(\mathbf{r}) \exp(i\mathbf{k} \cdot \mathbf{r}) \quad (3.8)$$

where n is the band index, $\hbar\mathbf{k}$ is the carrier crystal momentum and $u_{nk}(\mathbf{r})$ denotes the periodicity of the crystal. The Bloch states relate a carrier energy E to a state $\mathbf{k}$, with the function $E_n(\mathbf{k})$ often referred to as the energy dispersion relation. The $E_n(\mathbf{k})$ functions describe the band structure of the material for the given band n . In this work the material under study is silicon and the band index will be neglected in future references. Also, only the lowest minima conduction band for silicon, the X-valleys, will be considered as this work is concentrated on relatively low energy electron transport ($E < \sim 1.5\text{eV}$).

For the conduction band often a simple quadratic expression is used to represent the energy dispersion relation as

$$E(\mathbf{k}) = \frac{\hbar^2 \mathbf{k}^2}{2m^*} \quad (3.9)$$

In this expression all the detail of the band structure is contained within the effective mass, m^* . The effective mass plays a pivotal role in defining the bands and many other aspects of the physical

3.2 Monte Carlo Fundamentals

theory. As such there are several definitions of this term depending on the application. For a detailed review of the definitions see [71].

The basic model for the energy bands, given by equation (3.9), is sufficient to gain rough estimates on the transport of electrons in a material. In this work a slightly more advanced energy dispersion relation is employed by incorporating the non-parabolic band model. The non-parabolic band model improves the agreement with experiment for the energy bands at higher carrier energies [30]. Nonparabolicity is introduced by using an advanced energy dispersion relation given as

$$E(1 + \alpha E) = \gamma(\mathbf{k}) \quad (3.10)$$

$$\gamma(\mathbf{k}) = \frac{\hbar^2 \mathbf{k}^2}{2m^*} \quad (3.11)$$

where α is the nonparabolicity parameter and $\gamma(\mathbf{k})$ is essentially the quadratic expression, equation (3.11). The nonparabolicity parameter is often used as a fitting parameter for the transport data but it can be defined from band parameters with an expression for conduction bands given by equation (3.12) [74].

$$\alpha = \frac{1}{E_G} \left(1 - \frac{m^*}{m_0} \right)^2 \quad (3.12)$$

In this work an experimentally obtained value for the nonparabolicity parameter is used where $\alpha = 0.5 \text{ eV}^{-1}$ [30, 71, 79]. Obtaining the positive root of equation (3.10) (only the positive root is considered as negative energies are not physical), the energy dispersion relation can be written

$$E(\mathbf{k}) = \frac{-1 \pm \sqrt{1 + 4\alpha\gamma(\mathbf{k})}}{2\alpha} \quad (3.13)$$

Plotting the parabolic (equation (3.9)) and non-parabolic (equation (3.13)) energy dispersion functions in Figure 3.1, plot (a) demonstrates the differences between the models.

3.2 Monte Carlo Fundamentals

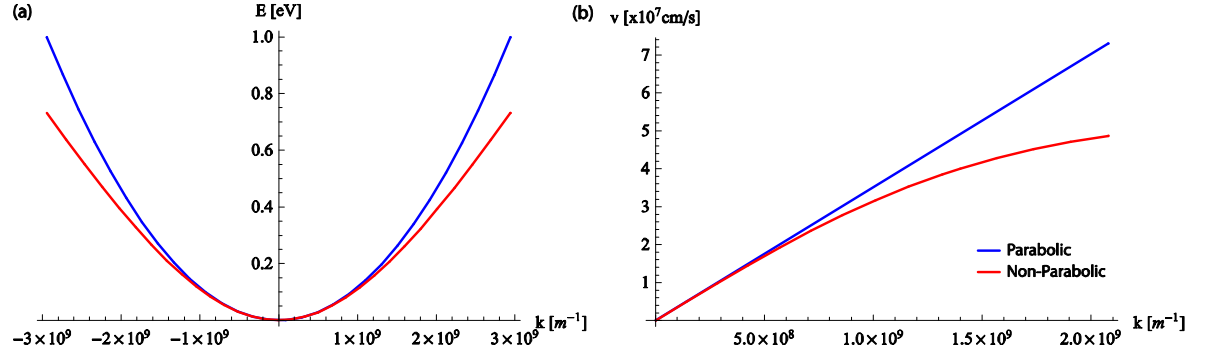


Figure 3.1: (a) Energy dispersion relations and (b) group velocity for parabolic and non-parabolic band structures.

As shown in plot (a) of Figure 3.1 the non-parabolic model increases the spread of energies at higher k states. This corresponds with an increase in the Density of States (DOS) which for non-parabolic bands is given by equation (3.14).

$$\rho(E) = \frac{3(2m^*)^{3/2}}{\pi^2 \hbar^3} E^{1/2} (1 + \frac{5}{2} \alpha E) \quad (3.14)$$

The DOS for the parabolic model (obtained from equation (3.14) by allowing $\alpha = 0$) and the non-parabolic model is shown plotted against a full numerical description of the band structure in Figure 3.2.

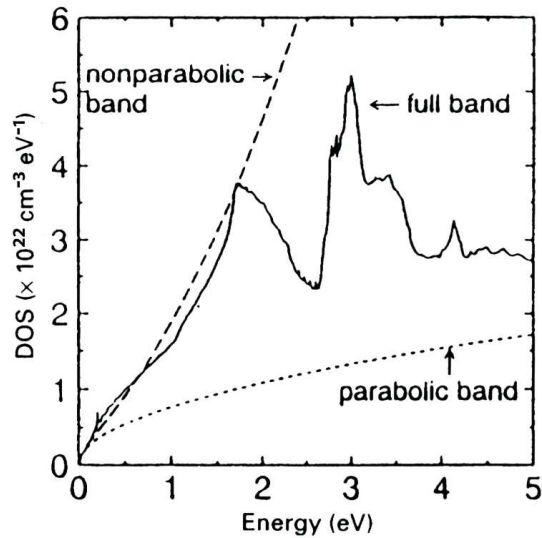


Figure 3.2: Comparison of parabolic and non-parabolic density of states models with a full numerical description. Reprinted with permission from T. Kunikiyo *et al*, J. Appl. Phys. 75, 297 (1994). Copyright 1994, American Institute of Physics [80].

3.2 Monte Carlo Fundamentals

It is clear from this figure that the DOS using the parabolic model is valid only for very low carrier energies. Whereas the non-parabolic model is much closer to the complete description of the band structure to roughly 1.5eV. Nonparabolicity also has the effect of reducing the carrier velocity for a given state $\mathbf{k}$. The group velocity for a state $\mathbf{k}$ for non-parabolic bands can be found from the energy dispersion relation, equation (3.13), as

$$v(\mathbf{k}) = \frac{1}{\hbar} \frac{\partial E}{\partial \mathbf{k}} = \frac{\hbar \mathbf{k}}{m^* (1 + 2\alpha E)} \quad (3.15)$$

Plotting the non-parabolic group velocity in part (b) Figure 3.1 highlights the drop in velocity at higher $\mathbf{k}$ states.

3.2.3 Herring-Vogt Transformation

In the equations discussed so far within this chapter the energy bands are assumed to have an isotropic effective mass such that the equi-energy surfaces are spherical. The energy bands for silicon that are under consideration in this work, the X-valleys, actually have ellipsoidal equi-energy surfaces, that is an anisotropic effective mass. For ellipsoidal bands the energy dispersion relation, neglecting nonparabolicity, can be written [32]

$$E(\mathbf{k}) = \frac{\hbar^2}{2} \left(\frac{k_x^2}{m_t^*} + \frac{k_y^2}{m_t^*} + \frac{k_z^2}{m_l^*} \right) \quad (3.16)$$

This representation of the energy dispersion relation makes analytical calculations such as those for the scattering mechanisms extremely challenging. To reduce the complexity of analytical calculations the Herring-Vogt transformation can be applied which reduces the ellipsoidal equi-energy surfaces to spherical surfaces. The Herring-Vogt transformation makes use of a starred-space which represents the ellipsoidal wave-vector transformed into the representative spherical system. The transformation is defined by

$$k_i^* = T_{ij} k_j \quad (3.17)$$

where $\mathbf{k}^*$ is the transformed wave-vector and the transformation matrix $\mathbf{T}$, in the valley frame of reference, is of the form

$$\mathbf{T} = \begin{bmatrix} \left(\frac{m_0}{m_i}\right)^{1/2} & 0 & 0 \\ 0 & \left(\frac{m_0}{m_i}\right)^{1/2} & 0 \\ 0 & 0 & \left(\frac{m_0}{m_i}\right)^{1/2} \end{bmatrix} \quad (3.18)$$

Finally, for non-parabolic bands the energy dispersion relation can then be written as

$$\gamma(\mathbf{k}) = \frac{\hbar^2 \mathbf{k}^{*2}}{2m_0} \quad (3.19)$$

with the corresponding non-parabolic group velocity as

$$v_i = \frac{\hbar}{m_0 (1 + 2\alpha E)} T_{ij} k_j^* \quad (3.20)$$

3.2.4 Fermi's Golden Rule

Scattering plays an important role in carrier transport as it defines the carrier interaction with the lattice, impurity ions and defects in the material. As discussed previously, carrier scattering in the definition of the BTE is a quantum mechanical concept. The collision operator of the BTE, expanded in equation (3.7), includes the quantum mechanical scattering probability transition rate, $P(\mathbf{k}, \mathbf{k}')$. The transition rate describes the probability per unit time of a carrier scattering from a state $\mathbf{k}$ to a state $\mathbf{k}'$. The probability transition rate is calculated using Fermi's Golden Rule, given by equation (3.21). For a complete discussion on the derivation of the Golden Rule see the textbooks [30, 32, 71].

$$P(\mathbf{k}, \mathbf{k}') = \frac{2\pi}{\hbar} |\mathbf{H}_{\mathbf{k}\mathbf{k}'}|^2 \delta(E(\mathbf{k}') - E(\mathbf{k}) \pm \hbar\omega) \quad (3.21)$$

Fermi's Golden Rule is the basic result of scattering theory which is used to describe carrier scattering in semiconductors. In the notation in this chapter, the upper and lower signs are for absorption and emission respectively. The Dirac-delta function $\delta(\cdot)$ ensures that energy is conserved during the scattering interaction by only allowing non-zero interaction probabilities for arguments that are zero.

3.2 Monte Carlo Fundamentals

The scattering matrix element, $\mathbf{H}_{\mathbf{k}\mathbf{k}}$, must be defined from the scattering potential and defines the particular scattering event. Once a scattering potential has been identified the scattering matrix element can be calculated as

$$\mathbf{H}_{\mathbf{k}\mathbf{k}} = \int_{\mathbf{r}} \exp(-i\mathbf{k}' \cdot \mathbf{r}) U_s(\mathbf{r}) \exp(i\mathbf{k} \cdot \mathbf{r}) d^3\mathbf{r} \quad (3.22)$$

where $U_s(\mathbf{r}) = eV(\mathbf{r})$ is the scattering potential energy. Here the overlap integral has been assumed to ≈ 1 which is an accurate approximation for non-parabolic conduction bands in silicon [79, 81].

In MC solutions of the BTE the carrier scattering is typically defined as a scattering rate, $\Gamma(\mathbf{k})$, that describes the number of scattering events per unit time of a carrier at an energy $E(\mathbf{k})$. The scattering rate can be calculated by integrating the probability transition rate over all final states $\mathbf{k}'$ described by equation (3.23).

$$\Gamma(\mathbf{k}) = N_k \int_{\mathbf{k}'} P(\mathbf{k}, \mathbf{k}') d^3\mathbf{k}' \quad (3.23)$$

Here $N_k = \Omega / (2\pi)^3$ is related to the number of electron states within the volume Ω .

It is important to note that Fermi's Golden Rule is valid when the duration of a collision is much smaller than the free time between collisions. This condition allows the effect of uncertainty in the carrier energy due to collisions to become significantly small that the carrier energy can be well defined.

3.2.5 Self-Scattering

An important development in the numerical solutions of the BTE and in particular MC simulations is the introduction of self-scattering. Self-scattering is a simplification of the free-flight time choice by introduction of a fictitious scattering event which greatly reduces the computational complexity of the choice of free-flight times for carriers.

The probability per unit time, $P(\tau)$, of a carrier travelling for a time τ and then being scattered is given by [32]

$$P(\tau) = \Gamma_T(\mathbf{k}(t)) \exp \left[- \int_0^\tau \Gamma_T(\mathbf{k}(t')) dt' \right] \quad (3.24)$$

where $\Gamma_T(\mathbf{k}) = \sum_i \Gamma_i(\mathbf{k})$ is the total scattering rate given by the sum of i scattering mechanisms, $\mathbf{k}(t) = \mathbf{k}_0 + e\mathbf{F}t/\hbar$ is the carrier wave vector at a given time t , $\mathbf{k}_0$ is the carrier wave-vector at the beginning of the free flight, $t = 0$.

To obtain the free-flight time from equation (3.24) requires that τ be evaluated for a given $P(\tau)/\Gamma_T(\mathbf{k})$ using random numbers distributed between 0 and 1. This is a complicated expression which requires numerical integration as the integral over all the scattering rates within the exponential cannot be solved analytically. A simple solution was proposed by Rees [82, 83] through introduction of a scattering rate that does not alter the carrier $\mathbf{k}$ state, aptly titled self-scattering. The simplification is achieved by introducing $\Gamma_0(\mathbf{k}(t))$, the self scattering mechanism into the total scattering rate such that

$$\Gamma_T^{\text{sc}}(\mathbf{k}(t)) = \sum_i \Gamma_i(\mathbf{k}(t)) + \Gamma_0(\mathbf{k}(t)) = \Gamma_T(\mathbf{k}(t)) + \Gamma_0(\mathbf{k}(t)) \quad (3.25)$$

Substituting this into the probability per unit time of free flight, equation (3.24) yields

$$P(\tau) = \{\Gamma_T(\mathbf{k}(t)) + \Gamma_0(\mathbf{k}(t))\} \exp \left[- \int_0^\tau \{\Gamma_T(\mathbf{k}(t')) + \Gamma_0(\mathbf{k}(t'))\} dt' \right] \quad (3.26)$$

This expression can be greatly simplified by allowing the value of $\Gamma_0(\mathbf{k}(t))$ to be carefully chosen to remove the energy dependent scattering rate term and introduce a constant value. This is represented as

$$\Gamma_0(\mathbf{k}(t)) = \Gamma - \Gamma_T(\mathbf{k}(t)) \quad (3.27)$$

where Γ is a constant value representing the self-scattering rate such that $\Gamma_0 \geq 0$ for all $\mathbf{k}$ states of interest (this value is selected at the start of simulation). Then the free flight probability becomes

$$P(\tau) = \Gamma \exp(-\Gamma \tau) \quad (3.28)$$

3.3 Carrier Scattering Mechanisms

which can be solved for the free-flight time τ through use of a random number r by rearranging the equation to give

$$\tau = -\frac{1}{\Gamma} \ln(1-r) \quad (3.29)$$

Although this method introduces more scattering events increasing the computational time, it is more than compensated by reducing the complexity of calculating the free-flight duration. The number of self-scattering events that occur in a simulation can be minimised by selecting the self-scattering rate, Γ , to be the largest value of the total scattering rate for the $\mathbf{k}$ states considered.

3.3 Carrier Scattering Mechanisms

3.3.1 Acoustic Phonons

Acoustic phonon scattering is the mechanism which describes the interaction of the carriers with the crystal lattice producing a relatively low frequency oscillation of the neighbouring atoms in the lattice. Modelling the exact change in the periodic crystal potential of the oscillating atoms is very challenging and a simplified approach making use of a deformation potential, D_{ac} , is typically employed [32].

The acoustic phonon scattering model used within this MC simulator is based on the inelastic approach given in Jacoboni's MC textbook [71] with a modification to the acoustic phonon dispersion relation taken from a journal paper by Pop [84]. The final scattering rate suitable for non-parabolic, ellipsoidal bands can be written as

$$\Gamma_{ac} = \frac{D_{ac}^2 m_d}{4\pi\rho\hbar^2 k^*} \int_{q_{min}^*}^{q_{max}^*} d\mathbf{q}^* \frac{\mathbf{q}^{*3}}{\omega_q(\mathbf{q}^*)} \left(N_q(\omega_q(\mathbf{q}^*)) + \frac{1}{2} \mp \frac{1}{2} \right) \frac{d\gamma}{dE} \quad (3.30)$$

where $m_d = (m_l m_t^2)^{1/3}$ is the density of states mass, ρ is the silicon density, k^* is magnitude of the carrier wave-vector in starred space, $\hbar\omega_q$ is the acoustic phonon energy and N_q is the phonon occupation number given by equation (3.31). Noting that the upper sign is for absorption of an acoustic phonon, the lower for phonon emission which is the convention used throughout this section. All silicon material and band parameters for this scattering rate are specified in Table 2 at the end of the chapter.

3.3 Carrier Scattering Mechanisms

$$N_q(\omega_q) = \frac{1}{\exp\left(\frac{\hbar\omega_q}{k_B T}\right) - 1} \quad (3.31)$$

To evaluate the scattering rate given by equation (3.30) the integral must be completed hence requiring that $\mathbf{q}_{\min}^*$ and $\mathbf{q}_{\max}^*$ be found. These bounds on the integral can be found from energy conservation using equation (3.32) [84].

$$\cos\theta = \mp \frac{\mathbf{q}^*}{2\mathbf{k}^*} + \frac{m_d\omega_q(\mathbf{q}^*)}{\hbar\mathbf{q}^*\mathbf{k}^*} \left(1 + \alpha(2E \pm \hbar\omega_q(\mathbf{q}^*))\right) \quad (3.32)$$

Here the RHS can be equated to a function $f(\mathbf{q}^*)$ and using the definition that $-1 \leq \cos\theta \leq 1$ allows the values of $\mathbf{q}_{\min}^*$ and $\mathbf{q}_{\max}^*$ to be defined as $f(\mathbf{q}_{\min}^*) = 1$ and $f(\mathbf{q}_{\max}^*) = -1$. Here and in the scattering rate the phonon frequency, ω_q , as a function of the momentum transfer, $\mathbf{q}^*$, is determined from equation (3.33)

$$\omega_q(\mathbf{q}^*) = \langle u \rangle |\mathbf{q}^*| + c |\mathbf{q}^*|^2 \quad (3.33)$$

where $\langle u \rangle = \frac{1}{3}(2u_t + u_l)$ is the average velocity and $c = -2 \times 10^{-3} \text{ cm}^2/\text{s}$ is a coefficient for the dispersion relation given by [84].

3.3.2 Optical Phonons

Optical phonon scattering also uses a deformation potential scattering methodology to simplify the description of the oscillating atoms in the crystal lattice. Optical phonons describe crystal oscillations at a much higher frequency than those of acoustic phonons and correspondingly have a much larger phonon energy.

In the MC simulator there are two distinct mechanisms for optical phonon scattering. The first to be considered here is intervalley scattering between equivalent valleys given by equation (3.34) [71].

$$\Gamma_{op} = \theta(E_f) \frac{m_d^{3/2} (D_t K)^2}{2^{1/2} \pi \rho \hbar^3 \omega_{op}} \left(N_q(\omega_{op}) + \frac{1}{2} \mp \frac{1}{2} \right) \gamma^{1/2} (1 + 2\alpha E_f) \quad (3.34)$$

3.3 Carrier Scattering Mechanisms

Here the upper signs are for absorption and the lower signs for emission of an optical phonon, $E_f = E \pm \hbar\omega_{op}$ is the final carrier energy with $\hbar\omega_{op}$ the optical phonon energy, $D_t K$ is the optical coupling constant, $\gamma = E_f (1 + \alpha E_f)$ is the non-parabolic carrier energy term and N_q is the phonon occupation number given by equation (3.31). Again all material and scattering constants used within the MC simulator are presented in Table 2.

The second optical phonon scattering mechanism is that of the f- and g-type phonons, which is also an intervalley scattering mechanism and is given by equation (3.35) [71]. The g-type phonons describe scattering between equivalent valleys and the f-type phonons describe scattering between non-equivalent valleys.

$$\Gamma_{op,i} = \theta(E_f) \frac{m_d^{3/2} (D_t K_i)^2}{2^{1/2} \pi \rho \hbar^3 \omega_{op,i}} Z_f \left(N_q(\omega_{op,i}) + \frac{1}{2} \mp \frac{1}{2} \right) \gamma^{1/2} (1 + 2\alpha E_f) \quad (3.35)$$

In this scattering rate the terms with a subscript index i relate to the particular f- or g-type phonon index, details of which are given in Table 2. The number of final valleys available for a particular phonon mode is given by Z_f and all other symbols are the same as defined previously.

3.3.3 Ionized Impurities

Ionized impurity (II) scattering is an elastic process and uses the screened Coulomb potential as the scattering potential. The screened Coulomb potential can be found from a solution of Poisson's equation for a point charge in a charge neutral region of a semiconductor (this method is presented in detail in [32] and discussed in section 2.3). The electrostatic screening introduced by the background charge is represented in the model employed here by the degenerate Debye-Hückel screening model for non-parabolic bands. This screening model is expressed as

$$k_C = \sqrt{\frac{e^2 n}{\epsilon_{Si} \epsilon_0 k_B T} \frac{(\mathfrak{F}_{-1/2}(\eta) + \frac{15}{4} \alpha k_B T \mathfrak{F}_{1/2}(\eta))}{(\mathfrak{F}_{1/2}(\eta) + \frac{5}{2} \alpha k_B T \mathfrak{F}_{3/2}(\eta))}} \text{ for } \eta = \frac{E_F}{k_B T} \quad (3.36)$$

where e is the electronic charge, n the electron density, $\mathfrak{F}_j$ is the Fermi integral of order j [54] and E_F the Fermi energy used in the reduced Fermi level η .

The II scattering model utilised in this MC simulator is Ridley's Third-Body Exclusion (TBE) model [51, 55, 60] in conjunction with an empirical fitting parameter which is calibrated such that

3.3 Carrier Scattering Mechanisms

the bulk mobility is matched to experimental data. The TBE model, along with other important II scattering models are discussed in detail in Chapter 2 of this thesis and further discussion on the model is not repeated here. It should be highlighted that in this work a new model for II scattering is developed in Chapter 5 which is a more accurate approach than the TBE model discussed here which has been traditionally been used in this MC simulator.

To compute the TBE model it is important to be able to express the Brooks-Herring (BH) II scattering rate which is given by equation (3.37). This is the standard BH expression for non-parabolic ellipsoidal bands.

$$\Gamma_{BH} = \left(\frac{Ze^2}{4\pi\epsilon_{Si}\epsilon_0} \right)^2 N_I \frac{2^{5/2}\pi}{m_d^{1/2}E_{k_c}^2} \frac{\gamma^{1/2}}{1 + 4\gamma/E_{k_c}} \frac{d\gamma}{dE} \quad (3.37)$$

Here N_I is the impurity density and $E_{k_c} = \hbar^2 k_c^2 / 2m^*$ is the screening length represented as an energy. From Van de Roer [60] the TBE scattering model can be expressed as

$$\Gamma_R = \frac{v(\mathbf{k})}{a} \left[1 - \exp \left(- \frac{a}{v(\mathbf{k})} \Gamma_{BH} \right) \right] \quad (3.38)$$

where $v(\mathbf{k})$ is the group velocity, given by equation (3.15), for the magnitude of the carrier wave-vector $k = \sqrt{2m_d^* \gamma} / \hbar$, $a = (2\pi N_I)^{-1/3}$ is half the average inter-ion separation distance and Γ_{BH} is given by equation (3.37).

Finally the II scattering rate used in the MC simulation can be obtained by multiplying the TBE rate by the empirical correction factor, K_n , to obtain the complete scattering rate as $\Gamma_{II} = \Gamma_R \times K_n(N_I)$ [85]. Values used for the fitting parameter are given in Table 1 which are tabulated and then interpolated for a given impurity density N_I . The empirical correction factor, K_n , is a fitting parameter which is calibrated such that the II scattering model is fitted to experimental bulk mobility data. This parameter highlights the difference between the physical model and experimental data over a wide range of impurity densities.

Table 1: Values used in empirical correction to II scattering

$\log_{10} N_I$	14	15	16	17	18	19	20	21	22
K_n	1	1	1.4	2.3	3.1	3.7	2.5	1.4	1.4

3.3.4 Interface Roughness

An important scattering mechanism for simulation of MOS devices is Interface Roughness (IR) scattering. This mechanism describes the perturbation in the potential due to roughness at the interface of the silicon substrate with the oxide insulator layer. This mechanism is only evident when (for a nMOS device) there is an inversion layer present in the device confining carriers close to the interface.

IR scattering is dependent on the electric field perpendicular to the interface, the vertical electric field, which controls the inversion charge and the corresponding confinement of carriers at the interface. As the electric field within the inversion layer varies with position, an average is introduced to simplify the scattering model. The average electric field in the inversion layer is expressed as the effective vertical field [30, 58], E_{eff} , written as [27]

$$E_{eff} = \frac{e}{\epsilon_{Si}\epsilon_0} \left(N_{depl} + \frac{n_s}{2} \right) \quad (3.39)$$

where N_{depl} is the depletion charge density and n_s is the inversion carrier density.

In order to describe the interface fluctuations a statistical function is introduced. The IR scattering model uses an exponential autocorrelation function to describe the rough interface as discussed in a paper by Goodnick [86]. The form of this autocorrelation function is

$$\langle \Delta(\mathbf{r}) \Delta(\mathbf{r} - \mathbf{r}') \rangle = \Delta_{rms}^2 \exp(-\sqrt{2} |\mathbf{r}| / L_e) \quad (3.40)$$

where $\mathbf{r}$ represents a position in the 2D plane parallel to the interface, Δ_{rms} is the RMS amplitude of the fluctuations in the interface and L_e is their correlation length.

Making use of the Ando model [86, 87] to define the scattering rate, the completed model can be found as

$$\Gamma_{IR}(\mathbf{k}) = \frac{e^2 m_d^*}{\hbar^3} (E_{eff}^2 \Delta_{rms}^2 L_e^2) \int_0^{2\pi} d\phi \frac{1}{(1 + \frac{1}{2} L_e^2 \mathbf{q}^2)^{3/2}} \quad (3.41)$$

3.4 Monte Carlo Process

where $\mathbf{q}^2 = 2\mathbf{k}^2(1 - \cos\varphi)$ is the momentum transfer of the scattering event. For all future device simulations the RMS amplitude of fluctuation is taken as $\Delta_{rms} = 0.35nm$ with a correlation length of $L_e = 1.3nm$.

It should be noted that at each scattering event the local effective vertical electric field is used in place of the definition given by equation (3.39). The scattering event with the local effective field is compared to the scattering rate with the definition using equation (3.39). Using a rejection technique, which is discussed in the appendix of [75], the scattering event will be allowed if the ratio is greater than a randomly selected number. This approach is similar to one discussed in a journal paper by Formicone [88].

3.4 Monte Carlo Process

3.4.1 Single Particle Monte Carlo

The single particle MC approach is the original approach to the modelling of carrier transport first developed in the 1960's. This approach is suitable for modelling transport of a semiconductor material under fixed electric fields and can be used to obtain such quantities as the drift velocity, mean carrier energy and the bulk mobility of the material.

The single particle method is an approximation of the complete system which consists of an ensemble of carriers which mutually interact. Allowing this system to be described as a system of independent carriers acting as an ensemble leads to the single particle simulation description. By simulating a single particle accelerating in an electric field and undergoing many scattering events, an approximate description of an ensemble of carriers can be found.

A typical breakdown of the single particle simulation process is given in part (a) of Figure 3.3. The program follows a simple procedure of stochastically selecting a free-flight time according to the self-scattering procedure discussed in section 3.2.5 where the particle is subject to acceleration by the electric field. Following this the particle scattering event which ends the free-flight is stochastically selected and the carrier is scattered. This procedure repeats until the simulation time, t_{sim} , has been completed.

An important stage in this process is the gathering of carrier data which of course provides the drift velocities, mean energy and other quantities of interest. This is completed at the end of each

3.4 Monte Carlo Process

iteration of the procedure and is generally completed as an average of the quantity of interest over the entire simulation period which can be written as [32, 71]

$$\langle A \rangle_T = \frac{1}{T} \sum_{\tau} \langle A \rangle_{\tau} \tau \quad (3.42)$$

where $\langle A \rangle_{\tau}$ is the quantity average over the free-flight period τ , T is total simulation time and $\langle A \rangle_T$ is the average quantity over the entire simulation period. Use of this method requires that T be long enough to ensure that the average quantity obtained can be considered an unbiased estimator, that is the results can be considered in a steady-state and independent of the initial conditions.

This approach has been used successfully to simulate many different materials and is discussed in more detail in [32, 74, 75]. It has an advantage in the simplicity of the procedure but is limited by the fact that it often requires very large simulation times to obtain stable results. This approach is not widely used in current times due to the increase in computational power which allows more advanced procedures to be implemented. Although the single particle MC is not the approach used in the simulator employed in this work, it is an important evolutionary stage of the MC procedure and explains the original background to the approach.

3.4 Monte Carlo Process

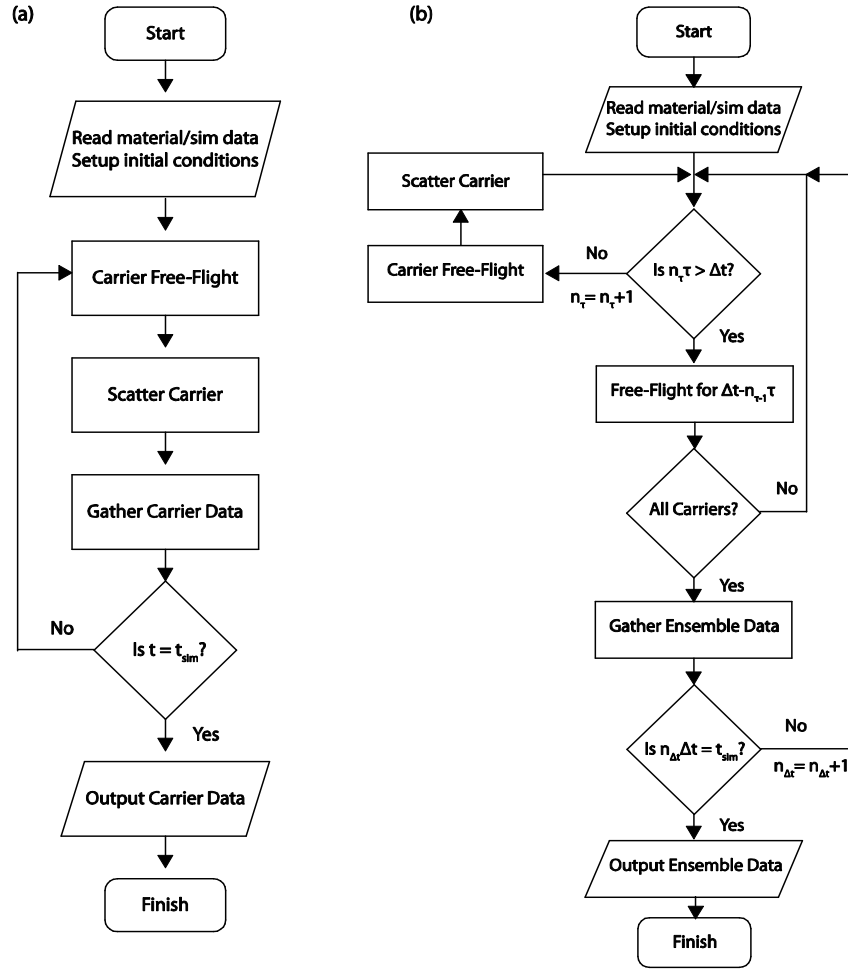


Figure 3.3: Flowchart of (a) the single particle and (b) ensemble Monte Carlo simulators.

3.4.2 Ensemble Monte Carlo

The Ensemble Monte Carlo (EMC) process is essentially an extension to the single particle approach by introduction of an ensemble of particles to the simulation. This allows the transient characteristics of carrier transport in semiconductors such as velocity overshoot to be simulated. The ensemble approach is necessary when simulating an inhomogeneous or non-stationary process although it can be used to solve stationary problems by allowing the simulation to continue until steady state.

The EMC approach is that used to simulate the properties of bulk semiconductors within this work. In particular the EMC approach is used to calibrate the simulator which is discussed in more detail in section 3.5. The program flow is described by part (b) of Figure 3.3 where the differences between this approach and the single-particle method become clear. Obviously the free-flight and scattering process is repeated for the entire ensemble of particles at each timestep.

3.4 Monte Carlo Process

A timestep, Δt , is no longer defined as a single free flight, τ , terminated by a scattering event and is instead defined externally as a fixed time period. Within a timestep each particle will have as many free flights terminated by scattering events as is required to fill the timestep (specified as n_τ free flights in the figure). In the final n_τ free-flight, for the case that $n_\tau \tau > \Delta t$, the carrier is only propagated for the time remaining in the current timestep and not for the full free-flight. This ensures that all carriers are propagated for the full timestep, Δt , only.

Similar to the single particle approach, the ensemble particle data is collected at the end of each timestep but a different procedure for obtaining results is required. An average for the quantity required is obtained at the end of each timestep from the average of the ensemble of particles [32, 71], which can be written as

$$\langle A(t) \rangle_N = \frac{1}{N} \sum_n A_n(t) \quad (3.43)$$

Here A_n is the quantity of particle number n at a time t , N is the total number of particles and $\langle A(t) \rangle_N$ is the quantity average over all particles at the given time. The time average of the quantity can be used to reduce the statistical error in ensemble simulations.

The number of particles in the ensemble is typically specified at the start of the simulation and is related to physical number of carriers in the device through the superparticle approach. Using the number of charges in the device, N , the superparticle charge can be found using [30]

$$Q = -e \frac{N}{N_{sim}} \quad (3.44)$$

where N_{sim} is the number of particles in the simulation. The superparticles are only considered in terms of the charge density and for all other calculations such as scattering the superparticles are treated as single carriers.

3.4.3 Device Monte Carlo

Simulation of semiconductor devices such as MOSFETs requires a more advanced technique for EMC simulation which allows for non-stationary transport through inhomogeneous materials. The Device Ensemble Monte Carlo (DEMC) approach is possible through extension of the EMC procedure by inclusion of a self-consistent solution of the electrostatic potential. A flowchart of the

3.4 Monte Carlo Process

general procedure of the DEMC approach is given in Figure 3.4 showing the extension to the EMC approach. In this figure the EMC procedure is essentially that of Figure 3.3 (b) without the feedback loop over all the timesteps which is re-specified in Figure 3.4.

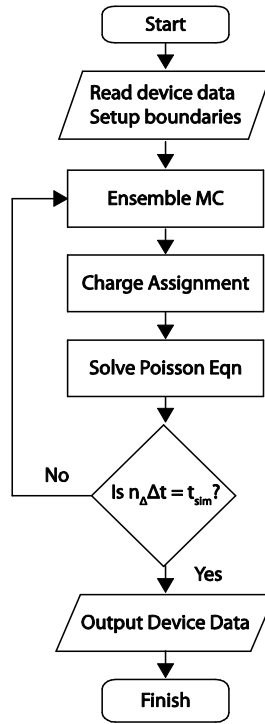


Figure 3.4: Flowchart for a device-ensemble Monte Carlo technique.

An important stage in the DEMC procedure is the specification of the boundaries as particles in a device are bounded. These boundaries must also be consistent with the solution for the electrostatic potential, which will be discussed later. Bulk material simulation such as those of the single-particle and EMC approaches use a boundless simulation (one that assumes an infinite material) but for a device a particle must be appropriately treated when reaching a surface. Typically there are two boundary conditions, one for a particle reaching an outer boundary for which the particle velocity normal to the surface is reflected. This boundary condition relates to the Neumann boundary condition for the electrostatic potential, that is a zero electric field component normal to the boundary surface.

The second boundary is for a particle reaching a contact where it is allowed to be absorbed. Of course as particles leave the device through a contact, particles must be injected to ensure that charge neutrality is kept within the contacts. The corresponding boundary condition for the electrostatic potential is the Dirichlet boundary which states that the boundary potential be set at the applied bias potential for the contact.

3.4 Monte Carlo Process

During the simulation, particles follow the EMC procedure of free-flight followed by a scattering event until the ensemble has completed the timestep. This movement of the particles causes the charge density to evolve with the simulation and will in turn cause the electrostatic potential to change. Before solution of the electrostatic potential can be completed the updated position of the particles and hence the charge density must be updated.

The DEMC simulator uses a Particle-Mesh (PM) method to resolve the particle charges to a mesh and define the forces for each particle. A full discussion on the PM technique can be found in the textbook by Hockney and Eastwood [89], here only a very brief discussion on the charge assignment mechanism will be undertaken. The particle charges are assigned to the mesh using a Cloud-In-Cell (CIC) technique originally developed for plasma simulations [90]. The CIC approach allows each particle charge to be assigned to the two nearest neighbour nodes which aids the smoothing of the forces and reduces the amplitude of fluctuations [71].

The electrostatic potential is found by solving Poisson's equation which relates the spatially varying charge density to the potential and is given by equation (3.6). There is extensive documentation in textbooks such as [32, 71, 89] regarding the solution of this equation in a PM system which is not repeated here. With the PM method the charge density is known at each mesh point thereby allowing the Poisson equation to be discretized over the mesh and solved using a finite difference approximation. Once the potential is found for each mesh point it is possible to define the electric fields and the corresponding forces for each particle.

When utilising a self-consistent PM approach the timestep, Δt , and the mesh spacing, Δx , must be considered to ensure that the DEMC simulation is stable. The timestep stability criterion is related to the plasma frequency for the highest carrier density, n , specified within the device model. The timestep criterion is given as [91, 92]

$$\Delta t \leq \frac{2v_c}{\omega_p^2} \quad (3.45)$$

where v_c is the momentum relaxation rate and the plasma frequency, ω_p , can be written

$$\omega_p = \sqrt{\frac{e^2 n}{\epsilon_{si} \epsilon_0 m^*}} \quad (3.46)$$

3.4 Monte Carlo Process

Taking a typical MOSFET device the peak carrier density can be estimated at $n \approx 5 \times 10^{19} \text{ cm}^{-3}$ giving the plasma frequency as $\omega_p \approx 2 \times 10^{14} \text{ s}^{-1}$. Estimating a typical momentum relaxation rate of $v_C \approx 2 \times 10^{15} \text{ s}^{-1}$ [33], this yields a stable time step of $\Delta t \leq 1 \times 10^{-13} \text{ s}$.

The mesh spacing criterion for resolution of the electrostatic potential is related to the expected charge variations within the simulation. The wavelength of the charge variations is typically approximated by the degenerate Debye length given by equation (3.36) which for $n = 5 \times 10^{19} \text{ cm}^{-3}$ gives a length of $\lambda_D = 0.8 \text{ nm}$. Hence for stable simulation the mesh spacing is generally taken such that $\Delta x < 2\lambda_D$ [93], hence a mesh spacing of $\Delta x = 0.5 \text{ nm}..1 \text{ nm}$ is suitable.

Although these stability criteria seem well specified there is a certain amount of freedom in the choice for the timestep and mesh spacing. A thorough study has recently been conducted by Palestri [91, 93] with the results given by Figure 3.5.

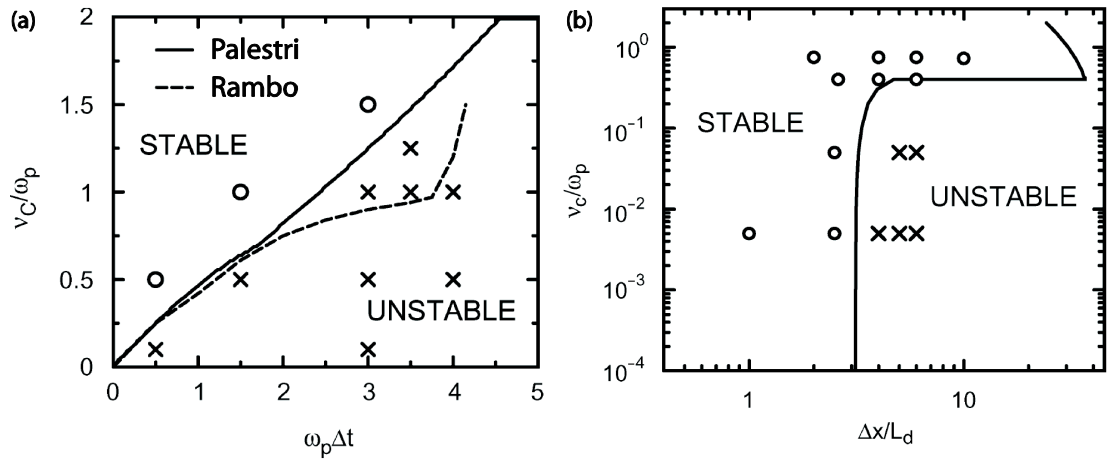


Figure 3.5: (a) Timestep stability plot (from Palestri [91]) and (b) mesh spacing stability (from Palestri [93]). Open symbols denote stable Monte Carlo simulations and crosses unstable simulations. (Both figures © 2006 IEEE)

This figure demonstrates that a large scattering rate, v_C , helps to stabilise the simulation by damping energy oscillations [93]. For the simulation data considered here, $v_C/\omega_p \approx 10$ which certainly allows for a greater range of timesteps and mesh spacing for stable MC simulation.

As a final stability criterion it is important to ensure that the timestep and mesh spacing are a correctly chosen pair. That is, within the chosen timestep the particles will not travel through several mesh spaces leading to greater charge oscillations and an increased instability. This can be checked by calculating the distance a particle will travel during the chosen timestep, which can be estimated by the maximum group velocity of a carrier in the semiconductor ($v_{sat} \approx 1 \times 10^7 \text{ cm/s}$).

Therefore, for this example a reasonable timestep of $\Delta t = 1 \times 10^{-14} \text{ s}$ can be chosen, then the maximum expected distance a particle can travel is $l_{\max} = v_{\text{sat}} \Delta t \approx 1 \text{ nm}$ which corresponds with the mesh spacing criterion. It should be noted that this timestep is suitable for bulk silicon simulations but for device simulations a timestep several orders of magnitude smaller is generally selected.

3.5 Monte Carlo Calibration

3.5.1 Bulk Silicon

Before using any MC simulator it is necessary to ensure that it has been calibrated against experimental data. For simulations of carrier transport in bulk silicon this requires calibration of the phonon scattering models and in the case of the II scattering model used here, the empirical correction factor discussed in section 3.3.3. The phonon scattering models are calibrated through adjustment of the corresponding deformation potential and phonon energy where there are several published sets of such data [30, 75, 94] which can be used. These parameters are chosen from the published data to match experimental energy- and velocity-field data for undoped silicon. Undoped silicon is used to remove the dependence of II scattering on the results.

To further simplify the phonon calibration process, many of the optical phonon mechanisms can be essentially frozen out by simulating the bulk silicon at a lattice temperature of 77K. This temperature is too low for most of the optical phonons which due to their high phonon energy, become statistically unimportant. Simulation at a lattice temperature of 300K then allows the full optical phonon model parameters to be calibrated. All calibrated parameters for the phonon models are given in Table 2 at the end of the chapter. In Figure 3.6, plots (a) and (b) are the results of the velocity-field and energy-field calibration respectively. Experimental data is taken from Canali [94] for an undoped sample of silicon at the temperatures of 77K and 300K.

3.5 Monte Carlo Calibration

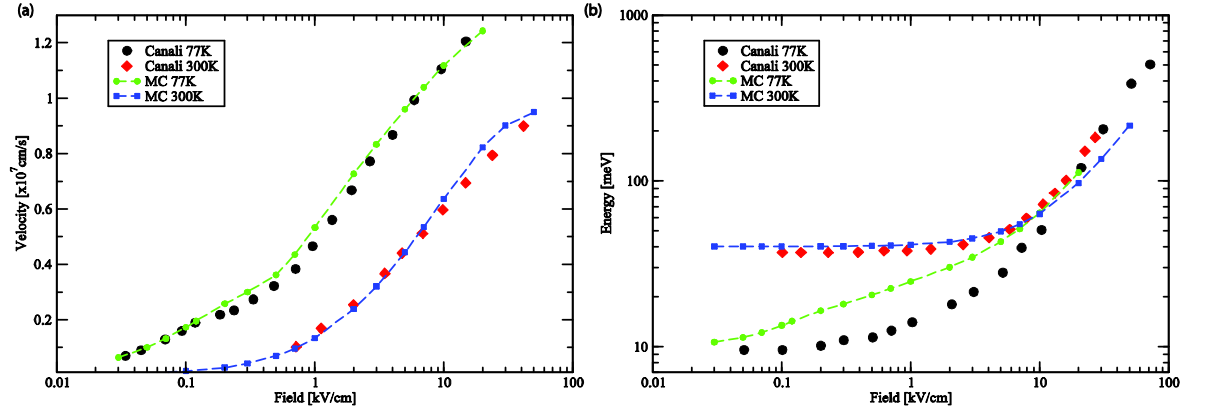


Figure 3.6: (a) Velocity-field and (b) energy-field calibration of Monte Carlo.

The velocity-field plot shows a good calibration with experimental data for both the low and high lattice temperatures over the range of applied fields. The energy-field figure also shows a close trend with experimental data. At 77K the low-field energy is higher than experimental data which, as reported in [31], is a cause of using an analytical band structure representation. As all future simulations in this work are completed for a lattice temperature of 300K, the calibration of the phonon models is considered a close match to experimental data at the simulation temperature.

The II scattering model used in this work utilises an empirical correction factor which improves the calibration of the II model with experimental data. To calibrate the correction factor the bulk silicon mobility is matched with experimental data over a wide range of dopant densities. Here the experimental data is taken from Thurber [29] and the values used for the II scattering empirical correction factor are given in Table 1. The result of the calibration is shown in plot (a) of Figure 3.7 and is clearly a close match with experimental data as is expected with the empirical II correction. It is also worthwhile to note that at impurity concentrations lower than $N_I = 10^{15} \text{ cm}^{-3}$ where II scattering is ineffective and phonon scattering dominates, that there is good agreement with experimental data.

3.5 Monte Carlo Calibration

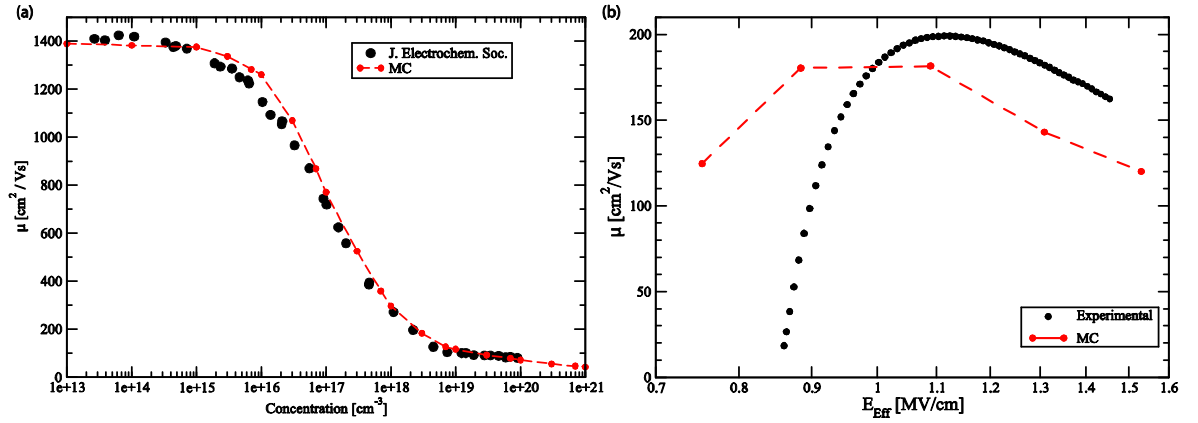


Figure 3.7: (a) Bulk mobility and (b) universal mobility calibration of Monte Carlo.

3.5.2 Inversion Layer

To accurately simulate MOSFET devices it is important to ensure that the MC simulator is calibrated to experimental data for carrier transport in the inversion layer. This process is required to calibrate the IR scattering model with experimental data as phonon and II scattering models should remain unchanged from the bulk silicon calibration.

Inversion layer calibration is completed by matching the universal mobility of carriers in an inversion layer with experimental universal mobility data. The experimental data is taken from Takagi [27, 28] for the substrate impurity concentration of $N_t = 2 \times 10^{18} \text{ cm}^{-3}$ and a applied lateral field of $E = 0.5 \text{ kV/cm}$.

The universal mobility trend is well replicated by the MC simulation as shown in plot (b) of Figure 3.7, with the correct drop in mobility at low effective field due to II scattering. At high effective fields the IR scattering model reduces the mobility and reproduces the universal curve [27] expected from the mobility.

The calibration of the simulator with the experimental data shown in plot (b) of Figure 3.7 is considered to be suitable despite the discrepancy between simulated and experimental data at low effective fields. This is based on the simulators ability to reproduce the overall trend of the universal mobility curve, specifically at high fields where interface roughness scattering dominates. At low effective fields the universal mobility is dominated by II scattering which in the current state-of-the-art simulators is modelled by a bulk 3D approach and is not an accurate solution to the II scattering problem in the inversion layer.

3.6 Conclusion

In this chapter the MC simulation procedure has been discussed in terms of the fundamentals of the simulation approach, the scattering mechanism involved, the procedure utilised in the numerical procedure through to the calibration of the MC code used in this work.

The discussion on the fundamentals of the MC procedure included the all-important BTE which is the core problem which the numerical procedure solves. The BTE can be described as a bookkeeping function for the distribution function which describes the state of the carrier ensemble in a device and through which all important quantities of interest can be calculated. Also discussed in the fundamentals section was the description of the silicon band structure used in the simulator. An analytical description of the band structure is utilised with the non-parabolic approximation. Ellipsoidal bands are also employed with the Herring-Vogt transformation which simplifies the description by transferring to and from a *starred* space.

Scattering in the BTE and the MC simulation procedure is typically completed using Fermi's Golden Rule approach which is discussed in section 3.2.4. The scattering in MC simulations is a quantum mechanical process which uses the interaction potential of a scattering event to obtain a probabilistic scattering rate.

Finally in the fundamentals section, the self-scattering procedure was discussed which greatly simplifies the way in which particle free-flights are selected by introducing a fictitious scattering event. This advancement in numerical simulation greatly advanced numerical MC simulations by vastly reducing the complexity of free-flight calculations.

The scattering mechanisms that are required for accurate simulation of silicon MOSFET devices are presented in section 3.3. These include the intravalley acoustic phonon, the intervalley optical phonons, II scattering and IR scattering. These scattering mechanisms are the minimum required to obtain accurate simulation data for bulk silicon and silicon MOSFET devices.

The evolution of the numerical procedure used within MC simulations was discussed in section 3.4 from the original 1960's single particle approach through to the state-of-the-art self-consistent DEMC approach. In the single particle model the simulation can only be used to obtain stationary homogeneous processes. The EMC approach allows transient, inhomogeneous systems to be modelled by simulating large numbers of particles and is the modern approach to simulating bulk semiconductor characteristics. For MOSFET simulation the required inclusion of a self-consistent Poisson solution leads to the DEMC approach.

3.6 Conclusion

The MC simulator calibration with experimental data is demonstrated in the final section. There the energy and velocity characteristics of carrier transport in silicon from the numerical MC simulation are shown to be in close match with experimental data. The carrier mobility for both the bulk and universal cases is also shown to be in good agreement with the experimental data.

Table 2: Silicon band parameters and constants.

Silicon Constants	$u_l = 5.34 \times 10^3 \text{ m/s}$	$\rho = 2.329 \text{ g/cm}^3$
	$u_t = 9.04 \times 10^3 \text{ m/s}$	$\epsilon_r = 11.7$
	$D_{ac} = 9 \text{ eV}$	$a_0 = 5.43 \text{ \AA}$
Band 1 (X-Valleys)	$m_l = 0.916 m_0$	$m_t = 0.190 m_0$
	$\alpha = 0.5 \text{ eV}^{-1}$	$E_G = 1.12 \text{ eV}$
Intervalley Optical equivalent X-valleys:	$D_t K = 1.75 \times 10^{10} \text{ eV/m}$	$\hbar \omega_{op} = 43 \text{ meV}$
	g-type:	$Z_f = 1$
		$(D_t K)_{g1} = 0.5 \times 10^{10} \text{ eV/m}$
		$(\hbar \omega_{op})_{g1} = 12.06 \text{ meV}$
		$(D_t K)_{g2} = 0.8 \times 10^{10} \text{ eV/m}$
		$(\hbar \omega_{op})_{g2} = 18.53 \text{ meV}$
		$(D_t K)_{g3} = 3 \times 10^{10} \text{ eV/m}$
		$(\hbar \omega_{op})_{g3} = 63 \text{ meV}$
	f-type:	$Z_f = 4$
		$(D_t K)_{f1} = 0.15 \times 10^{10} \text{ eV/m}$
		$(\hbar \omega_{op})_{f1} = 18.96 \text{ meV}$
		$(D_t K)_{f2} = 3.4 \times 10^{10} \text{ eV/m}$
		$(\hbar \omega_{op})_{f2} = 47.40 \text{ meV}$
		$(D_t K)_{f3} = 4 \times 10^{10} \text{ eV/m}$
		$(\hbar \omega_{op})_{f3} = 59.03 \text{ meV}$

Chapter 4 Scattering Potential Calculation

4.1 Introduction

Ionized impurity (II) scattering in modern MOSFET devices has a considerable effect on device performance. A great deal of research has been put into studying the electrostatic and transport effects of atomistic scattering [63, 67] yet little work has been done on the effect of impurity scattering close to interfaces. Here the intention is to formulate a scattering potential which describes the effect of a single atomistic impurity located next to highly-doped regions. The work will focus on looking at the effect of polarisation charges on channel IIs located close to highly doped source and/or drain regions of MOSFETs. The polarisation charges which are induced in the source and/or drain regions are shown here to remotely screen channel II ions.

Note that for the purpose of this work the typically named source-channel and channel-drain junctions shall be referred to as the source and drain interfaces respectively. This definition should not be confused with the typical device context definition of the interface between the silicon substrate and the silicon dioxide layer, which is not considered in this work.

This chapter presents and discusses scattering potentials which describe an atomistic impurity interacting with a single interface and also a double interface. The single interface case represents the II ion acting with the source, the double interface case represents the II interacting with the source and the drain. The structure of this chapter is split between the two potential models developed here, with section 4.2 presenting the single interface model and section 4.3 the double interface model. As the process of calculating and then verifying the models is identical in each case, the repetition in the content presented is carefully minimised.

The calculation of the single interface model in section 4.2 begins with the system definition before defining and solving the Poisson's equation for the potential in section 4.2.1. Much of the detail in calculation is avoided in this section with the full procedure given in Appendix A. Plots of the potential isolines for the single interface solution are shown in section 4.2.2 with a brief discussion. Validation of this solution is then completed in section 4.2.3 by checking the limits and ensuring that the behaviour is as expected of the model.

As the potential derived for the single interface model is an exact analytical solution of Poisson's equation it is important to validate the result with that of a fully self-consistent, non-linear

4.2 Single Interface Potential Model

Poisson's equation solution. This comparison is given in section 4.2.4 with a brief discussion of the method used to complete the comparison.

The solution found for the potential in the single interface model is very complex as it includes the detailed behaviour of a doped semiconductor source region. A simplified model has been calculated by taking a limit on the screening of the source, entitled the strong-screening limit and is presented in section 4.2.5. Although the use of the strong screening limit in this work simplifies the expressions involved, primarily it has been introduced to provide a worst-case scenario for this interaction. Utilising an upper limit on the interaction will allow an initial indication on the importance of remote screening effects of channel II ions on device performance.

This structure is repeated for the calculation and verification of the double interface model in section 4.3. The complete potential model is calculated in section 4.3.1 with the detailed procedure given in Appendix B. Validation of the model by means of the limits and comparison with the non-linear Poisson solver is given in sections 4.3.3 and 4.3.4 respectively. The strongly screened potential is obtained in section 4.3.5 for the double interface model.

4.2 Single Interface Potential Model

A self-consistent potential for a single impurity located close to the source –channel interface shall now be calculated by solving the Poisson equation over the source/channel region. The Linear Thomas-Fermi (LTF) approximation [95] is used to simplify this solution of the Poisson equation in conjunction with the Debye-Hückel screening model [53]. Due to the cylindrical symmetry of the system, cylindrical co-ordinates are used throughout the potential calculation [96]. Here the Z -axis is normal the source-channel interface with the $\mathbf{R}$ plane parallel to the interface.

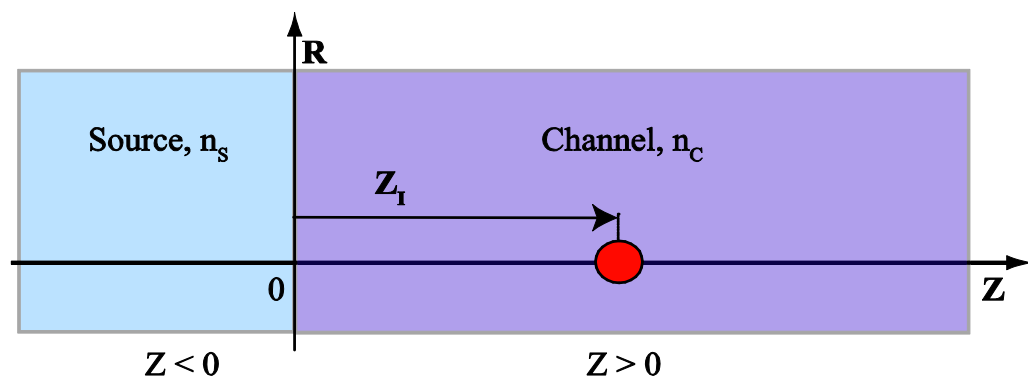


Figure 4.1: Physical picture of the problem system, defining source and channel regions with impurity located Z_I from interface.

4.2 Single Interface Potential Model

Figure 4.1 provides a pictorial representation of the physical system to be solved. Here the source and channel carrier densities are represented by n_s and n_c respectively. The source is assumed to have a larger carrier density in this figure, that is $n_s > n_c$ but this is not an assumption made in the calculation of the potential in section 4.2.1.

The impurity for which the potential is to be found is given by the red circle in the channel region for which $Z > 0$. In this case, the source interface is located at $Z = 0$ and the impurity is located at Z_I which must be in the channel region. To simplify the problem and incorporate radial symmetry around the Z axis, the impurity is assumed to be located at $\mathbf{R}_I = 0$.

4.2.1 Potential Solution

The solution for the electrostatic potential of this system can be found by solving the following Poisson equations for the free charge density.

$$\nabla^2 \phi_s = -\frac{\rho_s}{\epsilon_{si}\epsilon_0} \quad \text{for } Z < 0 \quad (4.1)$$

$$\nabla^2 \phi_c = -\frac{\rho_c}{\epsilon_{si}\epsilon_0} - \frac{Q}{2\pi\epsilon_{si}\epsilon_0} \frac{\delta(\mathbf{R})}{R} \delta(Z - Z_I) \quad \text{for } Z > 0 \quad (4.2)$$

Where ρ_s is the free charge density in the source region and ρ_c the free charge density in the channel region. On the right-hand side of equation (4.2) the atomistic impurity can be seen as a charge Q at position Z_I . For this model, the impurity is positioned at $\mathbf{R}_I = 0$ in the $\mathbf{R}$ plane. This simplifies the solution but retains the important Z dependence that controls the interaction with the source region.

The inverse bulk screening length, $k_x = \lambda_x^{-1}$, can be related to the free charge density with the LTF approximation by using the following relation

$$\rho_x = -\epsilon_{si}\epsilon_0 k_x^2 \phi_x \quad (4.3)$$

Here, the subscript X denotes either the source (S) or channel (C) region. This then gives the linearized Poisson equation, also known as a Helmholtz equation as

$$\nabla^2 \phi_s - k_s^2 \phi_s = 0 \quad \text{for } Z < 0 \quad (4.4)$$

4.2 Single Interface Potential Model

$$\nabla^2 \varphi_C - k_C^2 \varphi_C = -\frac{Q}{2\pi\epsilon_{si}\epsilon_0} \frac{\delta(\mathbf{R})}{R} \delta(Z - Z_I) \text{ for } Z > 0 \quad (4.5)$$

Solutions to equations (4.4)-(4.5) can be found by specifying boundary conditions on the potential, $\lim_{\mathbf{R}, Z \rightarrow \pm\infty} \varphi = 0$. Using a standardized solution of the Helmholtz equation using cylindrical coordinates in conjunction with the Bessel function [96], the electrostatic potential for the source and channel region can be found exactly as

$$\varphi_S = (1 - \theta(Z)) \int_0^\infty dk J_0(kR) A_S(k) \exp\left(Z\sqrt{k^2 + k_S^2}\right) \quad (4.6)$$

$$\begin{aligned} \varphi_C = \theta(Z) \int_0^\infty dk J_0(kR) \left\{ A_C(k) \exp\left(-Z\sqrt{k^2 + k_C^2}\right) \right. \\ \left. + \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \frac{k}{\sqrt{k^2 + k_C^2}} \exp\left(-|Z - Z_I|\sqrt{k^2 + k_C^2}\right) \right\} \end{aligned} \quad (4.7)$$

Here $\theta(Z)$ is the unit step function and J_0 is the zero order Bessel function of the first kind [97]. As we assume that $\mathbf{R}_I = 0$ giving symmetry around the Z axis, only the magnitude of $\mathbf{R}$ has any importance in these equations. This correctly allows the use of the magnitude of $\mathbf{R}$ in the Bessel function. It is important to note that the use of the variable k here shouldn't be confused with the typical notation for the carrier wave vector which has the identical symbol. In this case the variable is used to denote a separation constant used within the solution of the equation.

This leaves 2 coefficients, A_S and A_C , which need to be found to complete the solution for the potentials. This can be completed by using the static boundary continuity conditions on $\mathbf{E}$ and $\mathbf{D}$ for electric fields [26] such that

$$\mathbf{E}_{\parallel S} = \mathbf{E}_{\parallel C} \text{ or } \frac{\partial \varphi_S}{\partial \mathbf{R}} = \frac{\partial \varphi_C}{\partial \mathbf{R}} \quad (4.8)$$

$$\mathbf{D}_S = \mathbf{D}_C \text{ or } \epsilon_{si}\epsilon_0 \frac{\partial \varphi_S}{\partial Z} = \epsilon_{si}\epsilon_0 \frac{\partial \varphi_C}{\partial Z} \quad (4.9)$$

These define that the tangential electric field, $\mathbf{E}_{\parallel}$, must be the same along the interface and that the electric flux, $\mathbf{D}$, must be continuous across the interface. After solving the resulting simultaneous equations we find the solutions to the 2 unknown coefficients as

4.2 Single Interface Potential Model

$$A_s(k) = \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \frac{k}{\sqrt{k^2 + k_C^2} + \sqrt{k^2 + k_S^2}} \exp\left(-Z_I \sqrt{k^2 + k_C^2}\right) \quad (4.10)$$

$$A_C(k) = \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \frac{k}{\sqrt{k^2 + k_C^2}} \frac{\sqrt{k^2 + k_C^2} - \sqrt{k^2 + k_S^2}}{\sqrt{k^2 + k_C^2} + \sqrt{k^2 + k_S^2}} \exp\left(-Z_I \sqrt{k^2 + k_C^2}\right) \quad (4.11)$$

After some manipulation, the complete solutions for φ_s and φ_C can be written in the form

$$\begin{aligned} \varphi_s = (1 - \theta(Z)) & \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \int_0^\infty dk J_0(kR) \frac{2k}{\sqrt{k^2 + k_C^2} + \sqrt{k^2 + k_S^2}} \\ & \times \exp\left(Z \sqrt{k^2 + k_S^2}\right) \exp\left(-Z_I \sqrt{k^2 + k_C^2}\right) \end{aligned} \quad (4.12)$$

$$\begin{aligned} \varphi_C = \theta(Z) & \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \int_0^\infty dk J_0(kR) \frac{k}{\sqrt{k^2 + k_C^2}} \left\{ \exp\left(-|Z - Z_I| \sqrt{k^2 + k_C^2}\right) \right. \\ & \left. - \frac{\sqrt{k^2 + k_S^2} - \sqrt{k^2 + k_C^2}}{\sqrt{k^2 + k_S^2} + \sqrt{k^2 + k_C^2}} \exp\left(-(Z + Z_I) \sqrt{k^2 + k_C^2}\right) \right\} \end{aligned} \quad (4.13)$$

These potential equations define the self-consistent screened solution to an II located within the channel region which is coupled to the source, Figure 4.1. Here this calculation has been summarised to the major steps, for more detail of the procedure used to find these solutions see Appendix A.

Examining the solution to the channel potential of equation (4.13), we can see the additional term present from the polarisation charge effect. Looking at the two terms within the curly brackets of equation (4.13), the second term represents the potential from the polarisation charge. The sign of the impurity location, Z_I , is negative in this second term, representing the location of the fictitious polarisation (image) charge.

4.2.2 Contour Plots

Plotting the total potential given by equation (4.14) in some contour plots allows for examination of the effect of the interface on an atomistic impurity. Figure 4.2 shows contour plots of the total potential with an atomistic impurity located in four different locations in the channel region, $Z > 0$.

$$\varphi = \varphi_s + \varphi_C \quad (4.14)$$

4.2 Single Interface Potential Model

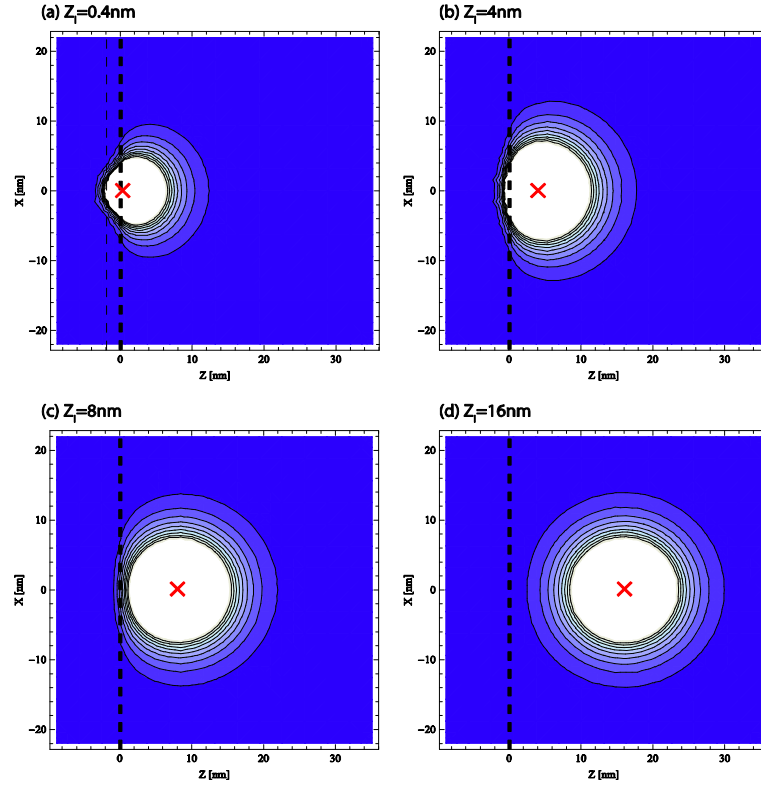


Figure 4.2: Contour plots of the potential for the single interface model. Plots (a)-(d) show four different impurity locations, Z_I , where the channel screening length, $\lambda_c = 4.133nm$, and the source screening length is $\lambda_s = 0.69nm$.

In Figure 4.2, the source region doping concentration is $N_I = 10^{20} cm^{-3}$ and the channel concentration is $N_I = 10^{18} cm^{-3}$ which yields screening lengths of $\lambda_s = 0.69nm$ and $\lambda_c = 4.133nm$ respectively. The screening lengths are calculated using the degenerate Debye-Hückel screening model, equation (3.36).

In plot (d) the impurity is located at $Z_I = 16nm$ from the source-channel interface and we see very little effect of the interface on the resulting potential isolines. This can be explained by the exponential roll-off of the polarisation charge effect with respect to the channel screening length and impurity position. At a position of $Z_I \approx 4\lambda_c$, the polarisation charge term is very small, e.g. $1 - \exp(-4) \approx 0.98$.

The case where the impurity is located far enough away from the interface so as to introduce no polarisation charge effects, $Z_I > 4\lambda_c$, will be termed the screened Coulomb limit. This is so called as the potential represents only the screened Coulomb component where the polarisation charge term tends to zero. This will be further demonstrated in section 4.2.3 where this limit and others will be analysed.

4.2 Single Interface Potential Model

At an impurity position of roughly two screening lengths from the interface, the potential contours in plot (c) show the increased screening effect induced from the interaction with the polarisation charge. This effect increases in plot (b) when the impurity is positioned roughly one screening length away. Notice the penetration of the impurity potential into the source region at this distance is minimal despite there being a strong interaction with the polarisation charge term. At $Z_I \approx 0.1\lambda_C$ from the source-channel interface, plotted in (a), the potential contours are highly distorted and the potential is being heavily screened by the polarisation charge. There is strong penetration of the impurity potential into the source region where, due to the much smaller screening length, the potential drops off much more rapidly.

4.2.3 Limits of Potential

It is important to confirm that the calculated potential is valid and yields the correct behaviour. This can be checked by testing the various limits of the equations (4.12)-(4.13) to ensure that the boundary conditions are properly held and that the expected result is obtained.

4.2.3.1 Screened Coulomb Limit

The first limit to check is to ensure that the model returns to the classic screened Coulomb potential when the impurity is located a large distance away from the source-channel interface, $Z_I k_C \gg 4$. Performing this limit on equations (4.12)-(4.13) gives

$$\lim_{Z_I k_C \gg 4} \varphi_S \approx (1 - \theta(Z)) \exp(-Z_I \sqrt{k^2 + k_C^2}) = 0 \quad (4.15)$$

$$\lim_{Z_I k_C \gg 4} \varphi_C = \theta(Z) \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} \int_0^\infty dk J_0(kR) \frac{k}{\sqrt{k^2 + k_C^2}} \exp(-|Z - Z_I| \sqrt{k^2 + k_C^2}) \quad (4.16)$$

The source potential term is dominated by the negative exponential which tends to zero in the limit $Z_I k_C \gg 4$. This is consistent with theory that if the impurity is a great distance from the source, there will be no interaction with polarisation charges in this region. Similarly the polarisation charge term within the channel potential, the second exponential on the RHS of equation (4.13), will tend to zero.

After use of the transformation theorem given by equation (4.17) [98] the channel potential can be given by equation (4.18). This form is identical to the screened Coulomb model with no boundary interactions such as polarisation effects.

4.2 Single Interface Potential Model

$$\int_0^{\infty} \frac{x}{\sqrt{x^2 + a^2}} J_0(xy) \exp\left(-b\sqrt{x^2 + a^2}\right) dx \equiv \frac{\exp\left(-a\sqrt{b^2 + y^2}\right)}{\sqrt{b^2 + y^2}} \quad (4.17)$$

$$\lim_{Z_I \gg 4k_C^{-1}} \varphi_C = \theta(Z) \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} \frac{\exp\left(-k_C\sqrt{\mathbf{R}^2 + (Z - Z_I)^2}\right)}{\sqrt{\mathbf{R}^2 + (Z - Z_I)^2}} \quad (4.18)$$

4.2.3.2 Matched Screening Limit

Ensuring that in the limit of matched screening in the source and channel regions, $k_s = k_C$, the polarisation charge terms disappear is the purpose of this check. This is the case if there is no boundary introduced via the screening in the source and channel region, then formation of polarisation charges is impossible.

$$\lim_{k_s = k_C} \varphi_S = (1 - \theta(Z)) \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} \int_0^{\infty} dk J_0(kR) \frac{k}{\sqrt{k^2 + k_C^2}} \exp\left((Z - Z_I)\sqrt{k^2 + k_C^2}\right) \quad (4.19)$$

$$\lim_{k_s = k_C} \varphi_C = \theta(Z) \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} \int_0^{\infty} dk J_0(kR) \frac{k}{\sqrt{k^2 + k_C^2}} \exp\left(-|Z - Z_I|\sqrt{k^2 + k_C^2}\right) \quad (4.20)$$

Completing the matched screening limit on the source and channel potential terms gives the equations (4.19) and (4.20). As expected the model returns to a screened Coulomb potential split over the source and drain regions. Again, if the impurity is located a large distance from the source region, the source potential will tend to zero as in the screened Coulomb limit discussed in the previous sub-section.

As the matched screening limit provides a solution of the screened Coulomb potential over the two regions, it is convenient to check the continuity of the solution at the interface. Taking the limit of $Z = 0$ on equations (4.19)-(4.20) and equating yields after some manipulation

$$\int_0^{\infty} dk \frac{J_0(kR)k}{\sqrt{k^2 + k_C^2}} \exp\left(-Z_I\sqrt{k^2 + k_C^2}\right) = \int_0^{\infty} dk \frac{J_0(kR)k}{\sqrt{k^2 + k_C^2}} \exp\left(-Z_I\sqrt{k^2 + k_C^2}\right) \quad (4.21)$$

$$\varphi_S(Z = 0) = \varphi_C(Z = 0)$$

Equation (4.21) clearly shows that the potentials match at the interface.

4.2.4 Comparison with Non-Linear Poisson Solution

As the newly-developed model for the potential of an impurity located close to a region of high-doping solves a linearized form of the Poisson equation, it is important to compare this with a numerical Poisson solver. This will allow for an accurate test of the quality of the solution obtained here. First the discrete impurity method will be discussed and demonstrated before the detailed comparison between the solution is completed.

4.2.4.1 Discrete Dopant Simulation

A fully self-consistent, Non-Linear Poisson (NLP) solution will be used to simulate an ideal device of a single atomistic impurity located close to an interface. The method used to solve for atomistic impurities with the Poisson equation is discussed in detail in the paper by Asenov [63]. The method involves including a single dopant via the mesh-resolved charge distribution by assigning the chosen mesh cell to contain the charge density e/h^3 where h is the mesh spacing. This mesh-resolved charge distribution is used within the Poisson solver to calculate the electrostatic potential for the system.

For this experiment a device has been constructed which closely represents the ideal system used to develop the single interface potential, Figure 4.1. This device takes the form of a highly doped n-region located adjacent to a p-doped region and is depicted in Figure 4.3.

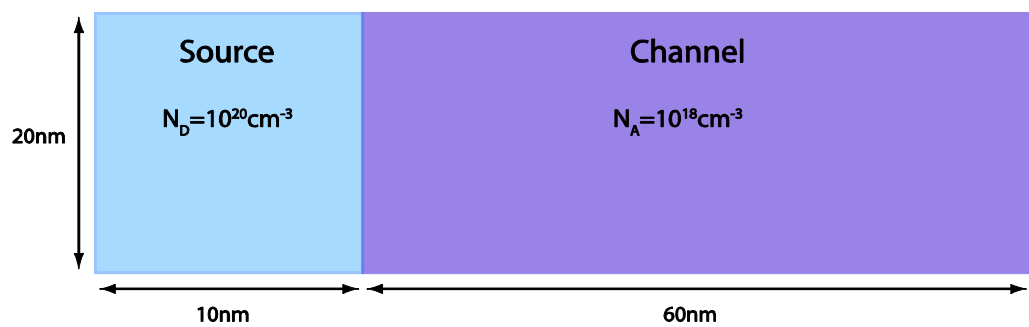


Figure 4.3: Figure demonstrating the doping profile of the Poisson test device for the single interface model. The doping transition from $N_D = 10^{20} \text{ cm}^{-3}$ to $N_A = 10^{18} \text{ cm}^{-3}$ is assumed to be abrupt.

The device has a 20nm square body and is 70nm long which is split into 10nm for the highly-doped source region and 60nm for the channel. Doping in the source region is given as $N_D = 10^{20} \text{ cm}^{-3}$ and the channel is doped at $N_A = 10^{18} \text{ cm}^{-3}$ with an abrupt doping transition between the regions.

4.2 Single Interface Potential Model

To improve the quality of this experiment a slight modification is made to the normal atomistic doping process. As the remote screening model developed here assumes a linear background charge density with a single atomistic impurity, a similar assumption is made when resolving the charge distribution for the Poisson solution. Hence, the inclusion of a single atomistic dopant is assumed not to alter the surrounding dopant concentration per unit volume of the simulated system.

Examining this assumption in more detail using equation (4.22) it is found that this assumption has little effect on the background doping. In the system described above the channel region has a volume of $V = 24 \times 10^{-18} \text{ cm}^3$ with a dopant density $N_I = 10^{18} \text{ cm}^{-3}$. Using the equation below, this leads to 24 dopant atoms in the channel volume. Adding one further dopant to the channel region roughly corresponds to a background doping concentration of $N_I = 1.042 \times 10^{18} \text{ cm}^{-3}$ which is less than a 5% shift in doping.

$$n_{ion} = V \times N_I \quad (4.22)$$

A mesh is applied to the structure with a node resolution of 0.25nm. This fine mesh is important to ensure that the atomistic impurity is accurately resolved within a discretized Poisson solution [99]. The channel length is chosen to be long enough to accommodate the source interface depletion width of $W_{dm} \approx 36.71 \text{ nm}$ calculated using the long-channel formula given in equation (4.23) [15].

$$W_{dm} = \sqrt{\frac{2\epsilon_{Si}\epsilon_0 \left(E_g/2 + k_B T \ln(N_A/n_i) \right)}{eN_A}} \quad (4.23)$$

The reference channel screening length is calculated using the Debye-Hückel screening model, equation (3.36), as $\lambda_c = 4.133 \text{ nm}$ where the carrier concentration is assumed to be fixed at the background dopant concentration, $n = N_A = 10^{18} \text{ cm}^{-3}$. This reference screening length is used only to provide a fixed length scale to measure the position of the impurity in the channel.

The potential solution for this device with a single atomistic impurity located at four different locations is shown in Figure 4.4. In part (a) of this figure, the atomistic impurity is placed at $Z_I = 52 \text{ nm}$ which is beyond the end of the depletion region. This is to ensure that the atomistic impurity will be minimally affected by the source interface. The potential isolines for this impurity are spherical close to the impurity and slowly disperse farther from the impurity centre.

4.2 Single Interface Potential Model

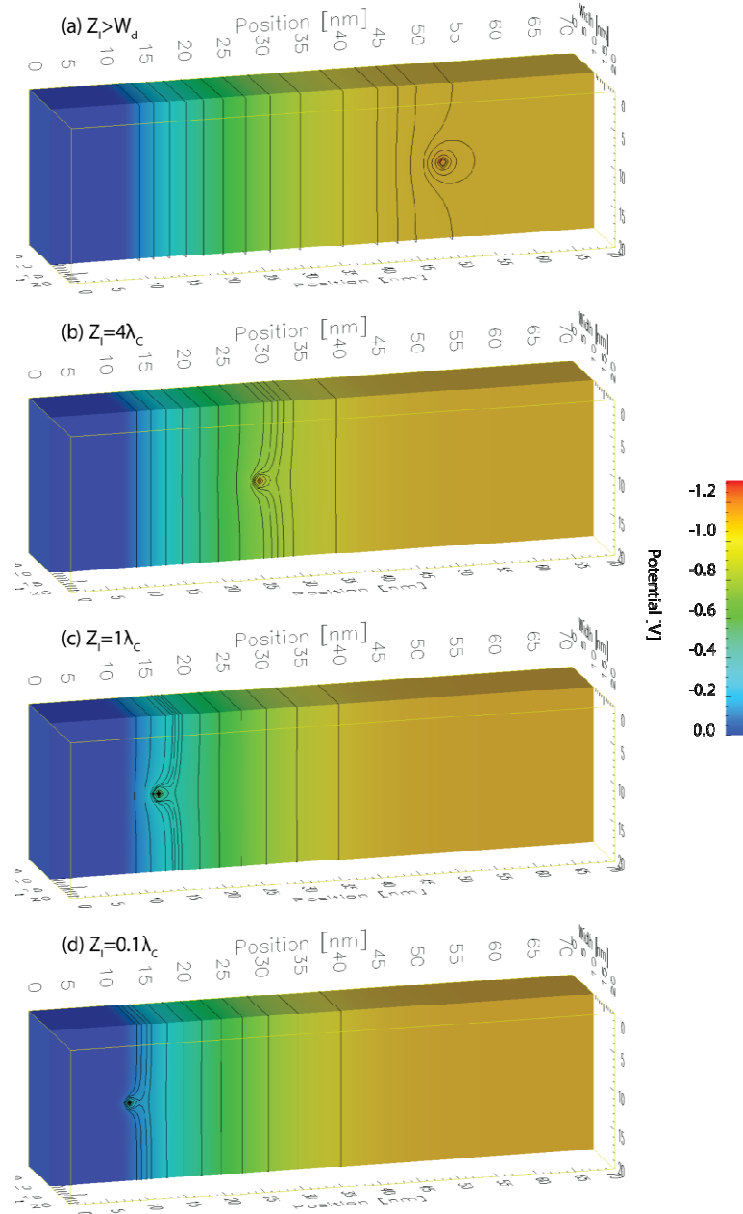


Figure 4.4: Plots of the potential iso-contours for an atomistic impurity in the ideal single interface structure. Plots (a)-(d) denote varying positions, Z_I , of the atomistic impurity given in relation to (a) the channel depletion width, or (b)-(d) the channel screening length.

In parts (b) and (c), the atomistic impurity is located around $4\lambda_c$ and $1\lambda_c$ from the source-channel interface. The potential contour lines change from being spherical to being teardrop shaped as the impurity is located closer to the interface. Clearly the vicinity of the interface is altering the screening of the atomistic impurity potential as is expected.

In part (d) of Figure 4.4, the impurity is located directly next to the interface at roughly $Z_I = 0.1\lambda_c$. At this distance the polarisation charge effect is very strong as the potential isolines demonstrate. The impurity is heavily screened and the impact of the impurity is felt over a cross-sectional area much smaller than the case where the interface plays little role such as in part (a) of this figure.

4.2 Single Interface Potential Model

These plots show a consistent result with the effect modelled by the single interface potential calculated earlier in this chapter, Figure 4.2.

4.2.4.2 Comparison with Analytical Model

To ensure that the calculated analytical potential is accurately modelling the impurity it is important to compare the results in more detail. This is possible by a comparison of the analytical model with the NLP solution from the previous section. In Figure 4.5, 1D slice plots of the potential obtained from the NLP solver are compared to the analytic solution calculated in section 4.2. As the analytical solution uses a linearized Poisson solution, the comparison in the models will differ as the full Poisson solution will include the depletion region of the p-n junction. This makes the comparison difficult but a simplifying solution has been utilised to compare the impurity potential solutions between the models.

Solving the model system described by Figure 4.3 with the NLP solver and with no atomistic impurities, a uniform device, provides a solution of the potential for the p-n junction. The potential and carrier density profiles for this uniform device solution can then be extracted giving a solution for the depletion region. Through the use of superposition the uniform device potential can be added to the analytical model to provide a solution comparable to the NLP solver. Likewise the uniform solution could have been subtracted from the NLP solver to compare the impurity potential alone, but the current method is perhaps closer to real simulation conditions.

4.2 Single Interface Potential Model

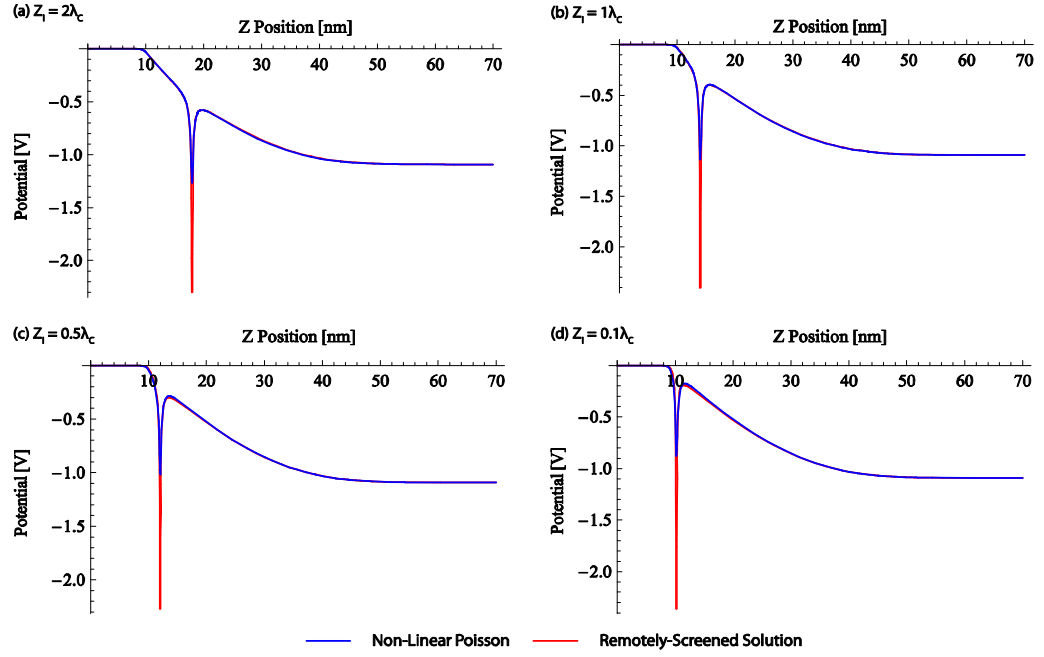


Figure 4.5: Comparison of the potential of a single atomistic impurity using a fully self-consistent, non-linear Poisson solution and the single interface, analytical solution obtained in section 4.2.

For all impurity positions in plots (a)-(d) of Figure 4.5, the analytical solution is found to be very close to the discretized NLP solution. The largest difference is in the resolution of the singular peak of a Coulomb point charge, the atomistic impurity centre, which is a known drawback of the discretized Poisson solution.

To be thorough in this comparison, a single impurity position from Figure 4.5 is chosen to complete a comparison in the axis parallel to the interface. This comparison is shown in Figure 4.6 for $Z_I = 2\lambda_c$ and again shows the close agreement between the models. Again there is a discrepancy in the singular peak of the point charge due to the discretization error induced from the numerical solution of the Poisson equation.

4.2 Single Interface Potential Model

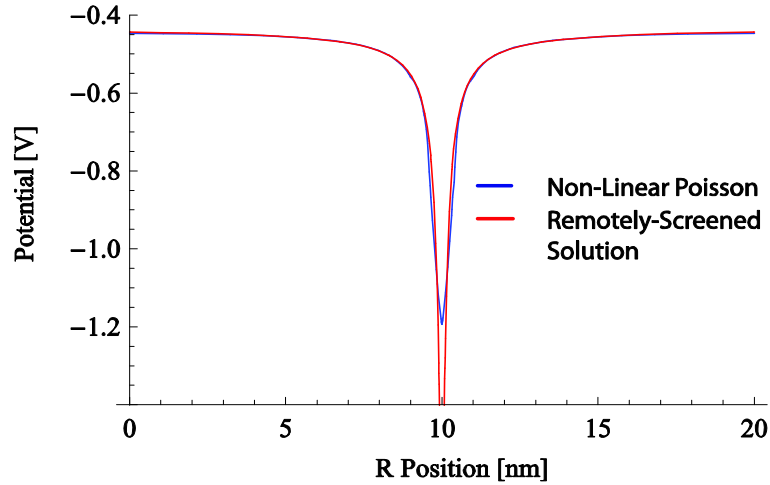


Figure 4.6: Comparison of the non-linear Poisson and analytical solutions of a single atomistic impurity located at $Z_I = 2\lambda_C$. Discrepancy between solutions of point charge due to numerical discretisation of Non-Linear Poisson solution at mesh spacing $\Delta x = 0.5nm$.

This comparison demonstrates that the calculated analytical model accurately provides a method to model the polarisation charge effect of an atomistic impurity located close to a region of higher doping.

4.2.5 Strong-Screening Limit

A set of equations has now been developed which model the potential of a single atomistic impurity located close to a reflecting interface. From the potential equation it is possible to develop a scattering mechanism which can be used in Monte Carlo simulation. The development of such a scattering mechanism and the application to Monte Carlo simulation will be the subject of the following chapters.

In their current form the potential solution for the single interface model, given by equation (4.14), is quite large and unwieldy. The calculation of a Monte Carlo appropriate scattering mechanism is a daunting procedure and is challenging to complete with the potential described above. A simplified form of the potential has been found which allows a straightforward calculation of the scattering mechanism, yet retains as much of the complete physical model as possible. This simplified model has been obtained here by using a limit which is appropriate to the model system that the potential solutions have been developed for.

This limit assumes that the source region is highly degenerately doped, becoming metallic-like, and the corresponding screening length becomes very much less than the channel screening length, $\lambda_s \ll \lambda_C$. This limit has been termed the strong-screening limit and is shown here to simplify the potential solution. Using the strongly screened limit constitutes a model which assumes the worst

4.2 Single Interface Potential Model

case scenario for this interaction in that the source region is a metal. This, as discussed below in section 4.2.5.2, leads to over estimation of the remote screening effect of the induced polarisation charges. For the purpose of this work, which is to study what effect polarisation charges have on modern device performance, this limit is considered viable. It is worthwhile mentioning that the strong-screening limit essentially reduces the problem to the classical image charge problem [100].

4.2.5.1 Strongly Screened Single Interface Model

The strong-screening limit for the single interface model greatly reduces the complexity whilst still retaining the important characteristics. Here it can be redefined as $k_s \gg k_c$ using the inverse screening length. Using the potential solutions from section 4.2, equations (4.12) and (4.13), and taking the limit yields

$$\begin{aligned} \lim_{k_s \gg k_c} \varphi_s &= (1 - \theta(Z)) \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \int_0^\infty dk J_0(kR) \frac{2k}{k_s} \exp(Z k_s) \exp(-Z_I \sqrt{k^2 + k_c^2}) \\ \lim_{k_s \gg k_c} \varphi_s &\simeq \frac{\exp(Z k_s)}{k_s} = 0 \quad \text{for } Z < 0 \end{aligned} \quad (4.24)$$

The source potential tends to zero as all of the impurity potential is screened out in a very small region on the source side of the interface. This is expected as the screening in the source becomes very strong.

The limit of the channel potential seems less effective but simplifies the coefficient of the polarisation charge term, the second term within the square brackets. Essentially, the strength of the polarisation charge term no longer depends on the ratio between the channel and source screening as the source is assumed to be an almost perfect reflecting surface.

$$\begin{aligned} \lim_{k_s \gg k_c} \varphi_c &= \theta(Z) \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \int_0^\infty dk J_0(kR) \frac{k}{\sqrt{k^2 + k_c^2}} \left[\exp(-|Z - Z_I| \sqrt{k^2 + k_c^2}) \right. \\ &\quad \left. - \frac{k_s}{k_s} \exp(-(Z + Z_I) \sqrt{k^2 + k_c^2}) \right] \\ \lim_{k_s \gg k_c} \varphi_c &= \theta(Z) \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \int_0^\infty dk J_0(kR) \frac{k}{\sqrt{k^2 + k_c^2}} \left[\exp(-|Z - Z_I| \sqrt{k^2 + k_c^2}) \right. \\ &\quad \left. - \exp(-(Z + Z_I) \sqrt{k^2 + k_c^2}) \right] \end{aligned} \quad (4.25)$$

The strong screening limit allows the form of equation (4.25) to be further simplified by using the theorem, given by equation (4.17), which removes the integral.

4.2 Single Interface Potential Model

$$\lim_{k_s \gg k_c} \varphi_C = \theta(Z) \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} \left[\frac{\exp\left(-k_c \sqrt{\mathbf{R}^2 + (Z - Z_I)^2}\right)}{\sqrt{\mathbf{R}^2 + (Z - Z_I)^2}} - \frac{\exp\left(-k_c \sqrt{\mathbf{R}^2 + (Z + Z_I)^2}\right)}{\sqrt{\mathbf{R}^2 + (Z + Z_I)^2}} \right] \quad (4.26)$$

This simplified form of the single interface potential consists of the recognisable screened Coulomb potential, the first term in the square bracket, minus the potential of the polarisation charge, the second term. The polarisation charge term can be distinguished by the change in the sign of the impurity position, Z_I . As the source potential has been screened to zero with the limit of strong-screening, the total potential becomes simply the channel potential. It is important to note that this potential is only valid for the channel region, that is for $Z > 0$.

4.2.5.2 Verification of Limit

Although the strong-screening limit provides a simpler model, it is necessary to check that the model still provides an accurate representation of the system. This can be easily shown by comparison of the potential for the complete model against that of the simplified strongly screened model. Such a comparison of the remotely screened impurity potentials is made in Figure 4.7.

For this comparison an ideal example device has been used which has a source region located at $Z < 0$ doped at $N_I = 10^{20} \text{ cm}^{-3}$ and a channel region, $Z > 0$, with doping at three concentrations, $N_I = \{10^{14}, 10^{16}, 10^{18}\} \text{ cm}^{-3}$. The screening length for these three channel densities has been calculated using the screening model given by equation (3.36) and corresponds to $\lambda_c = \{409, 41, 4.1\} \text{ nm}$ respectively. The source region is only considered in the complete model as the strongly screened model screens out the potential in this region. Hence for the figures in this section the source region is not plotted.

4.2 Single Interface Potential Model

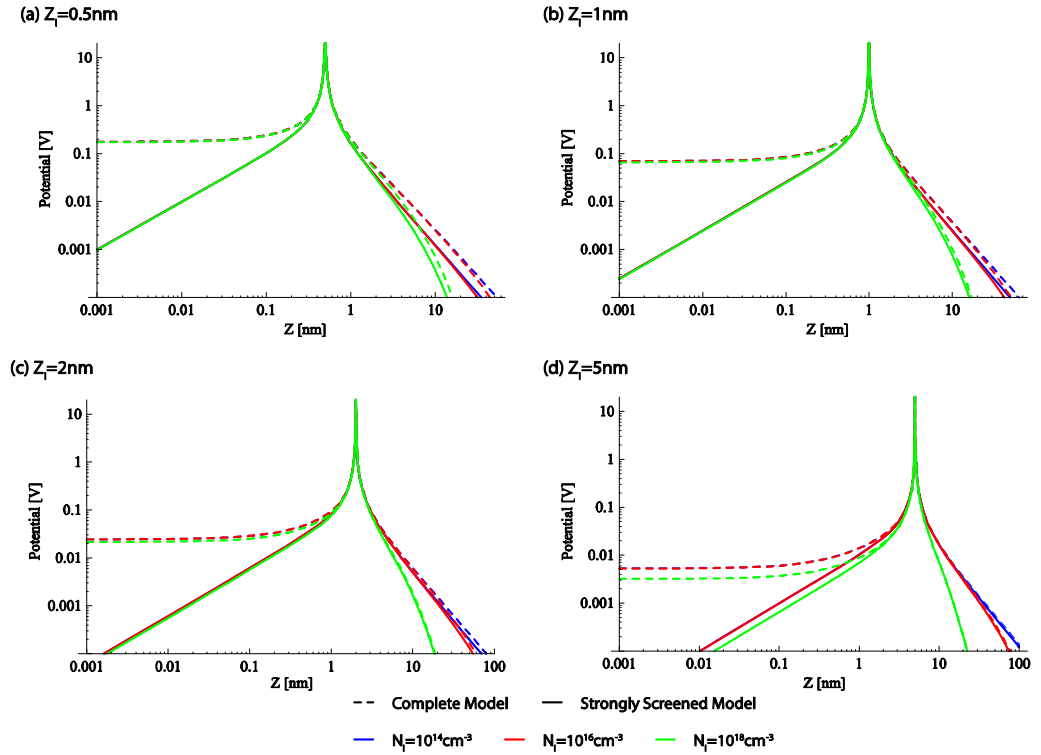


Figure 4.7: Comparison of the complete and strongly screened potentials for four impurity positions.

In Figure 4.7 are plots of the impurity potential at four different locations in the channel. In these plots the potential is given for both the complete and the strongly screened models over the three different channel impurity densities. In each plot of Figure 4.7 the strongly screened model shows an increased drop of the potential at the source interface. In plots (c) and (d) this drop in potential becomes appreciable at a distance roughly less than one nanometre from the source interface. When the impurity is located at one nanometre or less from the interface, as in plots (a) and (b), this drop in potential becomes quite large.

The increased screening of the potential at the source interface is expected from the strongly screened model as this limit forces the potential in the source region to zero. This acts as a strong boundary condition for the channel potential which ensures that the channel impurity charge is neutralised at the interface. The validity of this approach can be roughly analysed from the behaviour shown in Figure 4.7. As discussed above the limit induces a large shift for impurities very close to the interface. Examining the potential comparisons in more detail in the following figures will allow a better quantitative analysis.

4.2 Single Interface Potential Model

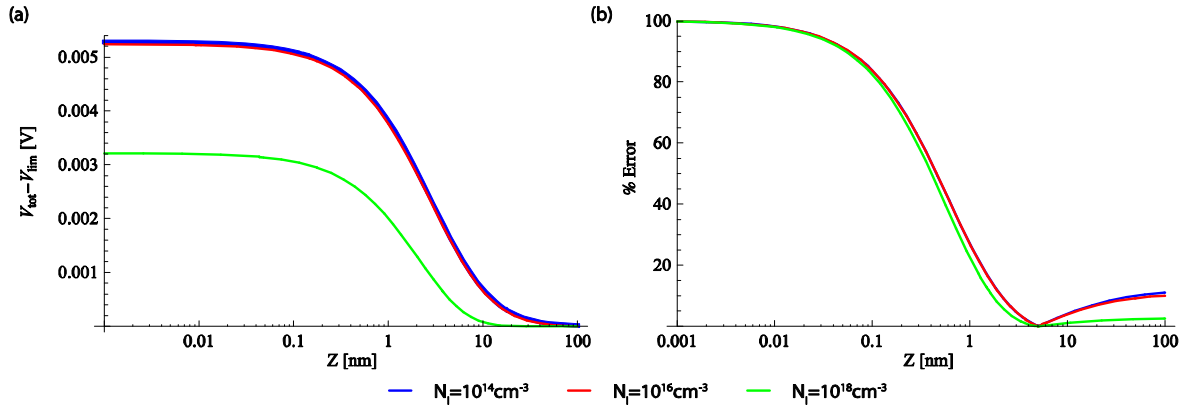


Figure 4.8: Detailed comparison of complete and strongly screened potential models for $Z_I = 5 \text{ nm}$.

At an impurity distance of $Z_I = 5 \text{ nm}$, as shown in Figure 4.8, the strong screening limit is adequate with a shift in impurity potential of around 5 mV at a tenth of a nanometre from the interface. Although this corresponds to a 100% error at the interface, the potential can be considered to be well screened at this distance and the strongly screened model is quite accurate. Beyond the impurity into the channel region, the limit yields an error of $\sim 5\text{-}10\%$ or less than a millivolt shift in potential.

Interestingly at this impurity position the channel impurity density has a noticeable effect on the quality of the strong screening limit. The higher the impurity density in the channel, and therefore the higher the screening density the closer the models are. This can be explained by the increased screening of the impurity potential in the channel minimising the interaction with the source as seen in Figure 4.7, plot (d).

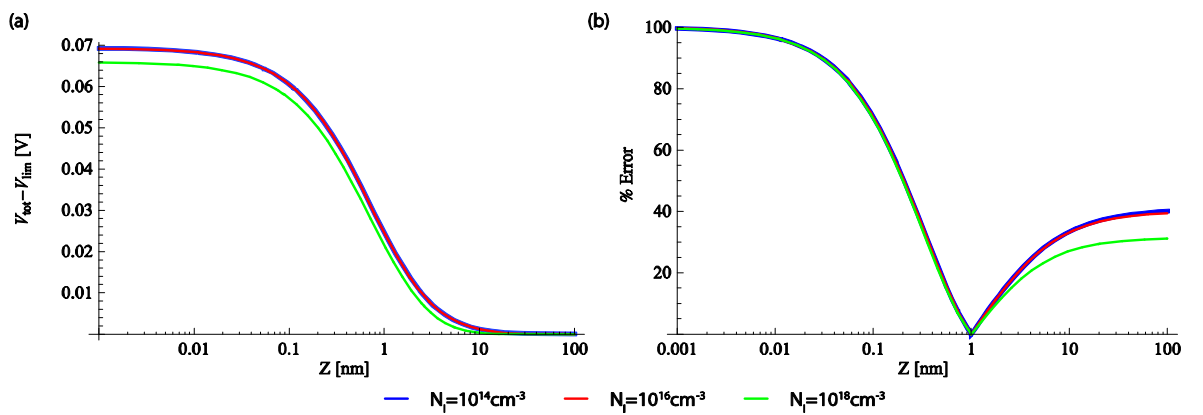


Figure 4.9: Detailed comparison of complete and strongly screened potential models for $Z_I = 1 \text{ nm}$.

4.2 Single Interface Potential Model

At the impurity position $Z_I = 1\text{nm}$, the detailed comparison plots of Figure 4.9 show a much larger shift in the potential, roughly 70mV at the interface. The percentage error plot of (b) highlights the problem of the strong screening limit at this distance from the source. Around this impurity position the error increases rapidly, but worryingly the error beyond the impurity into the channel bulk increases to 30-40%. At this distance the validity of this limit under these conditions is hard to justify given this increase in error.

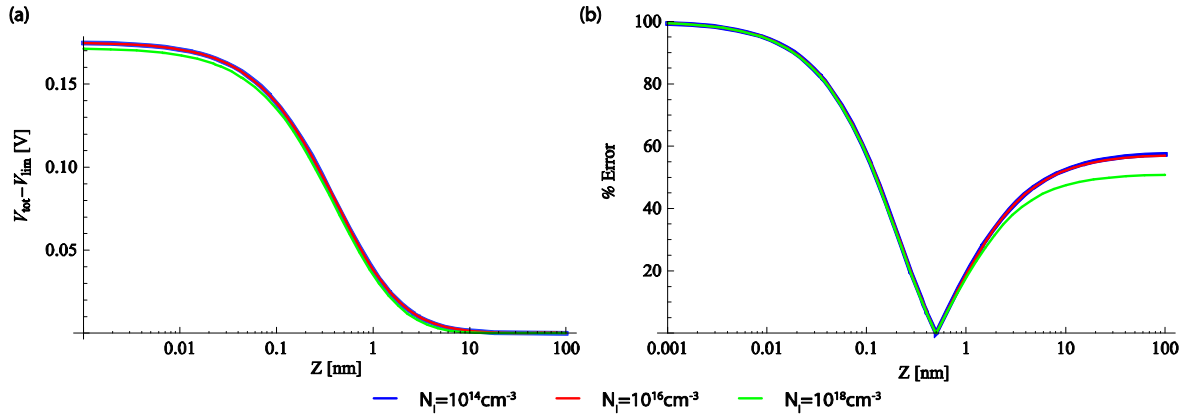


Figure 4.10: Detailed comparison of complete and strongly screened potential models for $Z_I = 0.5\text{nm}$.

Examining the effect of the limit at a closer impurity position in Figure 4.10 highlights the increasing error. The drop in the potential becomes very significant, rising to well over 150mV. The error induced in the bulk of the channel, beyond the impurity also show a drastic increase to almost 50%. At this impurity position, within 1nm of the interface, the strong screening limit for the source does not provide an accurate solution of the potential.

Looking at Figure 4.7 it is clear that the error in the approximation becomes appreciable within roughly a 1nm region from the source interface. For impurities located outwith this region, the error constitutes a small potential drop. From this analysis the limit has been shown to be close to the complete model over a range of channel impurity concentrations and impurity positions greater than 1nm of the interface. Modelling impurities within 1nm of the interface leads to an overestimation in the screening of the potential.

To further the verification of the strongly screened limit it is appropriate to compare the two models in a context of effect on device behaviour. It is difficult to estimate the effect that the strongly screened limit will have on carrier scattering from the comparisons on potential alone and therefore an analysis on ionized impurity limited mobility is ideal. A numerical calculation of the impurity scattering limited mobility using the momentum relaxation rates of the complete and strongly screened models is shown in Figure 4.11. Although the discussion and use of momentum

4.2 Single Interface Potential Model

relaxation rates in this chapter is a little out of sequence in the structure of this PhD thesis (see Chapter 5), it is necessary for the analysis of the mobility discussed here.

The electron mobility is calculated using the Kubo-Greenwood formula [33], equation (4.27), assuming a spherical, parabolic band structure. The momentum relaxation rate for the strongly-screened model is presented in Chapter 5 (assuming the non-parabolicity parameter $\alpha=0$) and Appendix C presents the momentum relaxation rate for the complete single interface model.

$$\mu = \frac{2e}{3m^*n} \int_0^\infty dE \rho(E) E \tau_m(E) \left(\frac{\partial f_0}{\partial E_F} \right) \quad (4.27)$$

Here e is the electronic charge, n is the electron density, $\rho(E)$ is the density of states, f_0 is the equilibrium Fermi function and E_F is the Fermi energy. The electron density and the density of states can be written for parabolic bands as

$$n = 2 \left(\frac{m^* k_B T}{2\pi \hbar^2} \right)^{3/2} \mathfrak{F}_{1/2}(\eta) \quad \text{for } \eta = \frac{E_F}{k_B T} \quad (4.28)$$

$$\rho(E) = \frac{3(2m^*)^{3/2}}{\pi^2 \hbar^3} E^{1/2} \quad (4.29)$$

In Figure 4.11 the ratio of the mobility between the two models is plotted against the position, Z_I , of a single II. The mobilities are calculated at three different background channel impurity concentrations where the carrier density is assumed to equal to impurity density in each case. Similar to the potential comparisons given above, the source impurity/carrier density is given as $n = N_I = 10^{20} \text{ cm}^{-3}$ and is only referenced in the complete model.

4.3 Double Interface Potential Model

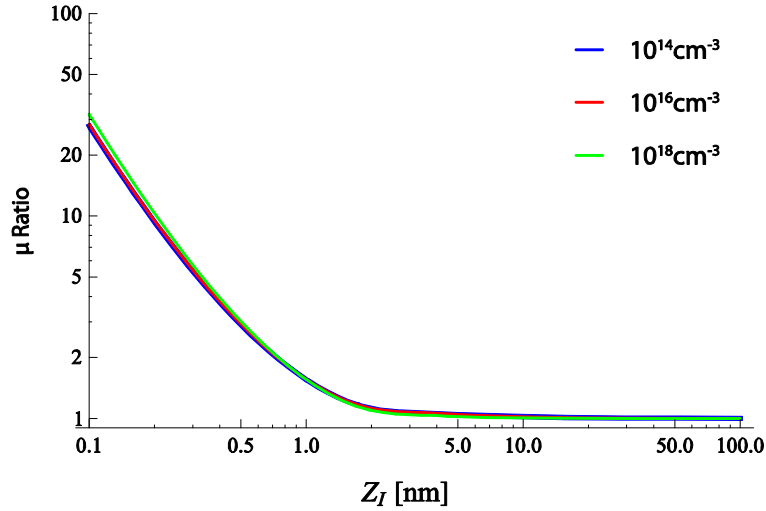


Figure 4.11: Mobility comparison of the complete and strongly screened models assuming a single ionized dopant at a range of positions Z_I , given three background doping concentrations.

It is clear from this plot that the strongly screened model does in fact become increasingly invalid when the impurity is located within 1nm of the source interface regardless of channel screening density. This is very much consistent with the conclusion of the potential comparison that the strongly screened limit will lead to an over-estimation of the effect of remote screening. At 1nm the strongly screened model gives a mobility approximately just over one and a half times larger than that of the complete model. This increases rapidly at decreasing impurity distance from the interface with a ratio of roughly three at $Z_I = 0.5nm$ and a peak of over twenty in the plot above.

Considering the context of this work which is to model the polarisation charge effect on ionized impurity scattering, the use of the strongly screened limit is deemed acceptable to obtain a worst-case value. Use of the strongly screened model will correctly yield an upper limit on the effect of this interaction in a device simulation as has been completed in Chapter 6.

4.3 Double Interface Potential Model

The double interface potential can be calculated following the identical procedure as the single interface model. Cylindrical co-ordinates are used throughout and the LTF approximation, in conjunction with the Debye-Hückel screening model, is used to simplify the Poisson solution. The physical system is defined in Figure 4.12 with the source interface located at $Z = 0$ and the drain interface located at $Z = L_C$. In this figure the source and drain regions have carrier densities larger than the channel, $n_s, n_d > n_c$. Again the impurity is assumed to be always located at $\mathbf{R}_I = 0$ to incorporate radial symmetry around the Z axis, simplifying the solution.

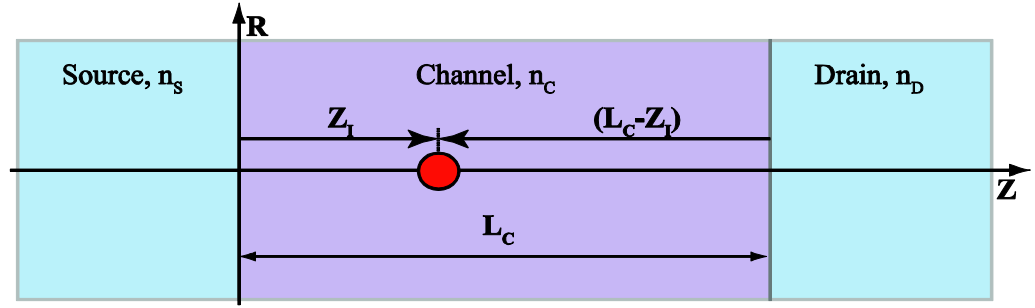


Figure 4.12: Pictorial representation of the double interface system with the impurity located at Z_I and the channel length is given by L_c .

The II is given by the red circle in the channel region and its position is defined relative to the source and drain interfaces, in this case Z_I and $(L_c - Z_I)$ respectively where L_c denotes the channel length.

4.3.1 Potential Solution

The Poisson equations defining the double interface system of Figure 4.12 using the LTF approximation can be given as

$$\nabla^2 \phi_s - k_s^2 \phi_s = 0 \quad \text{for } Z < 0 \quad (4.30)$$

$$\nabla^2 \phi_c - k_c^2 \phi_c = -\frac{Q}{2\pi\epsilon_{si}\epsilon_0} \frac{\delta(\mathbf{R})}{R} \delta(Z - Z_I) \quad \text{for } 0 < Z < L_c \quad (4.31)$$

$$\nabla^2 \phi_d - k_d^2 \phi_d = 0 \quad \text{for } Z > L_c \quad (4.32)$$

Using similar boundary conditions on the potential as the single interface model, $\lim_{\mathbf{R}, Z \rightarrow \pm\infty} \phi \rightarrow 0$, and using the Bessel functions within cylindrical co-ordinates, the following solutions can be found

$$\phi_s = (1 - \theta(Z)) \int_0^\infty dk J_0(kR) A_s(k) \exp(ZK_s) \quad (4.33)$$

$$\begin{aligned} \phi_c = (\theta(Z) - \theta(Z - L_c)) \int_0^\infty dk J_0(kR) & \left[\frac{Q}{4\pi\epsilon_{si}\epsilon_0} \frac{k}{K_c} \exp(-|Z - Z_I|K_c) \right. \\ & - A_c(k) \exp(-ZK_c) \\ & \left. - B_c(k) \exp(ZK_c) \right] \end{aligned} \quad (4.34)$$

4.3 Double Interface Potential Model

$$\varphi_D = \theta(Z - L_C) \int_0^{\infty} dk J_0(kR) A_D(k) \exp(-ZK_D) \quad (4.35)$$

Here the simplified terms , K_x , are given by equations (4.36)-(4.38) below.

$$K_C = \sqrt{k^2 + k_C^2} \quad (4.36)$$

$$K_S = \sqrt{k^2 + k_S^2} \quad (4.37)$$

$$K_D = \sqrt{k^2 + k_D^2} \quad (4.38)$$

The four coefficients, $\{A_S, A_C, B_C, A_D\}$, can be found by matching conditions at the interfaces using a simplified set of the electric field continuity equations specified in equation (4.39).

$$\begin{aligned} \frac{\partial \varphi_S}{\partial Z} &= \frac{\partial \varphi_C}{\partial Z} \text{ and } \frac{\partial \varphi_C}{\partial Z} = \frac{\partial \varphi_D}{\partial Z} \\ \frac{\partial \varphi_S}{\partial R} &= \frac{\partial \varphi_C}{\partial R} \text{ and } \frac{\partial \varphi_C}{\partial R} = \frac{\partial \varphi_D}{\partial R} \end{aligned} \quad (4.39)$$

These boundary condition have been simplified as the dielectric permittivity is constant throughout the system.

The solution for the four coefficients has been found using a matrix method to solve the simultaneous equations, which is not reproduced here (see Appendix B). The resultant form for the coefficients is large and after some manipulation can be reduced to the set of equations given by (4.40)-(4.45).

$$A_S(k) = \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} 2k A_m(k) \exp(-Z_I K_C) \quad (4.40)$$

$$A_C(k) = \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} \frac{k}{K_C} (K_S - K_C) A_m(k) \exp(-Z_I K_C) \quad (4.41)$$

$$B_C(k) = \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} \frac{k}{K_C} (K_D - K_C) A_n(k) \exp(-Z_I K_C) \quad (4.42)$$

4.3 Double Interface Potential Model

$$A_D(k) = \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} 2k A_n(k) \exp(-Z_I K_C) \exp(-L_C (K_C + K_D)) \quad (4.43)$$

The following two coefficients become common components which control the screened fields for the polarisation charges in the source, A_m , and in the drain, A_n .

$$A_m = \frac{K_C (\exp(2L_C K_C) + \exp(2Z_I K_C)) + K_D (\exp(2L_C K_C) - \exp(2Z_I K_C))}{(K_C^2 + K_D K_S)(\exp(2L_C K_C) - 1) + K_C (K_D + K_S)(\exp(2L_C K_C) + 1)} \quad (4.44)$$

$$A_n = \frac{K_C (\exp(2Z_I K_C) + 1) + K_S (\exp(2Z_I K_C) - 1)}{(K_C^2 + K_D K_S)(\exp(2L_C K_C) - 1) + K_C (K_D + K_S)(\exp(2L_C K_C) + 1)} \quad (4.45)$$

After some re-arrangement the potential for the source, channel and drain regions can be simplified to use only the coefficients $A_m(k)$ and $A_n(k)$. These simplified forms are:

$$\varphi_S = \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} (1 - \theta(Z)) \int_0^\infty dk J_0(kR) 2k A_m(k) \exp(-Z_I K_C) \exp(Z K_S) \quad (4.46)$$

$$\begin{aligned} \varphi_C = \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} (\theta(Z) - \theta(Z - L_C)) \int_0^\infty dk J_0(kR) \frac{k}{K_C} & \left[\exp(-|Z - Z_I| K_C) \right. \\ & - (K_S - K_C) A_m(k) \exp(-(Z + Z_I) K_C) \\ & \left. - (K_D - K_C) A_n(k) \exp((Z - Z_I) K_C) \right] \end{aligned} \quad (4.47)$$

$$\begin{aligned} \varphi_D = \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} \theta(Z - L_C) \int_0^\infty dk J_0(kR) 2k A_n(k) & \exp(-(Z_I - L_C) K_C) \\ & \times \exp(-(Z - L_C) K_D) \end{aligned} \quad (4.48)$$

$$\varphi = \varphi_S + \varphi_C + \varphi_D \quad (4.49)$$

Examining the forms of the calculated potentials, there are some distinct similarities with the single interface model defined in section 4.2. The source potential term, φ_S , is almost identical apart from a change in the coefficient. The channel potential is also very similar but has an additional component included from the drain polarisation charges, the third term within the square brackets of equation (4.47). More detail on the calculation of these potentials is given in Appendix B. This includes an outline of the matrix method used to solve for the coefficients.

4.3 Double Interface Potential Model

In the single interface model, the single induced polarisation charge could be represented by a simple coefficient which can be said to represent a ratio of the screening densities between the source and channel regions. In the double interface model above, the coefficients become considerably more complex although represent a similar ratio of screening between the source, channel and drain regions.

As mentioned earlier, the double interface model in certain conditions will induce multiple polarisation charges. This is a side-effect of having two reflecting interfaces a short distance apart, an analogy being that of having two mirrors facing each other reflecting the same image. Here this behaviour can be seen in the coefficients A_m and A_n which control the polarisation charges induced from the source and drain regions. Looking at the coefficients of equations (4.44) and (4.45), the extra complexity of the multiple polarisation charges can be seen by the introduction of the positive exponential components. The positive exponentials represent an infinite sum of polarisation charges which interact to increase the overall screening effect.

4.3.2 Contour Plots

Plotting the total potential, equation (4.49), for an impurity in three different locations in Figure 4.13 shows the effect of the double interface model. Polarisation charge effects are present at both ends of the channel and importantly, combine to further increase the screening effect.

4.3 Double Interface Potential Model

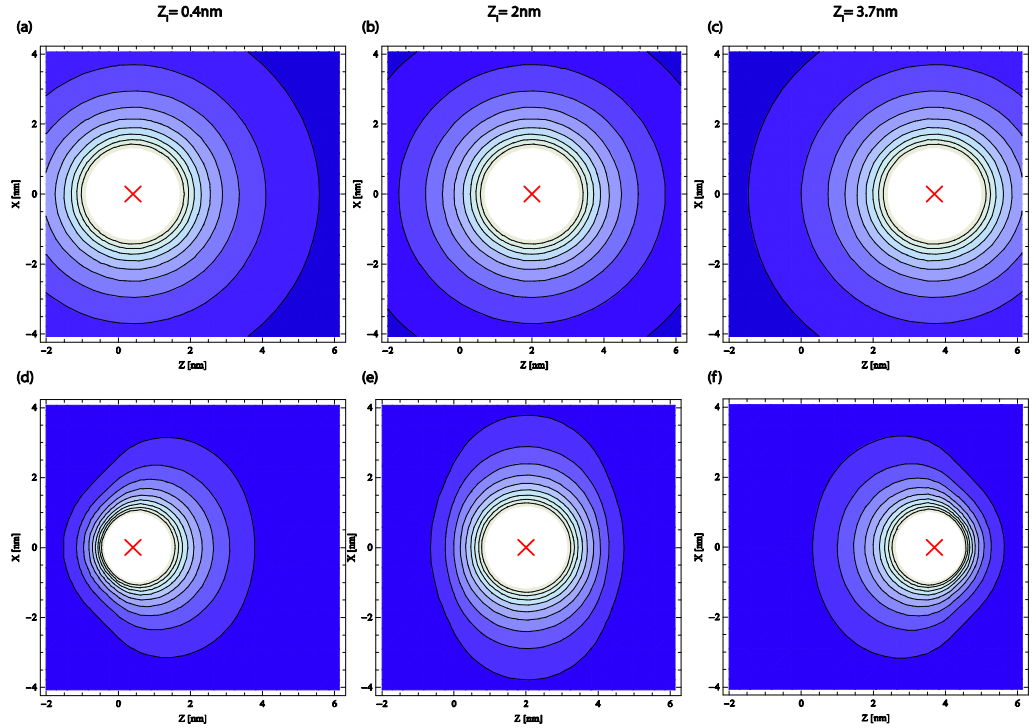


Figure 4.13: Potential contour plots of a device with a channel length $L_C = \lambda_C = 4.133\text{nm}$. Channel doping is $N_A = 10^{18}\text{cm}^{-3}$ and the source-drain doping is $N_D = 10^{20}\text{cm}^{-3}$. Plots (a)-(c) identical screening in the source, channel and drain. Plots (d)-(f) include the polarisation charge effects of the highly-doped source and drain regions.

The largest change between the single and double interface potential models comes in the form of the coefficients $A_m(k)$ and $A_n(k)$ given by equations (4.44)-(4.45). In this model the coefficients are large and complex as the polarisation charge effect develops beyond a reflection of charge from one surface to reflections between two surfaces. Polarisation charges or reflections between the heavily-doped source and drain regions is more complex than the single interface. Under circumstances that the channel length is sufficiently short and an atomistic impurity is not fully screened in the distance to the interfaces, the double interface model induces multiple polarisation charges. This situation will occur for channel lengths which are smaller than the channel screening length.

4.3.3 Long Channel Limit

As with the single interface model, it is important to check that the calculated potential behaves in the expected manner at appropriate limits. Due to the similarities between this model and the single interface model it is not felt necessary to repeat here the screened Coulomb and the matched screening limit. Instead the potentials for this model will be checked to ensure that in the appropriate limit they return to the single interface case. This limit has been entitled the long channel limit and can be found by allowing the channel length to become very large, that is the

4.3 Double Interface Potential Model

limit of $L_C \rightarrow \infty$. For this limit it is best to first take the limit on the coefficients $A_m(k)$ and $A_n(k)$ given by equations (4.44)-(4.45):

$$\begin{aligned} \lim_{L_C \rightarrow \infty} A_m &= \frac{\exp(2L_C K_C)(K_C + K_D) + \exp(2Z_I K_C)(K_C + K_D)}{\exp(2L_C K_C)(K_C^2 + K_D K_S + K_C(K_D + K_S))} \\ &= \frac{1}{K_C + K_S} \end{aligned} \quad (4.50)$$

$$\begin{aligned} \lim_{L_C \rightarrow \infty} A_n &= \frac{\exp(2Z_I K_C)(K_C + K_S) + K_C - K_S}{\exp(2L_C K_C)((K_C + K_S)(K_C + K_D))} \\ &= 0 \end{aligned} \quad (4.51)$$

The coefficient A_n which controls the drain polarisation charges correctly tends to zero as the channel length tends to infinity. The source controlled polarisation charge terms, given by A_m , simplifies vastly as the coefficient is reduced to modelling a single polarisation charge term within the source region. Substituting these coefficients into equations (4.46)-(4.48) gives the single interface model, which is not repeated here, as expected if the drain region is a large distance from the source and the atomistic impurity.

4.3.4 Comparison with Non-Linear Poisson Solution

Comparison of the single interface solution with the NLP solver in section 4.2.4 has shown excellent agreement. To ensure that the double interface model also agrees with a full solution of Poisson's equation, a similar test will be completed here. Again using a solution of the uniform device with the NLP solver to find the solution including the depletion region.

A simple example device will be used to test the double interface remotely screened impurity solution and is depicted in Figure 4.14. The device will have a channel length which is approximately equal to a single screening length at $N_A = 10^{18} \text{ cm}^{-3}$ of $L_C \approx \lambda_C \approx 4.25 \text{ nm}$. This device will be referred to as the lambda channel device, for want of a better name.

4.3 Double Interface Potential Model

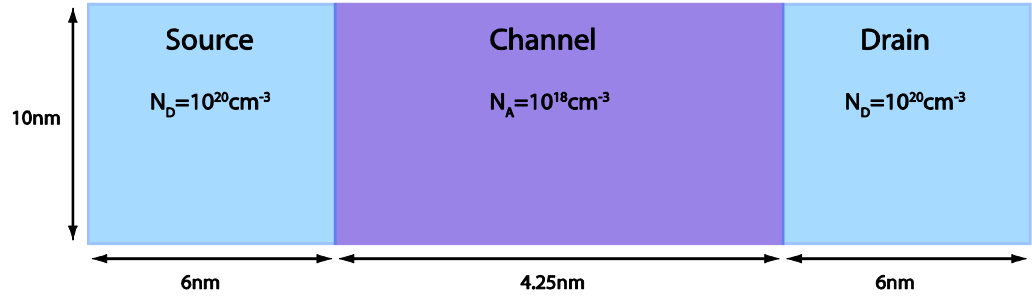


Figure 4.14: Lambda channel device for the comparison of the double interface potential with a non-linear Poisson solver.

This device is important to test because under conditions when the channel length is around the screening length, multiple polarisation charges are likely to be present in the system as discussed at the end of section 4.3.2. Figure 4.15 gives the plots of the lambda channel device with a single atomistic impurity in three different locations. Plots (a) and (b) give the dopant in positions which correspond roughly to $Z_I = 0.1\lambda_C, 0.9\lambda_C$ and plot (c) in position $Z_I = 0.5\lambda_C$.

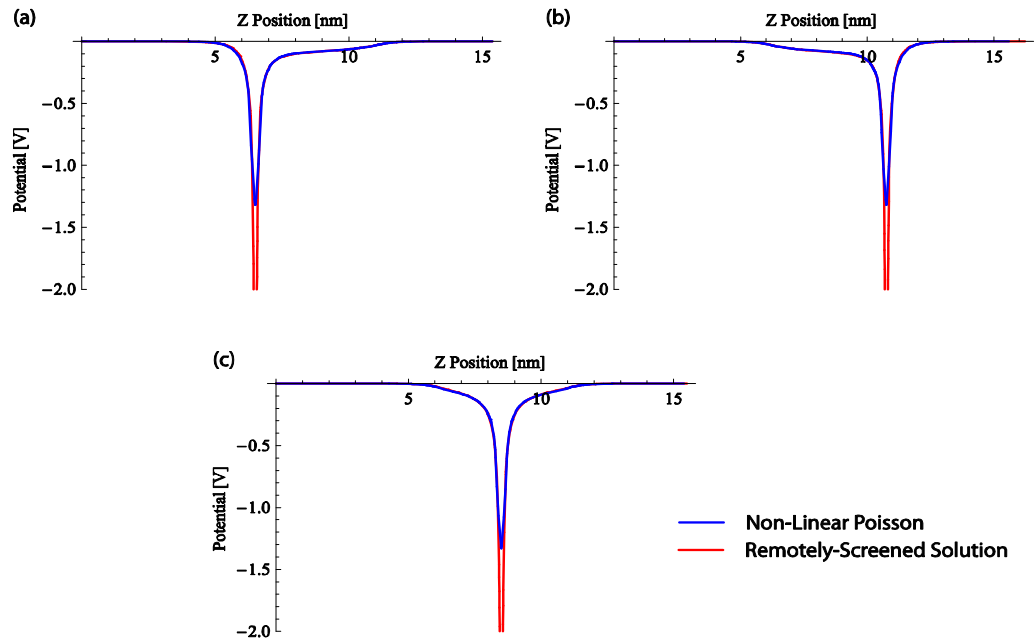


Figure 4.15: Plots of the non-linear Poisson comparison with the analytical model for remotely-screened impurities within the lambda channel device.

These plots show the excellent agreement between the analytical and numerical solutions. Regardless of the impurity position the match is almost indistinguishable neglecting the discretization error of the potential peak in the NLP solution.

4.3.5 Strong-Screening Limit

The strong screening limit of the double interface model, that is $k_s, k_D \gg k_C$, will also simplify the potential terms much like in the single interface case. Here the potential equations and coefficients from section 4.3.1 (equations (4.44)-(4.48)) are used for the double interface model. For simplicity when applying the limit, it will taken that for the limit of $k_s, k_D \gg k_C$, the K_x terms will become:

$$\lim_{k_s, k_D \gg k_C} \begin{cases} K_s = k_s \\ K_D = k_D \end{cases} \quad (4.52)$$

Taking the limit of the coefficients first:

$$\begin{aligned} \lim_{k_s, k_D \gg k_C} A_m &= \frac{k_D (\exp(2L_C K_C) - \exp(2Z_I K_C))}{k_D k_s (\exp(2L_C K_C) - 1) + k_D K_C \left(1 + \frac{k_s}{k_D}\right) (\exp(2L_C K_C) + 1)} \\ A_m^{\text{lim}} &= \frac{\exp(2L_C K_C) - \exp(2Z_I K_C)}{k_s (\exp(2L_C K_C) - 1)} \end{aligned} \quad (4.53)$$

$$\begin{aligned} \lim_{k_s, k_D \gg k_C} A_n &= \frac{k_s (\exp(2Z_I K_C) - 1)}{k_s k_D (\exp(2L_C K_C) - 1) + k_s K_C \left(1 + \frac{k_D}{k_s}\right) (\exp(2L_C K_C) + 1)} \\ A_n^{\text{lim}} &= \frac{\exp(2Z_I K_C) - 1}{k_D (\exp(2L_C K_C) - 1)} \end{aligned} \quad (4.54)$$

Substituting these coefficients into the limit of equations (4.46) and (4.48) gives the limiting form of the double interface source and drain potentials as

$$\lim_{k_s, k_D \gg k_C} \varphi_s \approx \frac{\exp(Zk_s)}{k_s} = 0 \quad \text{for } Z < 0 \quad (4.55)$$

$$\lim_{k_s, k_D \gg k_C} \varphi_D \approx \frac{\exp(-(Z - L_C)k_D)}{k_D} = 0 \quad \text{for } Z > L_C \quad (4.56)$$

Finally, substitution of the strongly screened coefficients into the channel potential term yields the following.

4.3 Double Interface Potential Model

$$\lim_{k_s, k_D \gg k_C} \varphi_C = \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} (\theta(Z) - \theta(Z - L_C)) \int_0^\infty dk J_0(kR) \frac{k}{K_C} \left[\exp(-|Z - Z_I|K_C) - k_s A_m^{\lim}(k) \exp(-(Z + Z_I)K_C) - k_D A_n^{\lim}(k) \exp((Z - Z_I)K_C) \right] \quad (4.57)$$

This is a substantial reduction in complexity of the model, yet still retains the important polarisation charge terms from the reflecting source and drain regions, the 2nd and 3rd terms in the square brackets of equation (4.57) respectively.

Importantly the coefficients $A_m^{\lim}, A_n^{\lim}$ retain the positive exponential components which can be considered to represent the *multiple-image* effect discussed earlier in this chapter. The *multiple-image* effect is the repeated reflection of the impurity point charge between the source and drain regions when the channel length is sufficiently small.

4.3.5.1 Verification of Limit

Repeating a procedure similar to that of the single interface case for the strongly-screened model, the strongly screened double interface model will now be compared to the complete potential. Again, the purpose of this limit is to provide an upper-bound on the remote screening effect of channel ionized impurities.

The comparison will initially be based on two test devices which have different channel lengths, a 25nm channel length device and a 15nm channel device. Both of these devices have a channel doping concentration of $N_I = 10^{15} \text{ cm}^{-3}$ which corresponds to screening length of $\lambda_C = 129.29 \text{ nm}$ using equation (3.36), the Debye-Hückel screening model. The source and drain regions of these devices which is referenced only within the complete model is doped to $N_I = 10^{20} \text{ cm}^{-3}$.

4.3 Double Interface Potential Model

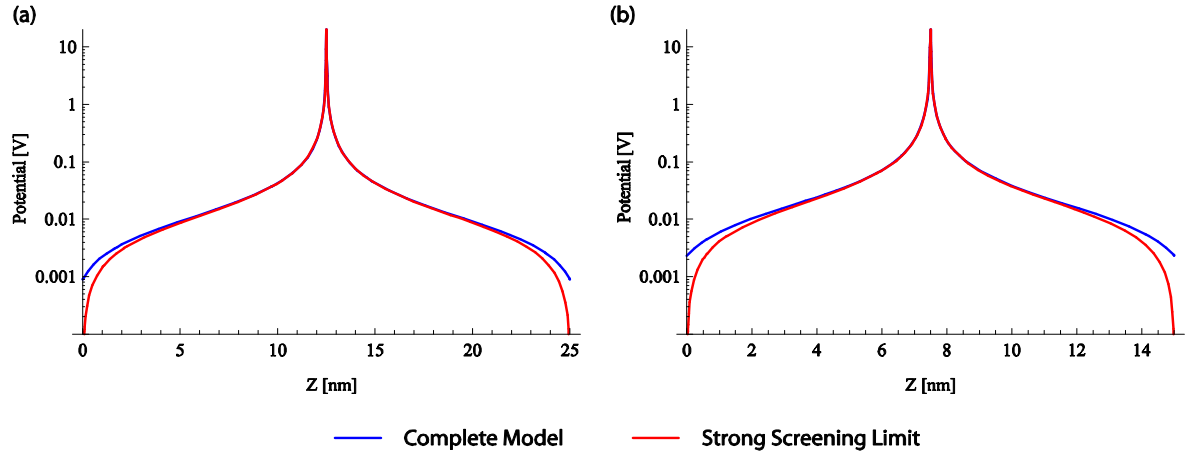


Figure 4.16: Comparison of the complete double interface potential with the strongly screened model for two different channel length devices. Atomistic impurity located exactly mid-channel of each device.

Figure 4.16 shows the comparison between the potentials for (a) the 25nm device and (b) the 15nm channel device. The potential of the strongly screened model is a close match to the complete model surrounding the impurity as expected. Again there is an increased screening of the potential close to the interfaces which is consistent with the strongly screened single interface model.

With the strongly screened interface model discussed in section 4.2.5.2, the region over which the limit caused a notable error in the potential was within roughly 1nm of the interface. It was shown that modelling an impurity within this region of the interface caused a significant error in the potential. Essentially the limit over estimated the polarisation charge effect and over screened the impurity potential. In the double interface model this error in the potential seems evident over a larger region from the interface. Looking at Figure 4.16 the difference in the potential becomes appreciable at around $\sim 2\text{nm}$ from each interface. Plotting the comparison in more detail in Figure 4.17 allows a better analysis of the error.

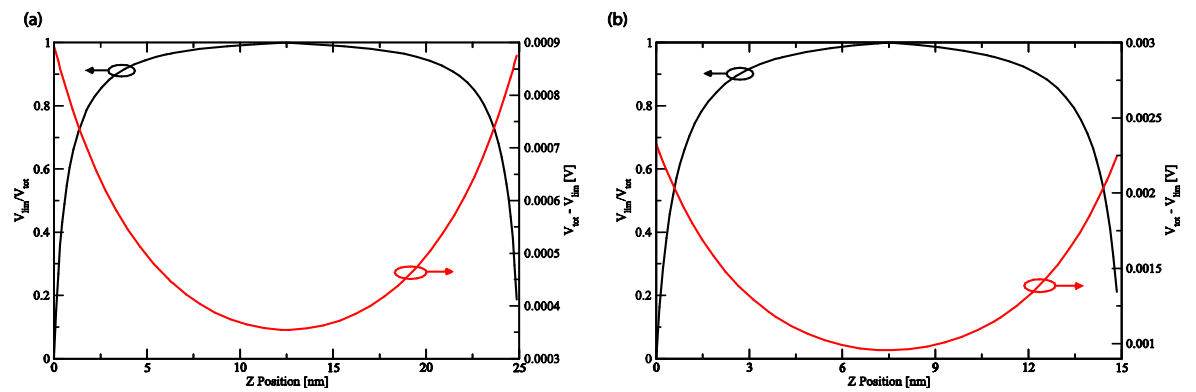


Figure 4.17: Detailed comparison of the strongly screened and complete double interface potential models.

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Figure 4.17 shows that at $\sim 2\text{nm}$ from the interface the strongly screened model is approximately 80% of the complete model. This corresponds to around a 1-1.5mV potential difference for the 25nm and 15nm channel length devices.

To further test the validity of the strongly screened model another comparison has been completed with a device whose channel length is equal to the channel screening length, for want of a better name, the lambda channel device. This device has a channel doped to $N_I = 10^{18}\text{cm}^{-3}$ which corresponds to a screening length of $\lambda_C = 4.133\text{nm}$. The source and drain regions are doped to $N_I = 10^{20}\text{cm}^{-3}$, again this is only referenced with the complete model.

In Figure 4.18 and Figure 4.19 are the potential comparisons between the models in the lambda channel device. Initially this comparison looks at an atomistic impurity at three different locations in the channel but the detailed comparison will look at only two positions due to the symmetry between the left and right positions.

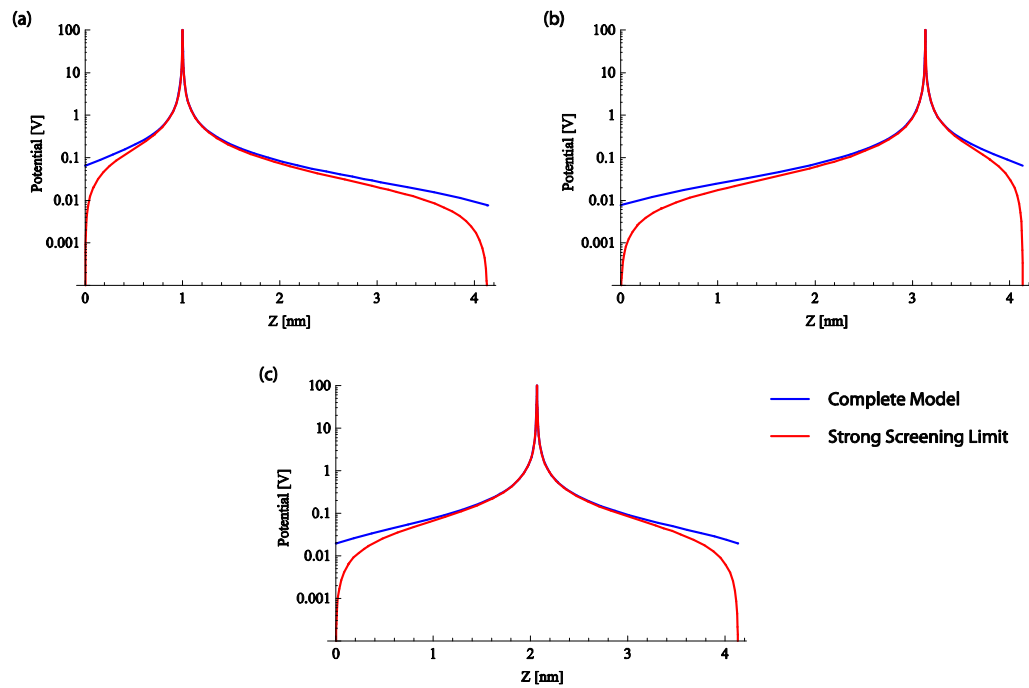


Figure 4.18: Comparison between the strongly screened and complete double interface model using the lambda channel device. Atomistic impurity located at (a) $Z_I = 1\text{nm}$, (b) $Z_I = 0.5\lambda_C$ and (c) $Z_I = \lambda_C - 1\text{nm}$.

Plot (c) of Figure 4.18 shows a single atomistic impurity located exactly mid channel, just over 2nm from each interface. There is an appreciable drop in the potential within 1nm of the interface which is given in more detail in plot (b) of Figure 4.19. At 1nm, the strongly screened model is

4.3 Double Interface Potential Model

around 80% of the complete model with a corresponding drop of roughly 10mV. For an impurity here within 2nm of the interface, 50% of the potential between the interface is above 80%.

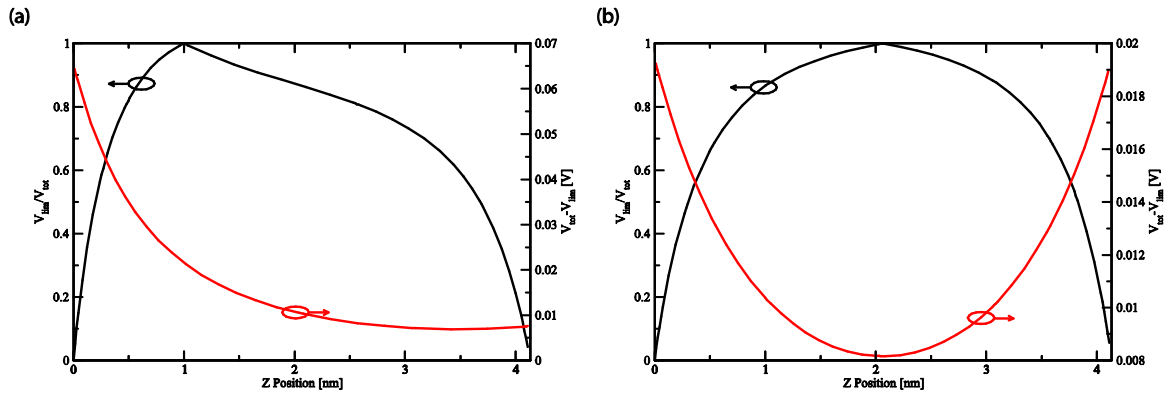


Figure 4.19: Plots of the ratio and potential difference between the strongly screened model and the complete model for the lambda channel device. Plot (a) shows the impurity at $Z_I = 1\text{nm}$ and (b) the impurity positioned at $Z_I = 0.5\lambda_C = 0.5L_C$.

Looking at the case of the impurity located close to the source interface given by plot (a) of Figure 4.18 and Figure 4.19. An impurity located at 1nm from the interface the maximum potential difference is increased by a factor of 2-3 times the mid channel impurity. At this distance the validity of the strong screening limit is questionable. This behaviour is not completely dissimilar to that of the single interface model with an impurity at this distance from the interface given by Figure 4.9.

It is clear that as the impurity is moved closer to the interface the error in the strongly screened model will increase and is very much appreciable within 2nm of an interface. At impurity positions greater than this distance from either the source or drain interface, the limited model is shown above to be close to the complete model with small shifts in the potential of several mV's near the interfaces.

Unfortunately due to time constraints in the PhD project, the complete double interface momentum relaxation rate and therefore the mobility has not been calculated for this model. As discussed in the above examination of the strong screening effect on the potential, it can be said that the limit will induce an increasing error as impurities are located close to either the source or drain interface (or both). This said, the objective of using this limit is to obtain a worst-case condition for the remote screening of channel impurities induced from polarisation charge effects in the source and drain regions. This is certainly achieved by imposing a limiting condition on the screening density in these regions.

4.4 Conclusion

In sections 4.2 and 4.3 of this chapter a potential solution for a single atomistic impurity located close to one or two highly doped regions has been obtained. This has been completed by solving Poisson's equation using the LTF approach to obtain an exact analytical solution. This solution naturally includes polarisation charge effects induced by the boundaries which are the focus of this work. Polarisation charge effects are shown to increase the screening of an atomistic impurity located close to abrupt interface with a highly doped region. Hence these potentials represent the remotely screened impurity potential for the cases of an impurity located close to the source and/or drain regions.

The mathematical limits of the potential solutions have been checked to ensure the correct behaviour. It has been shown that polarisation charge effects disappear when the impurity is a large distance from the interfaces. Under this condition the model returns to the screened Coulomb potential which is the classic potential for an impurity and is an important limit for this model.

To further prove the validity of the approach and solution presented, in section 4.2.4 and 4.3.4 a comparison between a fully self-consistent, non-linear Poisson solver and the calculated analytical approach has been completed. This comparison shows a close agreement between the approaches and highlights the accuracy of the remotely-screened impurity potentials.

Finally, a simplified model has been obtained by introduction of the strong screening limit in sections 4.2.5 and 4.3.5, which assumes that the source and drain regions are degenerately doped and become metallic like. The limit has the resultant effect of screening all the induced impurity potential in the source/drain regions at the interface, thereby reducing the potentials in these regions to zero.

In the single interface model, the strongly screened potential is shown to be almost exact for impurities which are located greater than 1nm from the source interface. For impurities located closer than 1nm from the interface the strongly screened potential greatly over-estimates the screening effect. Similar behaviour is seen in the double interface strongly screened potential for impurities located close to either interface.

The purpose of using the strongly screened models is to represent a worst-case scenario of this model in order to obtain an estimate of the effect on device performance. The strongly screened potentials can easily be used in scattering rate calculations whilst providing an upper bound on the remote screening features of polarisation charge effects.

Chapter 5 Scattering Rate Calculation

5.1 Introduction

In typical Monte Carlo (MC) simulations Ionized Impurity (II) scattering is based on a simple model of a single II located in a semiconductor material. Complex boundary effects such as polarisation charge effects are not included in this simple physical picture. Existing II scattering models based on this simple physical picture have been given a thorough review in Chapter 2. It should also be noted here that the *ab initio* atomistic approach to II scattering developed in this research group [62, 63] does include the complex boundary effects through the Poisson equation solution. Although, the *ab initio* approach is a classical approach to the problem in that the II scattering is achieved through the classical particle transport in MC, here the intention is to obtain a quantum description of the polarisation charge effect.

In this chapter the aim is to develop a scattering model for MC simulation which extends the existing II scattering model. This new scattering rate will allow the II scattering model to include the complex effects of IIs that are located close to the source and drain regions. The impurity potential equations developed in the previous chapter will be used to develop this new model. In this new model the effect of highly-doped regions located close to an ionized dopant is to alter the screening of the impurity potential. Hence, the new model has been entitled remotely screened impurity scattering to reflect the nature of the induced screening from polarisation charge induced from the source and/or drain regions.

Initially, the scattering matrix element and then the scattering rate will be calculated for both the single interface and double interface models in sections 5.2 and 5.3 respectively. The method used to obtain the scattering rate will be based on Fermi's Golden Rule approach. Calculation of the momentum relaxation rates and differential cross-section will also be included, which are very useful for analysis of the scattering model.

In section 5.4 the application of this new scattering model in sub-threshold device conditions is discussed where screening is very low. Low-screening densities cause large problems with II scattering in MC simulations as will be highlighted and resolved for this scattering model. This involves the development of a new II scattering approach which is presented in detail.

5.2 Single Interface Scattering Model

Following this, a brief discussion of the numerical implementation into the MC simulator will be covered in section 5.5. This section will cover the techniques used within the MC simulator to calculate the scattering rate and complete the scattering process.

5.2 Single Interface Scattering Model

In the previous chapter the scattering potential for an atomistic impurity located close to a reflecting interface was calculated. This scattering potential can be used to develop a scattering rate for MC simulation. For such a scattering rate, the matrix element must first be evaluated from the scattering potential.

In the case for the remotely screened impurity model, the strong screening limit potentials shall be used as they simplify the model whilst retaining the important polarisation charge effect of the source region. As discussed in the previous chapter, use of this limit is a worst-case condition which leads to an overestimation of the remote screening effect induced from the source region for impurities located close to the source interface. The aim of this work is to look at what effect remote screening has on device performance, therefore the use of strongly screened model is considered suitable as it will provide an upper limit on remote screening.

The scattering potential for the remotely-screened II model is not spherically symmetric like the standard II scattering models. With the remotely-screened model the scattering potential is anisotropic and therefore varies depending on the angle with which the carrier sees the impurity. The typical textbook approach for the scattering in Monte Carlo makes use of isotropic scattering potentials. Anisotropy in scattering is typically found through the band structure via anisotropic effective masses which can also be modelled using an isotropic effective mass with an anisotropic scattering potential [101-104]. There are several approaches for modelling anisotropic scattering potentials such as a spherical harmonics expansion of the Schrödinger equation as discussed by Boardman [105], or through solutions to the linear Boltzmann equation [106-109]. Due to the complexity of these approaches and the context of this work which is to analyse what effect remote screening may have, a simpler approach is employed here. This simpler approach will allow for an initial examination of the strength of remote screening of ionized impurity scattering in a Monte Carlo simulation.

For the purposes of this work a simplifying approximation is made such that the anisotropy of the scattering potential is removed by allowing the incoming carrier angle to be aligned with the principle scattering axis. In other words, we make an assumption on the alignment of the scattering potential with the scattering carrier which removes the anisotropy. This alignment is discussed and

5.2 Single Interface Scattering Model

analysed in detail later in this chapter and is shown to lead to a negligible error in all cases. Further discussion of this simplification is left to section 5.2.3.

Initially the scattering matrix element suitable for use with Fermi's Golden Rule will be calculated from the scattering potential defined in the previous chapter, section 4.2. Following this, in section 5.2.2 the scattering rate for use in the MC simulation technique will be developed. Here other important scattering model equations are calculated such as the differential cross-section and momentum relaxation rate. These have a specific importance in the analysis of the scattering model, allowing the magnitude of the scattering probability and the effect on carrier transport to be examined. In section 5.2.3 the incoming angle simplification will be discussed in detail and the effect the simplification has on the model will be presented. Finally in section 5.2.4 the scattering model developed in this section will be analysed.

5.2.1 Scattering Matrix Element

The matrix element for a scattering rate is defined as [30]

$$\mathbf{H}_{\mathbf{k}'\mathbf{k}} = \frac{1}{\Omega} \int_{-\infty}^{\infty} d^3\mathbf{r} \exp(-i\mathbf{k}' \cdot \mathbf{r}) U_s(\mathbf{r}) \exp(i\mathbf{k} \cdot \mathbf{r}) \quad (5.1)$$

where electron plane wave functions have been assumed. The matrix element has been normalised over the 3D unit volume, Ω , and $U_s(\mathbf{r})$ is the scattering energy. Simplifying this using $\mathbf{q}^2 = |\mathbf{k}' - \mathbf{k}|^2$ and separating into cylindrical co-ordinates, the matrix element definition may be written as a Fourier transform over the variables $\mathbf{q}_\perp$ and q_z .

$$\mathbf{H}_{\mathbf{k}'\mathbf{k}} = \frac{1}{\Omega} \int_{-\infty}^{\infty} dZ \int_0^{2\pi} d\phi \int_0^{\infty} dR U_s(\mathbf{R}, Z) \exp(-i\mathbf{q}_\perp \cdot \mathbf{R}) \exp(-iq_z Z) \quad (5.2)$$

Throughout this section the scattering momentum transfer variables will be expressed in cylindrical co-ordinates using the perpendicular and Z-directed momentum transfer wave vectors, $\mathbf{q}_\perp$ and q_z . A more detailed discussion on the exact definition of the scattering momentum transfer wave-vectors for this scattering model is left to section 5.2.3. For now it is sufficient to know that the definition of the scattering momentum transfer in cylindrical co-ordinates is given by equations (5.3)-(5.4).

$$\mathbf{q}_\perp^2 = |\mathbf{k}'_\perp - \mathbf{k}_\perp|^2 \quad (5.3)$$

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$$q_z^2 = |k'_z - k_z|^2 \quad (5.4)$$

For the single interface model, the scattering potential to be used is the strong screening limit of the model. This potential which was calculated in section 4.2 of the previous chapter can be written as

$$V(\mathbf{R}, Z) = \theta(Z) \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} \left[\frac{\exp\left(-k_c \sqrt{\mathbf{R}^2 + (Z - Z_I)^2}\right)}{\sqrt{\mathbf{R}^2 + (Z - Z_I)^2}} - \frac{\exp\left(-k_c \sqrt{\mathbf{R}^2 + (Z + Z_I)^2}\right)}{\sqrt{\mathbf{R}^2 + (Z + Z_I)^2}} \right] \quad (5.5)$$

Substituting this scattering potential into the scattering matrix definition equation (5.2) using the transform $U_s(\mathbf{R}, Z) = eV(\mathbf{R}, Z)$ gives equation (5.6). As the strongly screened potential is valid only for the $Z > 0$ region, the integral over the Z space in the Fourier transform has been corrected accordingly.

$$\mathbf{H}_{\mathbf{k}'\mathbf{k}} = \frac{1}{\Omega} \int_0^\infty dZ \int_0^{2\pi} d\phi \int_0^\infty d\mathbf{R} eV(\mathbf{R}, Z) \exp(-i\mathbf{q}_\perp \cdot \mathbf{R}) \exp(-iq_z Z) \quad (5.6)$$

After some lengthy integration, the Fourier transform above can be completed to give

$$\mathbf{H}_{\mathbf{k}'\mathbf{k}} = \frac{eQ}{4\pi\epsilon_{Si}\epsilon_0} \frac{1}{\Omega} \frac{4\pi}{\mathbf{q}_\perp^2 + q_z^2 + k_c^2} \left[\exp(-iq_z Z_I) - \exp\left(-Z_I \sqrt{\mathbf{q}_\perp^2 + k_c^2}\right) \right] \quad (5.7)$$

Taking the magnitude-squared of this matrix element, also known as the Born approximation, provides us with a form suitable for use in Fermi's Golden Rule. After some algebraic manipulation the scattering matrix element becomes

$$|\mathbf{H}_{\mathbf{k}'\mathbf{k}}|^2 = \left(\frac{eQ}{4\pi\epsilon_{Si}\epsilon_0} \right)^2 \frac{1}{\Omega^2} \left(\frac{4\pi}{\mathbf{q}_\perp^2 + q_z^2 + k_c^2} \right)^2 \times \left[1 + \exp\left(-2Z_I \sqrt{\mathbf{q}_\perp^2 + k_c^2}\right) - 2\cos(q_z Z_I) \exp\left(-Z_I \sqrt{\mathbf{q}_\perp^2 + k_c^2}\right) \right] \quad (5.8)$$

Equation (5.8) is the scattering matrix element for the single interface, remotely screened impurity scattering model. As is expected the matrix element has some similarities with that of the Brooks-Herring (BH) approach (see section 2.3) albeit given here in cylindrical co-ordinates. The terms

5.2 Single Interface Scattering Model

within the square brackets represents the remote screening coefficient and defines the extent of the polarisation charge effects in screening the impurity. These terms are dominated by the $\exp(-Z_I \dots)$ components which reduce the interaction as the impurity position Z_I increases. In other words the remote screening effect drops off roughly exponentially as the impurity is located farther from the source region.

As discussed in the previous chapter it is important for this scattering rate to return to the BH model when the atomistic impurity is located a large distance from the interface. Looking at the second and third terms in the square brackets of the matrix element, the exponentials of negative power, it is clear that in the limit of $Z_I \rightarrow \infty$ these terms will tend to zero and will yield the BH model.

5.2.2 Scattering Rate

Having found the scattering matrix element in section 5.2.1 for the remotely screened impurity model, it is now possible to define the total scattering rate for use in MC simulation. This calculation will follow the method of Fermi's Golden Rule which defines the scattering transition probability for a carrier wave vector $\mathbf{k}$ to a state $\mathbf{k}'$. In addition to the total scattering rate, the differential scattering cross-section and the momentum relaxation rate will be calculated for the new impurity scattering model.

Equation (5.9) is the Fermi Golden Rule for an elastic scattering event [110], which is a scattering event where the incoming and outgoing energies are equal. Here the overlap integral for electrons is assumed to equal one and the band structure is modelled by an ellipsoidal and non-parabolic model. The effective mass, which is a 2nd rank tensor with a single diagonal component, is represented by the isotropic density of states effective mass, $m_d^* = \sqrt[3]{m_l m_t^2}$, by making use of the Herring-Vogt transformation as discussed in section 3.2.3 [71]. The Herring-Vogt transformation allows the ellipsoidal bandstructure to be represented as a spherical bandstructure.

$$P(\mathbf{k}, \mathbf{k}') = \frac{2\pi}{\hbar} |\mathbf{H}_{\mathbf{k}'\mathbf{k}}|^2 \delta(E(\mathbf{k}^*) - E(\mathbf{k}')) \quad (5.9)$$

Here $\mathbf{k}^*$ is the carrier wave vector after the Herring-Vogt transformation into starred space (see section 3.2.3). This equation calculates the probability of scattering from a state $\mathbf{k}$ to a state $\mathbf{k}'$ but the calculation must be completed using the Herring-Vogt transformed vectors, hence the change of the vector in this expression. Inserting the scattering matrix element of equation (5.8) into equation (5.9) for the probability of scattering gives

5.2 Single Interface Scattering Model

$$P(\mathbf{k}, \mathbf{k}') = \frac{2\pi}{\hbar} \left(\frac{eQ}{4\pi\epsilon_{Si}\epsilon_0} \right)^2 \frac{1}{\Omega^2} \left(\frac{4\pi}{\mathbf{q}_\perp^2 + q_z^2 + k_C^2} \right)^2 \delta(E(\mathbf{k}^{*'}) - E(\mathbf{k}^*)) \quad (5.10)$$

$$\times \left[1 + \exp\left(-2Z_I \sqrt{\mathbf{q}_\perp^2 + k_C^2}\right) - 2\cos(q_z Z_I) \exp\left(-Z_I \sqrt{\mathbf{q}_\perp^2 + k_C^2}\right) \right]$$

There are various quantities which can be obtained from the scattering probability, $P(\mathbf{k}, \mathbf{k}')$, which allow various different properties of the scattering model to be analysed. The differential scattering cross-section is found using equation (5.11) which integrates the scattering probability over all $\mathbf{k}$ -space. Here v is the velocity of a state $\mathbf{k}$ given by equation (5.12) where α is the non-parabolicity parameter.

$$\sigma = \frac{\Omega^2}{v(\mathbf{k})} \int_0^\infty d\mathbf{k}^{*'} \mathbf{k}^{*'} P(\mathbf{k}, \mathbf{k}') \quad (5.11)$$

$$v(\mathbf{k}) = \frac{1}{\hbar} \frac{\partial E}{\partial \mathbf{k}} = \frac{\hbar k^*}{m_d (1 + 2\alpha E)} \quad (5.12)$$

The differential scattering cross-section is a function of angle and allows for analysis of the strength of a scattering centre. Using the scattering probability in equation (5.11) and completing the integral yields

$$\sigma = \left(\frac{Ze^2}{4\pi\epsilon_{Si}\epsilon_0} \right)^2 \frac{2^2 m_d^2}{\hbar^4} (1 + 2\alpha E)^2 \frac{1}{(\mathbf{q}^2 + k_C^2)^2} \quad (5.13)$$

$$\times \left[1 + \exp\left(-2Z_I \sqrt{\mathbf{q}_\perp^2 + k_C^2}\right) - 2\cos(q_z Z_I) \exp\left(-Z_I \sqrt{\mathbf{q}_\perp^2 + k_C^2}\right) \right]$$

Here the impurity charge, Q , has been replaced by the number of free unit charges of the II, Z , multiplied by the electron charge, e .

The total scattering rate and the momentum relaxation rate are calculated in a similar manner to each other and are specified in equations (5.14) and (5.15) respectively. The momentum relaxation rate includes a weighting term by the change in the momentum of a scattering event, hence the extra term within the integral on the RHS of equation (5.15).

$$\Gamma(\mathbf{k}) = \sum_{\mathbf{k}^{*'}} P(\mathbf{k}, \mathbf{k}') = N_k \int_{\mathbf{k}^{*'}} P(\mathbf{k}, \mathbf{k}') d\mathbf{k}^{*'} \quad (5.14)$$

5.2 Single Interface Scattering Model

$$\frac{1}{\tau_m(\mathbf{k})} = \sum_{\mathbf{k}'} P(\mathbf{k}, \mathbf{k}') \left(1 - \frac{\mathbf{k}'}{\mathbf{k}^*} \cos \theta_s \right) = N_k \int_{\mathbf{k}'} P(\mathbf{k}, \mathbf{k}') \left(1 - \frac{\mathbf{k}'}{\mathbf{k}^*} \cos \theta_s \right) d\mathbf{k}' \quad (5.15)$$

$$N_k = \frac{\Omega}{(2\pi)^3} \quad (5.16)$$

where θ_s is the angle between the incident and scattered wave-vector. The exact definition of the scattering angle is left to section 5.2.3.

The total scattering rate can be found by substituting (5.10) into equation (5.14) and after expanding the integral using spherical co-ordinates, the scattering rate is given as

$$\begin{aligned} \Gamma(\mathbf{k}) = & \left(\frac{Ze^2}{4\pi\epsilon_{Si}\epsilon_0} \right)^2 \frac{1}{\Omega} \frac{2^2}{\hbar} \int_0^{2\pi} d\varphi_{k'} \int_0^\pi d\theta_{k'} \sin \theta_{k'} \int_0^\infty dk'^* k'^*{}^2 \frac{1}{(\mathbf{q}^2 + k_C^2)^2} \\ & \times \left[1 + \exp\left(-2Z_I \sqrt{\mathbf{q}_\perp^2 + k_C^2}\right) - 2 \cos(q_Z Z_I) \exp\left(-Z_I \sqrt{\mathbf{q}_\perp^2 + k_C^2}\right) \right] \\ & \times \delta\left(E(\mathbf{k}') - E(\mathbf{k}^*)\right) \end{aligned} \quad (5.17)$$

The integral over the range of final electron wave vectors, k' , can be completed easily due to the Dirac delta function which ensures energy conservation. This leaves the integral over the final angles $\theta_{k'}$ and $\varphi_{k'}$. These integrals have not been completed here and will be discussed in the next section. After some algebraic manipulation and multiplication by the II density of the unit volume, $N_I \Omega$, the total scattering rate is found as

$$\begin{aligned} \Gamma(\mathbf{k}) = & \left(\frac{Ze^2}{4\pi\epsilon_{Si}\epsilon_0} \right)^2 N_I \frac{2^2 m_d k^*}{\hbar^3} (1 + 2\alpha E) \int_0^{2\pi} d\varphi_{k'} \int_0^\pi d\theta_{k'} \frac{\sin \theta_{k'}}{(\mathbf{q}^2 + k_C^2)^2} \\ & \times \left[1 + \exp\left(-2Z_I \sqrt{\mathbf{q}_\perp^2 + k_C^2}\right) - 2 \cos(q_Z Z_I) \exp\left(-Z_I \sqrt{\mathbf{q}_\perp^2 + k_C^2}\right) \right] \end{aligned} \quad (5.18)$$

Here and in the following expressions the magnitude of the incoming vector after the Herring-Vogt transformation is written as k^* for simplicity. The momentum relaxation rate for the scattering process can be defined by inserting the momentum relaxation weighting term into the $\theta_{k'}$ integral of the total scattering rate and using the elastic scattering definition that $E(\mathbf{k}') = E(\mathbf{k})$.

$$\frac{1}{\tau_m(\mathbf{k})} = \left(\frac{Ze^2}{4\pi\epsilon_{si}\epsilon_0} \right)^2 N_I \frac{2^2 m_d k^*}{\hbar^3} (1 + 2\alpha E) \int_0^{2\pi} d\phi_{k'} \int_0^{\pi} d\theta_{k'} \frac{\sin\theta_{k'} (1 - \cos\theta_s)}{(\mathbf{q}^2 + k_c^2)^2} \times \left[1 + \exp\left(-2Z_I \sqrt{\mathbf{q}_{\perp}^2 + k_c^2}\right) - 2\cos(q_z Z_I) \exp\left(-Z_I \sqrt{\mathbf{q}_{\perp}^2 + k_c^2}\right) \right] \quad (5.19)$$

5.2.3 Scattering Reference Frame

The II scattering models of BH and Conwell-Weisskopf (CW) have scattering potentials which are spherically symmetric. In a spherically symmetric scattering potential the angle of the incoming carrier doesn't affect the potential the carrier interacts with. This allows the scattering and device reference frames to be aligned reducing the complexity of the model. The scattering reference frame being that used to describe the scattering event and the device reference frame describing the physical device for the direction of carrier momentum.

In the remotely screened model developed here the scattering potential given by equation (5.5) is not spherically symmetric. An example of the potential contours is given in Figure 5.1 below. There is rotational symmetry around the Z-axis due to the assumption that the II is located at $\mathbf{R}_I = 0$ (see Figure 5.4 and Figure 5.5). To properly describe the scattering event for this model the scattering reference frame must be fixed and be consistent with the potential model.

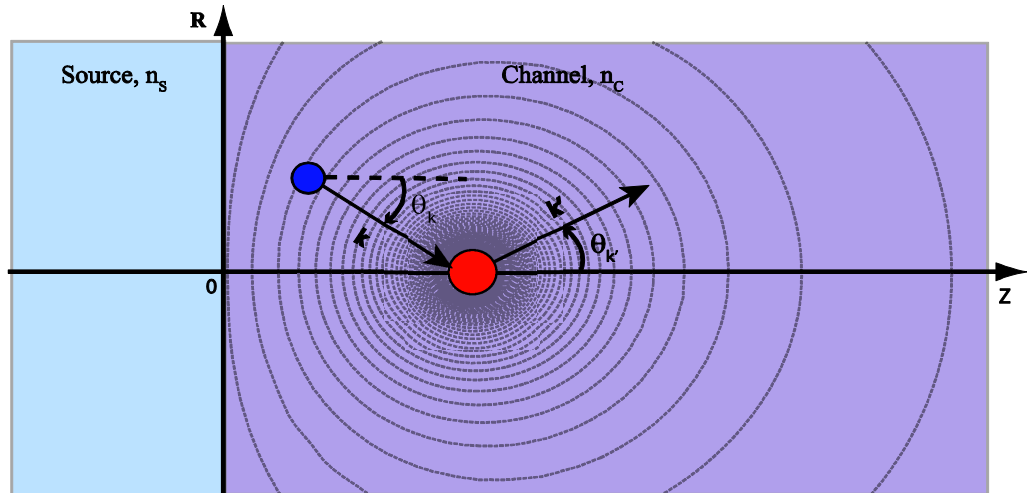


Figure 5.1: Fixed scattering reference frame with example case of remotely screened impurity potential contours and incoming/outgoing carrier wave-vectors.

The fixed scattering reference frame used here is identical to the reference frame defined within the calculation of the potential (see Figure 4.1) and is closely related to the device reference frame which is aligned on the same axes within a cartesian coordinate system. An example of the fixed scattering reference frame is given by Figure 5.1 with the remotely screened II given by the red

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circle and the incoming carrier by the blue circle. Figure 5.1 also shows example potential contours from a II located close to the source interface where the potential contours become slightly egg-shaped with a flat spot close to the source region, demonstrating the non-spherical nature.

Also demonstrated in this figure is an example scattering carrier with the incoming angle θ_k and outgoing angle θ_k' (the angle θ_k assumes a rotation of π around the Z axis). It is clear that the incoming angle of the carrier will affect the scattering potential that it sees and will alter the scattering rate.

For the Monte Carlo simulator used in this work, which is a 3D bulk Monte Carlo simulator it is ideal to express the wave-vectors in the spherical co-ordinate system. This ensures compatibility with the existing code and scattering processes.

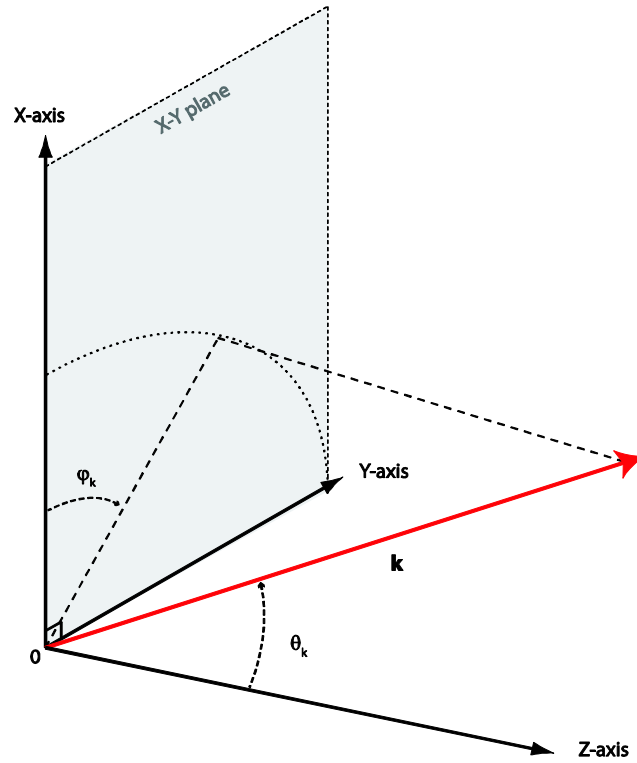


Figure 5.2: Definition of the fixed scattering reference frame using a spherical co-ordinate system.

Figure 5.2 gives the fixed reference frame for this scattering model in more detail using the spherical co-ordinate system. Here the X-Y plane denoted in the figure represents the R-plane of the cylindrical co-ordinate system and of the R plane in Figure 5.1, the angle φ_k provides the angle of rotation around the Z-axis and θ_k gives the angle of the vector from the Z-axis. This is the

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generic spherical co-ordinate reference system rotated such that it matches the axis definition of the scattering potential given by Figure 4.1.

Using the fixed reference frame, given in detail by Figure 5.2, the momentum transfer wave-vectors of equations (5.3)-(5.4) can now be defined. Expanding the components in terms of Cartesian co-ordinates initially gives

$$\begin{aligned} \mathbf{q}_{\perp}^2 &= |\mathbf{k}'_{\perp} - \mathbf{k}_{\perp}|^2 = |k'_x - k_x|^2 + |k'_y - k_y|^2 \\ &= (k'^2_x + k^2_x - 2k'_x \cdot k_x) + (k'^2_y + k^2_y - 2k'_y \cdot k_y) \end{aligned} \quad (5.20)$$

$$q_z^2 = |k'_z - k_z|^2 = k'^2_z + k^2_z - 2k'_z \cdot k_z \quad (5.21)$$

Using the following textbook transforms [96] and allowing the magnitude of the vector $\mathbf{k}$ to be written simply as k

$$k_x = k \sin \theta_k \cos \varphi_k \quad (5.22)$$

$$k_y = k \sin \theta_k \sin \varphi_k \quad (5.23)$$

$$k_z = k \cos \theta_k \quad (5.24)$$

the scattering momentum transfer wave-vectors can be expressed in spherical terms as

$$\begin{aligned} \mathbf{q}_{\perp}^2 &= k^2 \sin^2 \theta_k + k'^2 \sin^2 \theta_{k'} - 2kk' \sin \theta_k \sin \theta_{k'} \cos(\varphi_k - \varphi_{k'}) \\ &= k^2 (\sin^2 \theta_k + \sin^2 \theta_{k'} - 2 \sin \theta_k \sin \theta_{k'} \cos(\varphi_k - \varphi_{k'})) \end{aligned} \quad (5.25)$$

$$\begin{aligned} q_z^2 &= k^2 \cos^2 \theta_k + k'^2 \cos^2 \theta_{k'} - 2kk' \cos \theta_k \cos \theta_{k'} \\ &= k^2 (\cos \theta_k - \cos \theta_{k'})^2 \end{aligned} \quad (5.26)$$

These forms assume an elastic scattering process such that the incoming energy is conserved and so $E(\mathbf{k}) = E(\mathbf{k}')$ which is applicable to the II scattering process. Using equation (5.25) and (5.26), the full momentum transfer wave-vector can be written

$$\begin{aligned} \mathbf{q}^2 &= \mathbf{q}_{\perp}^2 + q_z^2 \\ &= 2k^2 (1 - \cos \theta_k \cos \theta_{k'} - \sin \theta_k \sin \theta_{k'} \cos(\varphi_k - \varphi_{k'})) \end{aligned} \quad (5.27)$$

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The effect that the incoming carrier has on the scattering model can now be analysed using the momentum transfer relations defined above. Substituting equations (5.25)-(5.27) into the total scattering rate of equation (5.18) gives the model including the incoming wave-vector dependence.

Care must be taken with the momentum relaxation rate as the weighting term depends on the scattered angle between the carriers. As the angle between the incident and scattered wave-vector is defined here within a fixed reference frame system, the momentum relaxation weighting term must be given as

$$1 - \cos \theta_S \equiv 1 - \cos \theta_k \cos \theta_{k'} - \sin \theta_k \sin \theta_{k'} \cos(\varphi_k - \varphi_{k'}) \quad (5.28)$$

Substitution of the momentum transfer relations and the weighting term of equations (5.25)-(5.28) into the momentum relaxation rate, equation (5.19), gives the incoming angle dependent momentum relaxation rate.

To test these relations are correct it is ideal to initially check that in the limit of $Z_I \rightarrow \infty$ the model returns to a spherically symmetric case. That is, the BH limit of the model which has no remote screening interaction. In Figure 5.3 the scattering rate is plotted over all incoming angles for such a limit.

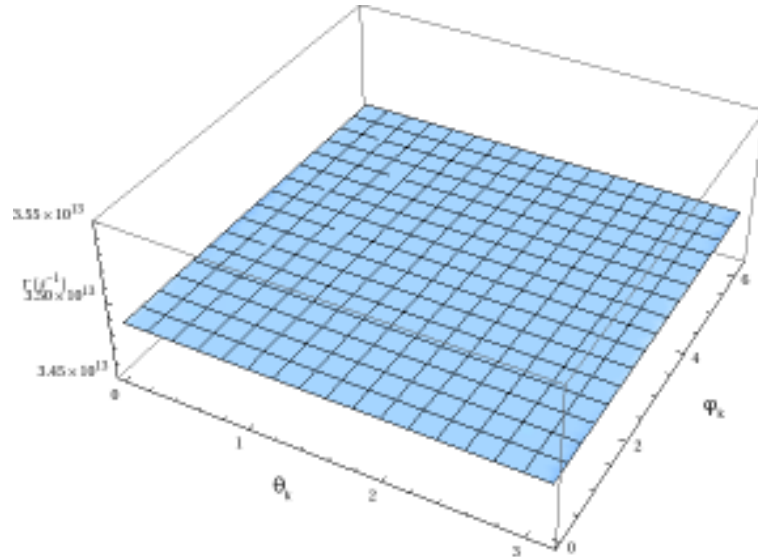


Figure 5.3: Plot of the remotely screened scattering rate at $Z_I k_C \gg 4$ over all possible incoming carrier angles.

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For this figure the impurity density matches the screening density and is given as $n = N_I = 10^{17} \text{ cm}^{-3}$. The incoming carrier energy is calculated as the average energy at a lattice temperature of $T = 300 \text{ K}$ using equation (5.29), yielding $\langle E \rangle \approx 40 \text{ meV}$.

$$\langle E \rangle = \frac{3}{2} k_B T \frac{\mathfrak{F}_{\frac{3}{2}}(\eta) + \frac{25}{4} \alpha k_B T \mathfrak{F}_{\frac{5}{2}}(\eta)}{\mathfrak{F}_{\frac{1}{2}}(\eta) + \frac{15}{4} \alpha k_B T \mathfrak{F}_{\frac{3}{2}}(\eta)} \quad (5.29)$$

where $\mathfrak{F}_j$ is the Fermi-Dirac integral of order j [54] and η is the reduced Fermi level given by $\eta = E_F / k_B T$. It is very clear that the scattering rate in Figure 5.3 is independent of the incoming carrier angle. This is expected as the scattering model returns to the classic BH case.

Plotting the incoming angle dependent scattering and momentum relaxation rates for the remotely screened model at an impurity distance closer to the interface will show the anisotropic behaviour. Using the same impurity density and average carrier energy as Figure 5.3 with an impurity located at $Z_I = 1\lambda_C$, the scattering rate is then plotted in Figure 5.4 and the momentum relaxation rate in Figure 5.5.

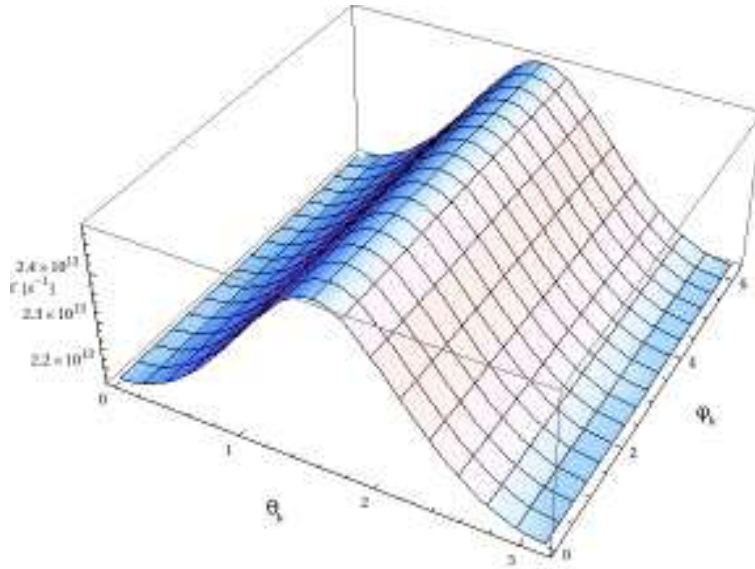


Figure 5.4: Plot of the remotely screened scattering rate at $Z_I k_C \approx 1$ over all possible incoming carrier angles.

The anisotropic behaviour of the incoming carrier angle on the scattering model is demonstrated in these figures with a change in the rates with the incoming angle θ_k . Referring to Figure 5.1 (and given in more detail in Figure 5.2), the angle θ_k is the angle of the carrier from the Z-axis. For an angle of $\theta_k = 0$ the carrier is aligned with the Z-axis and is travelling away from the source

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interface, and for an angle of $\theta_k = \pi$ the carrier is aligned with the Z-axis and travelling towards the interface.

It is interesting to note that for $\theta_k = 0$ and $\theta_k = \pi$ the scattering and momentum relaxation rates are identical. This behaviour can be understood from the magnitude-squared of the scattering matrix element, equation (5.8), being an even function around q_z . Therefore the rates for $\theta_k = x\pi$ will be identical to that of $\theta_k = \pi - x\pi$ for $0 \leq x \leq 1$.

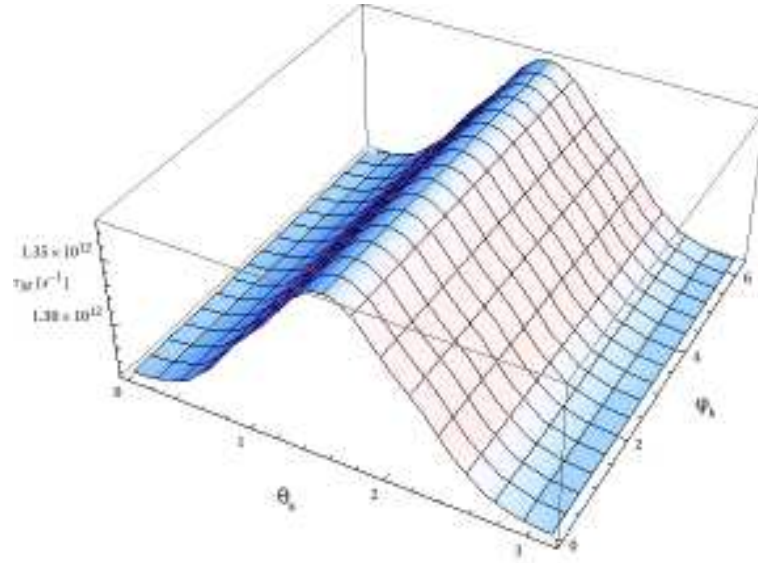


Figure 5.5: Plot of the remotely screened momentum relaxation rate at $Z_I k_C \approx 1$ over all possible incoming carrier angles.

In both Figure 5.4 and Figure 5.5 the rates reach a maximum at $\theta_k = \pi/2$ which corresponds to the point at which the Z-directed momentum transfer, q_z , is at a minimum (the carrier angle is perpendicular to the Z-axis). Examining the scattering matrix element of equation (5.8) again, the third term of the remote screening coefficient (the terms within the square brackets) contains the q_z component as a parameter of the cosine function. When this component, the Z-directed momentum transfer, becomes small the frequency of the cosine function will decrease rapidly. At high frequency the cosine function averages to a value close to zero, but at low frequency the function average becomes much larger. Therefore, as $q_z \rightarrow 0$ the third term of the coefficient will increase in value and will therefore increase the scattering rate.

The rotational symmetry around the Z-axis is highlighted in these plots, where the φ_k angle doesn't alter the scattering or momentum relaxation rate in any way. This is plotted in more detail in Figure 5.6 where the momentum relaxation rate has been plotted at three different θ_k angles

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showing the constant nature of the φ_k dependence. This is expected as the II is assumed to always lie on the same radial position as the carrier (at the origin) due to the assumption in the potential derivation that $\mathbf{R}_I = 0$.

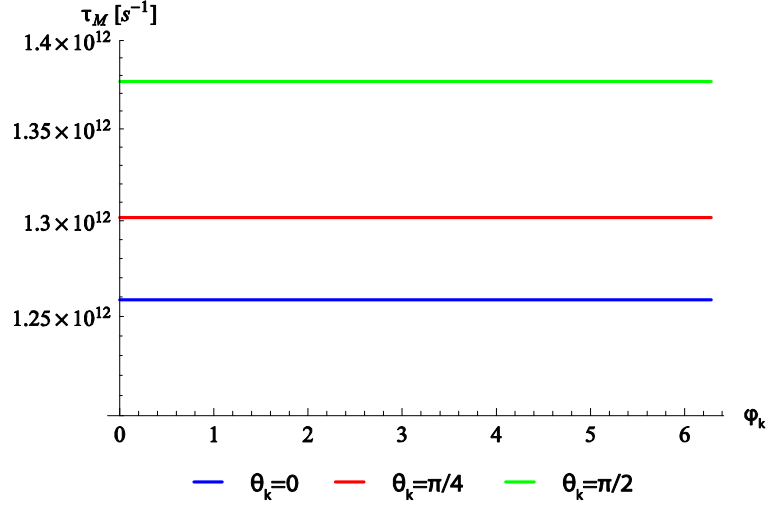


Figure 5.6: Momentum relaxation rate showing dependence on φ_k for incoming carrier dependent model at $n = N_I = 10^{17} \text{ cm}^{-3}$.

As mentioned previously the scattering model used in this work is simplified by removing the incoming angle dependence. As this work is to analyse the effect that remote screening has on device performance, the incoming angle dependence is considered to be unnecessary additional complexity. The simplification employed within this model is to assume that the incoming carrier is aligned with the Z-axis such that $\theta_k = 0$ which drastically reduces the momentum transfer wave-vector definitions. Using this simplification in equations (5.25)-(5.27) gives

$$\mathbf{q}_{\perp}^2 = \mathbf{k}'^2 \sin^2 \theta_{k'}, \quad (5.30)$$

$$q_z^2 = \mathbf{k}'^2 (1 - \cos \theta_{k'})^2 \quad (5.31)$$

$$\mathbf{q}^2 = \mathbf{q}_{\perp}^2 + q_z^2 = 2\mathbf{k}'^2 (1 - \cos \theta_{k'}) \quad (5.32)$$

It is important to state here that this assumption means that all scattering events assume that the carrier is aligned such that it is on the Z-axis. Although scattering events will occur that assume the wrong scattering potential, this simplification provides on average a good estimate of the overall scattering effect. A more detailed examination of the effect of the incoming carrier dependence is given below along with a comparison of the models to examine the quality of the

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simplification. For reference, the use of the Z-aligned (incoming carrier) simplification, for want of a better name, means that the momentum relaxation weighting term becomes

$$1 - \cos \theta_s = 1 - \cos \theta_k. \quad (5.33)$$

Below the incoming carrier dependent scattering model is examined for three different impurity concentrations with a corresponding comparison between the models. The impurity and screening concentrations are equal and the average carrier energy is calculated using equation (5.29) for the scattering & momentum relaxation rate plots.

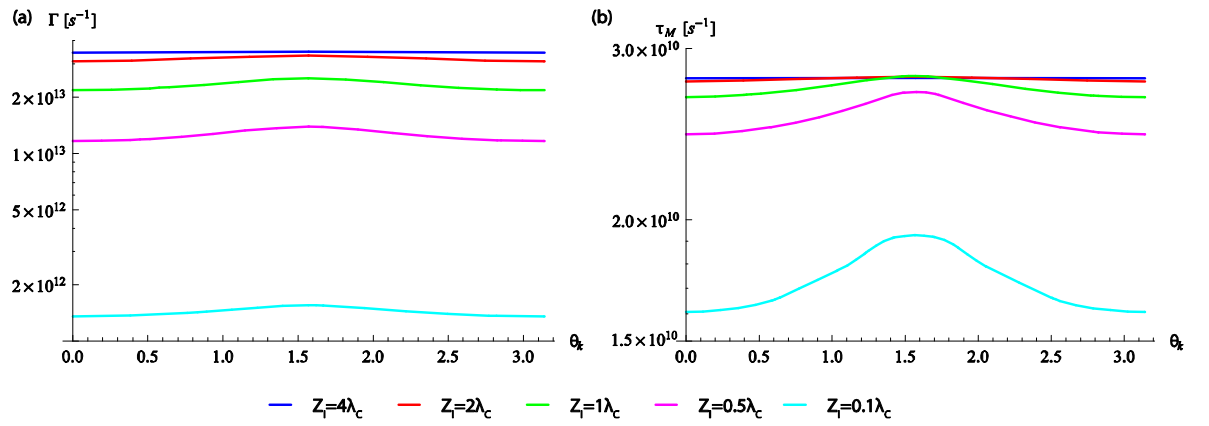


Figure 5.7: (a) Scattering and (b) momentum relaxation rates for an impurity concentration of $N_I = 10^{15} \text{ cm}^{-3}$ over a range of impurity positions for the incoming carrier dependent remote screening model.

Starting with Figure 5.7 by examining the incoming carrier dependence on the (a) scattering and (b) momentum relaxation rates for the lowest concentration of $n = N_I = 10^{15} \text{ cm}^{-3}$. Here the plots show the rates over a range of impurity positions and as expected, become smaller with decreasing distance from the source interface. Both plot (a) and (b) of this figure are plotted against the angle θ_k of the incoming carrier and show the large shift in the scattering model at $\theta_k = \pi/2$.

Figure 5.8 shows (a) the ratio of mobility and (b) the momentum relaxation rate ratio between the incoming angle dependent model and the Z-aligned model. Here the mobility is calculated from the momentum relaxation rate using the Kubo-Greenwood formula of equation (5.34) [33].

$$\mu = \frac{2e}{3n_0} \int_0^\infty dE \rho(E) E \tau_m(E) m_c(E)^{-1} \left(\frac{\partial f_0}{\partial E_F} \right) \quad (5.34)$$

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Here e is the electronic charge, n is the electron density, $\rho(E)$ is the density of states, $m_c(E)$ is the conductivity effective mass, f_0 is the equilibrium Fermi function and E_F is the Fermi energy. The electron density and the density of states can be written for non-parabolic bands as

$$n = 2 \left(\frac{m^* k_B T}{2\pi\hbar^2} \right)^{3/2} \left[\mathfrak{F}_{1/2}(\eta) + \frac{5}{2} \alpha k_B T \mathfrak{F}_{3/2}(\eta) \right] \text{ for } \eta = \frac{E_f}{k_B T} \quad (5.35)$$

$$\rho(E) = \frac{3(2m^*)^{3/2}}{\pi^2 \hbar^3} E^{1/2} \left(1 + \frac{5}{2} \alpha E \right) \quad (5.36)$$

In Figure 5.8, the data is arranged such that in plot (a) it is ratio of the Z-aligned model to the full incoming angle model and (b) the ratio of the complete model to the Z-aligned model. Therefore for values greater than one, the Z-aligned model is (a) over-estimating the mobility or (b) under-estimating the momentum relaxation rate of the full incoming carrier model. This is arranged such that the plots show similar behaviour to each other as the mobility calculation depends on the inverse of the momentum relaxation rate.

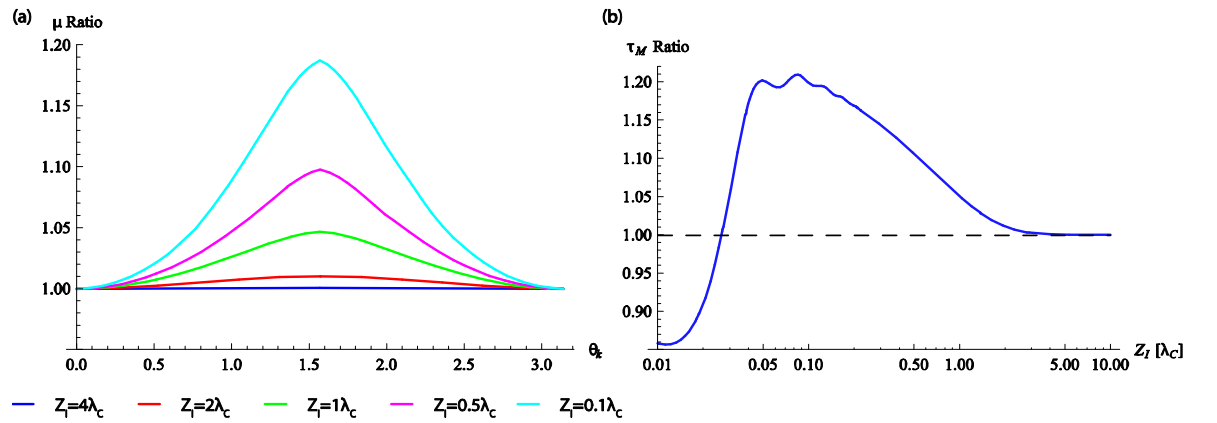


Figure 5.8: (a) Ratio of mobilities between the remote screening models over incoming carrier angle θ_k and (b) momentum relaxation ratios between models over impurity position.

Plot (a) of Figure 5.8 shows the mobility ratio over a range of impurity positions against the incoming carrier angle with the Z-axis, θ_k . For an impurity located at $Z_I = 4\lambda_c$ the mobility ratio is one at all incoming carrier angles which is expected as the remote screening nature at this distance is very small. As the impurity moves closer to the interface, the effect of the incoming carrier angle becomes much larger and the simplified Z-aligned model over-estimates the mobility by up to $\sim 20\%$.

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The behaviour of the mobility is shown in plot (b) of Figure 5.8. It should be noted that in this plot the momentum relaxation rate for the complete incoming carrier angle model is fixed at an angle of $\theta_k = \pi/2$, the alignment which yields the largest change from the Z-aligned model. This is the case for all the momentum relaxation ratio plots in this section, that is plots (b) of Figure 5.8, Figure 5.10 and Figure 5.12.

Plot (b) shows that the momentum relaxation time, the inverse of the momentum relaxation rate, is over-estimated by the Z-aligned model for $\sim 0.03\lambda_c < Z_I < 4\lambda_c$ with a peak at $Z_I = 0.1\lambda_c$, consistent with the mobility ratio. For values less than this the momentum relaxation rate is under-estimated. Although not shown in the mobility ratio plot for this density, this behaviour is repeated for the mobility. There also is some small oscillation in the momentum relaxation ratio around $Z_I = 0.1\lambda_c$.

This oscillating behaviour can be understood by examining the scattering matrix element of equation (5.8), specifically the remote screening coefficient within square brackets. Expanding the exponential terms of this coefficient into a power series and retaining only the first order terms gives

$$f_{sgl} = 2 \left(1 - k_c Z_I \sqrt{1 + \frac{q_z^2}{k_c^2}} \right) (1 - \cos(q_z Z_I)) \quad (5.37)$$

Plot (b) of Figure 5.8 shows that the oscillatory behaviour occurs for small $k_c Z_I$, which mean that the value of the term given by the first bracket of equation (5.37) will be close to one. As discussed earlier in this section, the q_z component has a minimum for an incoming carrier angle at $\theta_k = \pi/2$ which will lead to a smaller argument of the cosine function. Therefore, for incoming carrier angles close to perpendicular to the Z-axis (small q_z) and impurity positions close to the interface (small Z_I), the frequency of the cosine function will be greatly reduced. This will cause an increasingly oscillatory behaviour of the coefficient and scattering model, leading to the apparent *flip* from increased scattering to reduced scattering.

To obtain a quantitative measure of the quality of the simplification, an average of the mobility ratio has been taken over a range of impurity positions taking the worst incoming angle case for the complete model. This range of impurity positions, Z_I , is the complete range of positions where remote screening is effective. Using the mean value theorem for integrals, the following expression is used to obtain this average.

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$$\langle R_\mu \rangle = \frac{1}{10\lambda_c} \int_0^{10\lambda_c} dZ_I \frac{\mu_z}{\mu(\theta_k = \pi/2)} \quad (5.38)$$

where μ_z is the mobility of the Z-aligned model and $\mu(\theta_k)$ is the complete incoming angle mobility model. The upper limit of $10\lambda_c$ is chosen such that the remote screening effect is negligible, correct at this impurity distance from the interface. Evaluating equation (5.38) for the impurity density of $N_I = 10^{15} \text{ cm}^{-3}$ yields an average of 1.01325, or an over-estimation of 1.3% of the mobility over the range of impurity positions. Of course, this is for the worst-case scenario, assuming that all carriers scatter with $\theta_k = \pi/2$.

Continuing the examination of the Z-aligned simplification with a higher density of $n = N_I = 10^{17} \text{ cm}^{-3}$ in Figure 5.9 and Figure 5.10. In plots (a) and (b) we see the consistent reduction in scattering strength with decreasing Z_I . Also evident is the effect of the incoming angle on the scattering model with a shift near the $\theta_k = \pi/2$ point. Although at this higher density the change or *flip* in the scattering behaviour is clear in plot (b) for an impurity position of $Z_I = 0.1\lambda_c$.

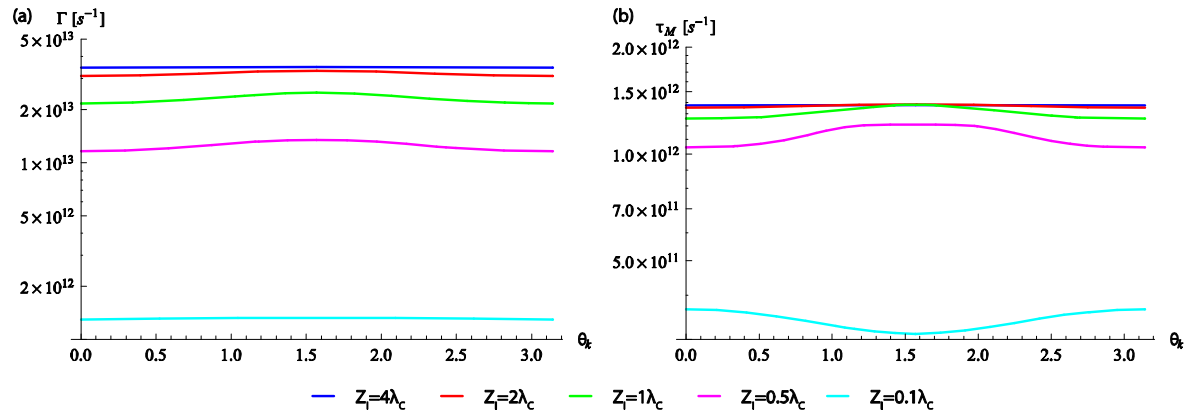


Figure 5.9: (a) Scattering and (b) momentum relaxation rates for an impurity concentration of $N_I = 10^{17} \text{ cm}^{-3}$ over a range of impurity positions for the incoming carrier dependent remote screening model.

In Figure 5.10 the (a) mobility ratio and (b) momentum relaxation ratios are plotted for this impurity concentration. The underestimation of the momentum relaxation at $Z_I = 0.1\lambda_c$ is very noticeable and is highlighted in the mobility ratio plot of Figure 5.10. The oscillatory behaviour of the scattering model is clear within plot (b) of Figure 5.10 when plotted over the range of impurity positions. For impurity positions greater than $Z_I \approx 0.3\lambda_c$ the mobility is over-estimated and for impurity positions closer to the interface the mobility is under-estimated. This change in behaviour

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occurs for electrons interacting with the II at angles perpendicular to the Z-axis where the magnitude of the scattering potential oscillates with the cosine function at small $k_c Z_I$.

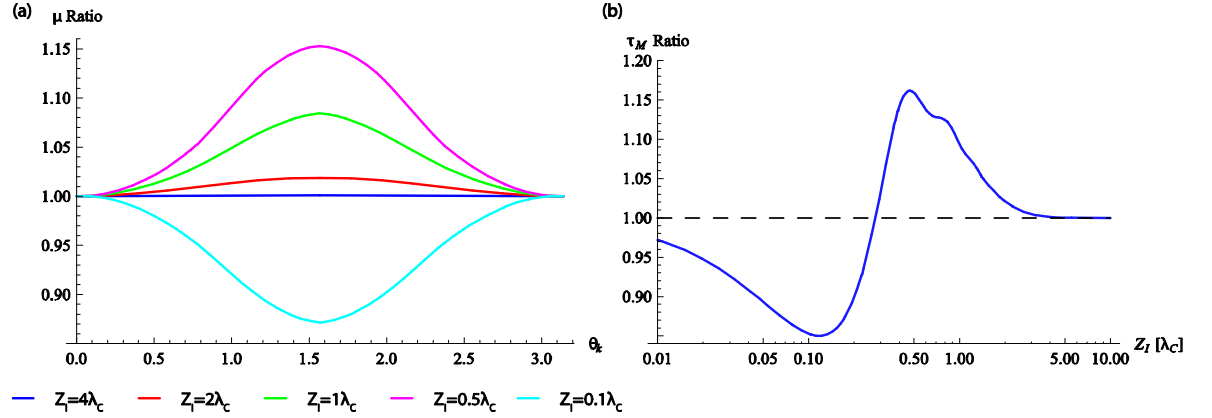


Figure 5.10: (a) Ratio of mobilities between the remote screening models over incoming carrier angle θ_k and (b) momentum relaxation ratios between models over impurity position.

At this impurity density of $n = N_I = 10^{17} \text{ cm}^{-3}$ the oscillatory behaviour is more compressed over the range of impurity positions, Z_I . Referring to the earlier discussion regarding the oscillatory behaviour, this compression in the fluctuation can be understood from the larger value of $k_c Z_I$. That is, the screening length will be smaller at higher concentrations leading to larger values of k_c and reduced oscillation. Completing the average mobility ratio using equation (5.38) yields an average overestimation of roughly 1.4% for this density.

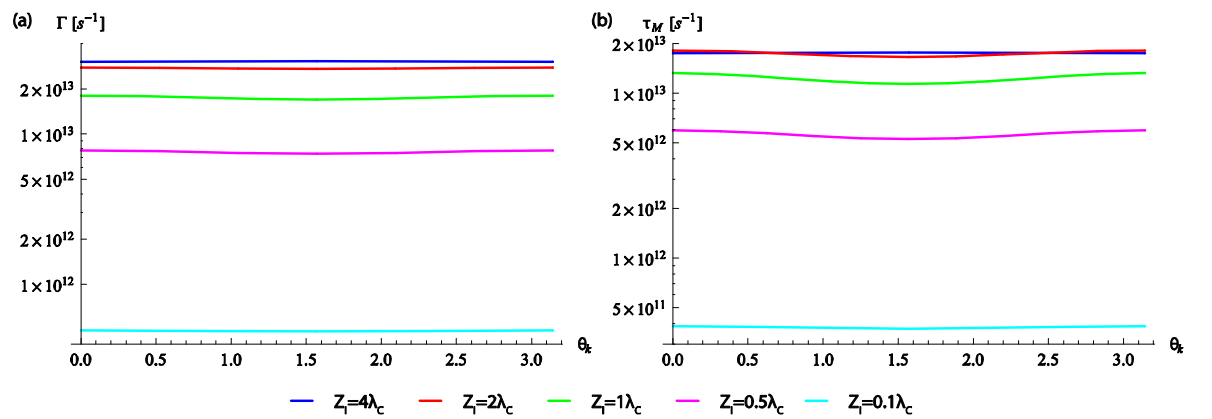


Figure 5.11: (a) Scattering and (b) momentum relaxation rates for an impurity concentration of $N_I = 10^{19} \text{ cm}^{-3}$ over a range of impurity positions for the incoming carrier dependent remote screening model.

Continuing the evaluation of the Z-aligned approximation at an impurity density of $n = N_I = 10^{19} \text{ cm}^{-3}$, the reduction in the oscillatory behaviour seems to be further enhanced with the

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increasing density. The scattering and momentum relaxation rates of Figure 5.11 don't show a significant shift with the incoming carrier angle.

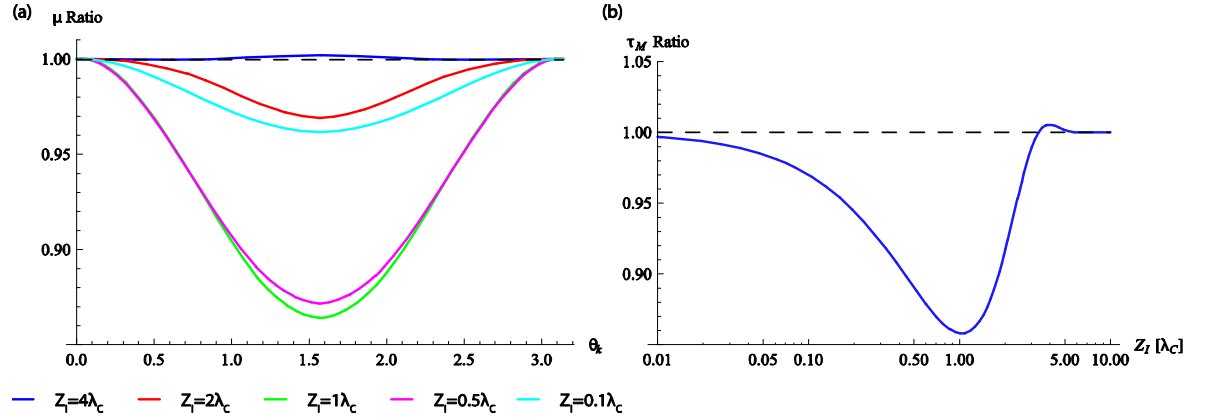


Figure 5.12: (a) Ratio of mobilities between the remote screening models over incoming carrier angle θ_k and (b) momentum relaxation ratios between models over impurity position.

The mobility ratio, plot (a) of Figure 5.12 shows a majority under-estimation of the mobility over the range of impurity positions plotted. Looking at the momentum relaxation rates of plot (b), there is a very small region of overestimation around $Z_l = 3 - 5\lambda_c$ and a large region of underestimation. It is clear that at this high impurity density the oscillations of the model are reduced in comparison to lower densities but lead to underestimation of the mobility. Completing the average mobility ratio from equation (5.38) for this density gives an average underestimation of around 2%.

In summary the alignment of the incoming carrier to the Z-axis reduces the complexity of the scattering model and preserves the remote screening effect. For remotely screened II scattering the average mobility using the Z-aligned model is within 1.5-2% of the complete model over the region that remote screening is effective.

5.2.3.1 Z-Aligned Model

Use of the Z-aligned momentum transfer wave-vectors of equations (5.30)-(5.32) in the scattering model allows the integral over the φ_k angles to be completed. As there is no longer a φ_k dependence, the integral over those angle can be completed to yield 2π . For reference, the Z-aligned scattering model equations can then be written as

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$$\sigma(\theta_{k'}) = \left(\frac{Ze^2}{4\pi\epsilon_{Si}\epsilon_0} \right)^2 \frac{2^3\pi m_d^2}{\hbar^4} (1+2\alpha E)^2 \frac{1}{(\mathbf{q}^2 + k_C^2)^2} \times \left[1 + \exp\left(-2Z_I\sqrt{\mathbf{q}_\perp^2 + k_C^2}\right) - 2\cos(q_Z Z_I)\exp\left(-Z_I\sqrt{\mathbf{q}_\perp^2 + k_C^2}\right) \right] \quad (5.39)$$

for the differential scattering cross section,

$$\Gamma(\mathbf{k}) = \left(\frac{Ze^2}{4\pi\epsilon_{Si}\epsilon_0} \right)^2 N_I \frac{2^3\pi m_d k^*}{\hbar^3} (1+2\alpha E) \int_0^\pi d\theta_{k'} \frac{\sin\theta_{k'}}{(\mathbf{q}^2 + k_C^2)^2} \times \left[1 + \exp\left(-2Z_I\sqrt{\mathbf{q}_\perp^2 + k_C^2}\right) - 2\cos(q_Z Z_I)\exp\left(-Z_I\sqrt{\mathbf{q}_\perp^2 + k_C^2}\right) \right] \quad (5.40)$$

for the total scattering rate and

$$\frac{1}{\tau_m(\mathbf{k})} = \left(\frac{Ze^2}{4\pi\epsilon_{Si}\epsilon_0} \right)^2 N_I \frac{2^3\pi m_d k^*}{\hbar^3} (1+2\alpha E) \int_0^\pi d\theta_{k'} \frac{\sin\theta_{k'}(1-\cos\theta_{k'})}{(\mathbf{q}^2 + k_C^2)^2} \times \left[1 + \exp\left(-2Z_I\sqrt{\mathbf{q}_\perp^2 + k_C^2}\right) - 2\cos(q_Z Z_I)\exp\left(-Z_I\sqrt{\mathbf{q}_\perp^2 + k_C^2}\right) \right] \quad (5.41)$$

for the momentum relaxation rate.

5.2.4 Analysis of Scattering Rate

Using the different methods of utilising the scattering probability the remotely screened impurity scattering process will now be analysed. Looking at the differential scattering cross-section given by equation (5.39) first, which is plotted in a set of polar plots over the scattering angle $\theta_{k'}$ in Figure 5.13. These plots are for two different screening densities at different carrier energies and impurity locations.

Plot (a) in the figure corresponds to a moderate screening density of approximately $n = 10^{17} \text{ cm}^{-3}$. At this screening density the differential cross-sectional scattering area is very large which will lead to large scattering rates. In the screening conditions of plot (a) it is clear to see that the scattering process favours forward scattering events. That is, events for which the electron scatters through angles of less than $\pi/2$. The differential scattering cross-section for scattering angles greater than $\pi/2$ or back-scattering, depicted by the negative component of the horizontal axis, is very small in comparison.

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At higher energies the tendency to forward scatter is increased as shown by the dotted lines in plot (a) of Figure 5.13. The back-scattering component is extremely small in this case and the range of angles for forward scattering is greatly decreased to a narrow range around zero degrees. From this behaviour it can be deduced that the scattering interaction has a lesser effect at higher carrier energies.

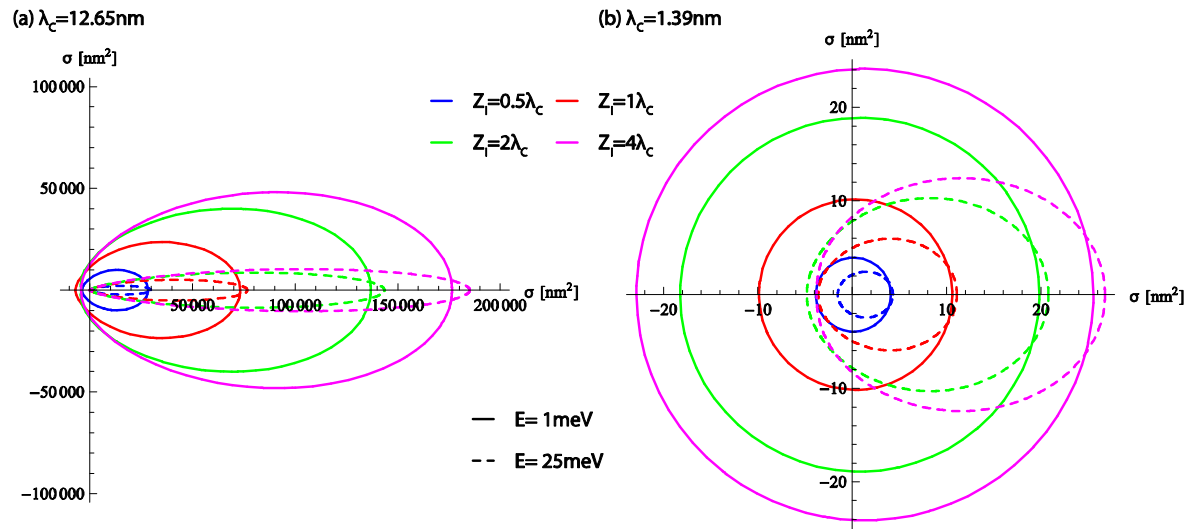


Figure 5.13: Polar plots of the differential scattering cross-section for an electron at low (solid lines) and high energy (dashed lines) at various impurity locations.

At the higher screening density of $n = 10^{19} \text{ cm}^{-3}$ plotted in (b), the differential scattering cross-section is considerably smaller. At low carrier energies the scattering cross-section in plot (b) has an almost isotropic nature with no particular scattering angle favoured. This suggests that impurity scattering will have a larger effect at this screening density and carrier energy due to the wide range of probable scattering angles. For higher carrier energies the scattering cross-section shifts towards a forward-angle scattering preference which is comparable with the situation at the lower screening density of plot (a).

This can be understood by examining the differential scattering cross section given by equation (5.39), in particular the terms involving an angular dependence. These angular dependent terms have been rewritten here as a separate function, f_θ ,

$$f_\theta = \frac{1}{\mathbf{q}^4 (1 + k_c^2 / \mathbf{q}^2)^2} \times \left[1 + \exp\left(-2q_\perp Z_I \sqrt{1 + k_c^2 / \mathbf{q}_\perp^2}\right) - 2 \cos(q_z Z_I) \exp\left(-q_\perp Z_I \sqrt{1 + k_c^2 / \mathbf{q}_\perp^2}\right) \right] \quad (5.42)$$

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where the momentum transfer wave-vectors are given by equations (5.30)-(5.32). This function highlights the relation between the screening density and the carrier energy given by the terms $(1 + k_C^2/\mathbf{q}^2)$ and $(1 + k_C^2/\mathbf{q}_\perp^2)$. When the screening density is large, the inverse screening length k_C is large and these terms are also very large ($\gg 1$) which causes the function f_θ to become very small and the scattering more anisotropic. Conversely when the screening density is low along with the inverse screening length, the terms are very small ($\ll 1$) and the function will lead to more isotropic scattering. This behaviour is of course dependent on carrier energy with higher carrier energies always leading to more anisotropic scattering.

With decreasing distance between the impurity and the source interface, Z_I , the scattering cross-section is reduced in both cases of Figure 5.13. As the remote screening interaction is expected to increase the screening of an impurity, as discussed in Chapter 4, the reduction in scattering cross-section is logical. The increased screening of the scattering impurity centre as it moves towards the interface clearly reduces the scattering cross-section and will lead to a reduction in the scattering rate.

Plots of the scattering and momentum relaxation rates, equations (5.40) and (5.41), for the same conditions in the above polar plots are given in Figure 5.14 and Figure 5.15. In both of the figures below the II concentration is taken to equal the screening density, that is $n = N_I$.

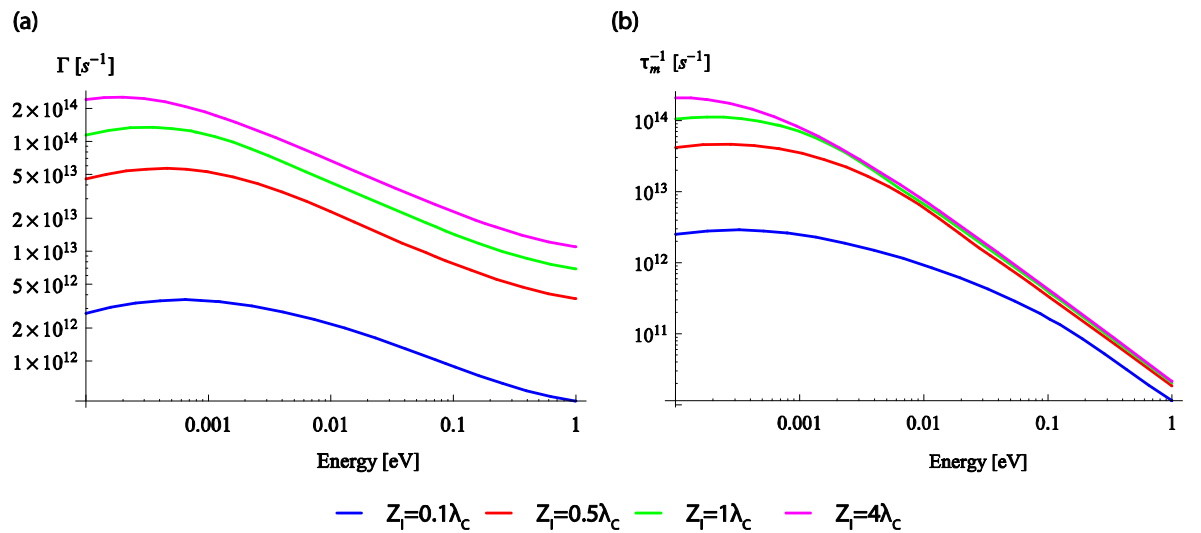


Figure 5.14: (a) Scattering and (b) momentum relaxation rates under the low screening conditions of $n = N_I = 10^{17} \text{ cm}^{-3}$ for various impurity locations.

As discussed above, the scattering differential cross-section is reduced with decreasing Z_I and becomes less effective at higher energies. This behaviour is clearly seen in the plots of Figure 5.14

5.2 Single Interface Scattering Model

which give the scattering rates (a) and momentum relaxation rates (b) for the lower concentration of $n = N_I = 10^{17} \text{ cm}^{-3}$. Figure 5.15 of the higher screening density $n = N_I = 10^{19} \text{ cm}^{-3}$ also shows this common behaviour which is expected for the remotely screened impurity scattering model.

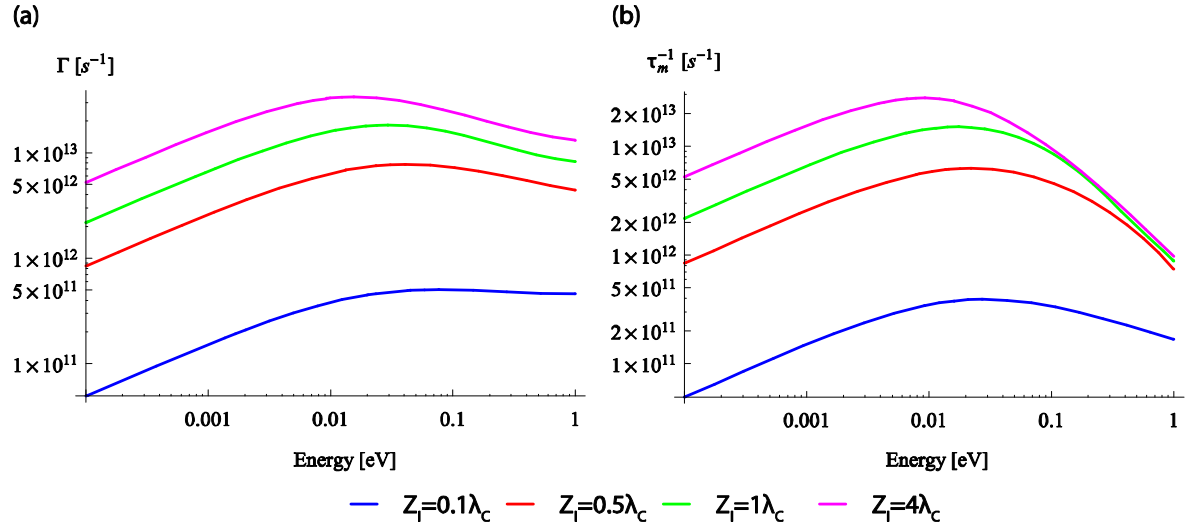


Figure 5.15: (a) Scattering and (b) momentum relaxation rates under the high screening conditions of $n = N_I = 10^{19} \text{ cm}^{-3}$ for various impurity locations.

Comparing the scattering rates between the two figures shows around an order of magnitude decrease at the higher concentration following the trend in the radius of the differential scattering cross-section.

In part (b) of Figure 5.14 the momentum relaxation rate for carriers greater than 10meV doesn't show much effect of remote-screening as the impurity position is varied between $Z_I = \{0.5..4\}\lambda_c$. Looking at the high energy polar plot of this case, plot (a) of Figure 5.13, the differential scattering cross-section varies dramatically in radius around scattering angles close to zero degrees.

This behaviour can be understood by looking at the momentum relaxation rate given by equation (5.41), particularly the weighting term, $(1 - \cos\theta_k)$. For small angle forward scattering this weighting term becomes very small and the momentum is relaxed on much longer scale. Therefore, in this case the scattering rate will be affected by the decreasing scattering cross-section radius but the momentum relaxation rate will show little change as the range of scattering angles remains close to zero.

Using the momentum relaxation rate of equation (5.41) the electron mobility can be analytically calculated providing more insight into the remote screening effect. Using the Kubo-Greenwood formula of equation (5.34) allows the electron mobility to be calculated. Here the ratio between the

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mobilities of the remotely screened model and the BH model are plotted to allow comparison. The BH model is found as the limit $Z_I \rightarrow \infty$ of the remotely screened model, given as equation (5.43). Noting of course, that the BH model is independent of Z_I .

$$\frac{1}{\tau_m(\mathbf{k})} = \left(\frac{Ze^2}{4\pi\epsilon_{Si}\epsilon_0} \right)^2 N_I \frac{2^3 \pi m_d k^*}{\hbar^3} (1 + 2\alpha E) \int_0^\pi d\theta_k \frac{\sin\theta(1 - \cos\theta_k)}{(\mathbf{q}^2 + k_c^2)^2} \quad (5.43)$$

In the figures below the ratio between the mobilities is given for different doping concentrations where the screening density is assumed to equal the doping concentration. In both figures the ratio is taken as the remotely screened mobility over the BH mobility.

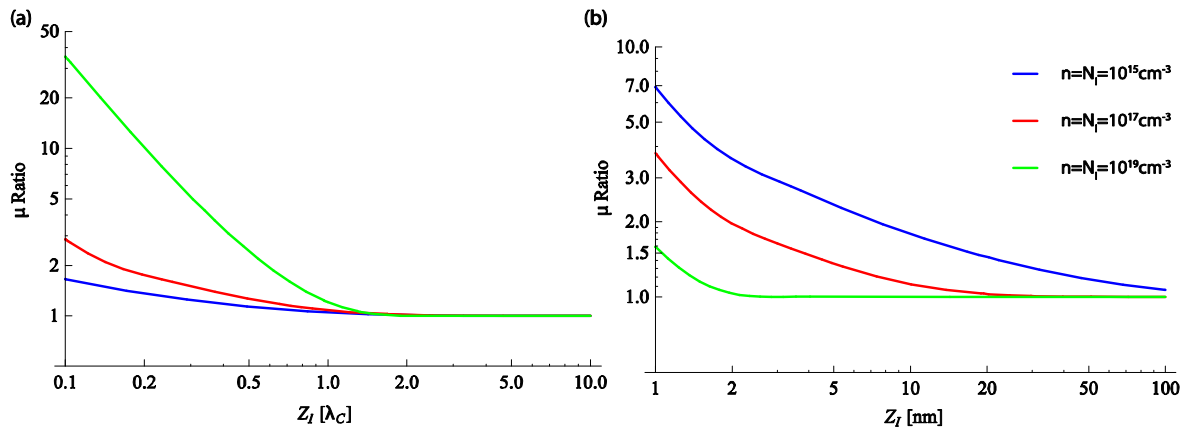


Figure 5.16: Ratio between the mobilities of the remotely screened and Brooks-Herring models. The impurity position from the source interface, Z_I , is given in (a) units of the respective channel screening length, λ_c , and (b) nanometres from the source interface.

In plot (a) of Figure 5.16 the ratio between the mobilities of the two models is plotted over the impurity distance from the source interface in units of the respective channel screening length. This follows the representation used in the plots of the differential scattering cross-section and the scattering/momentum relaxation rates. Plot (a) of Figure 5.16 shows that remote screening effect begins to strongly affect the impurity limited mobility at positions less than two screening lengths from the source interface. Beyond two screening lengths the remotely screened model is a close match with the BH model.

For impurity positions closer to the interface the remotely screened mobility increases heavily as the effect of polarisation charges becomes stronger. In particular, the mobility for the high channel density given by the green curve shows a dramatic increase to over 30x the BH mobility. This increase is very large and is a side-effect of the strong-screening limit. Using equation (3.36), the screening length for the screening/dopant concentration of $n = N_I = 10^{19} \text{ cm}^{-3}$ is $\lambda_c = 1.39 \text{ nm}$. As

5.3 Double Interface Scattering Model

discussed at the end of the previous chapter, the strongly screened model over-estimates the remote-screening effect for impurities located closer than 1nm from the source interface. Therefore at this density the point that the strongly screened model begins to overestimate the remote screening effect corresponds to $Z_I \approx 0.7\lambda_C$.

The figures in this section have all been plotted with a length scale normalised to the channel screening length which allows the scattering model to be analysed and compared over a wide range of screening densities and impurity concentrations as well as comparison with the previous figures in this section. Despite this, it is important here to also examine the mobility using a fixed length scale. In plot (b) of Figure 5.16 the mobility ratio between the remotely screened and BH model is given over a physical impurity distance from the source interface.

Using a physical length scale for each screening/background doping concentration in plot (b) of Figure 5.16 provides an example closer to a real scenario of the remote screening effect on the impurity limited mobility. This figure highlights the dependence of the channel screening density, where the lower the screening density the stronger the mobility increase due to remote screening. This plot does not follow the trend of Figure 5.16 which reports that the higher the screening density, the larger the remote screening effect. This reversal in behaviour between the figures can be understood from the screening length.

Using equation (3.36) the screening length can be found as $\lambda_C = \{126.27, 12.64, 1.39\} \text{ nm}$ for the screening densities of $n = \{10^{15}, 10^{17}, 10^{19}\} \text{ cm}^{-3}$ respectively. As discussed above, the remote screening effect starts to alter the mobility at roughly $Z_I = 2\lambda_C$. Therefore, at the highest screening density the remote screening effect will only alter impurities located within $\sim 2.8 \text{ nm}$ whereas at the lowest density we can expect a shift at distances up to $\sim 250 \text{ nm}$. For the lowest density involved at one nanometre from the interface, Z_I corresponds to roughly $8 \times 10^{-3} \lambda_C$ which leads to a large increase in the mobility of plot (b).

5.3 Double Interface Scattering Model

The double interface scattering model is found using an identical procedure to the single interface model. A scattering rate is defined using Fermi's Golden Rule approach based on the strongly screened impurity potential found for this model in the last chapter. The scattering potential is again not spherically symmetric and the Z-aligned incoming carrier simplification is applied.

5.3 Double Interface Scattering Model

This section will start with the calculation of the scattering matrix element in section 5.3.1. Following this the differential scattering cross-section, total scattering rate and the momentum relaxation rate will be obtained in section 5.3.2. The incoming carrier Z-alignment simplification is discussed in section 5.3.3 and finally the double interface remotely screened scattering model will be analysed in section 5.3.4.

5.3.1 Scattering Matrix Element

The strongly screened double interface potential found in section 4.3 is used to calculate the scattering matrix element for this model. The potential for the double interface remotely screened impurity potential is valid only in the channel region, that is the region of $0 < Z < L_C$. The calculation for the scattering matrix element must be integrated over this region only. Correcting the Z-space integral of equation (5.2) gives the following form for the scattering matrix element

$$\mathbf{H}_{\mathbf{k}'\mathbf{k}} = \frac{1}{\Omega} \int_0^{L_C} dZ \int_0^{2\pi} d\phi \int_0^{\infty} d\mathbf{R} eV(\mathbf{R}, Z) \exp(-i\mathbf{q}_{\perp} \cdot \mathbf{R}) \exp(-iq_Z Z) \quad (5.44)$$

Substituting the scattering potential into the matrix element definition and completing the integrals gives, after some lengthy manipulation

$$\begin{aligned} \mathbf{H}_{\mathbf{k}'\mathbf{k}} = & \frac{eQ}{4\pi\epsilon_{si}\epsilon_0} \frac{2\pi}{\Omega} \frac{1}{K_C^2} \left\{ 2\exp(-iq_Z Z_I) - \exp(-Z_I K_C) \left(1 + \frac{iq_Z}{K_C} \right) \right. \\ & - \exp(-iq_Z L_C) \exp((Z_I - L_C)K_C) \left(1 - \frac{iq_Z}{K_C} \right) \\ & - \exp(-Z_I K_C) (1 - \exp(-iq_Z L_C) \exp(-L_C K_C)) \left(1 - \frac{iq_Z}{K_C} \right) A_m \\ & \left. - \exp(-Z_I K_C) (\exp(-iq_Z L_C) \exp(L_C K_C) - 1) \left(1 + \frac{iq_Z}{K_C} \right) A_n \right\} \end{aligned} \quad (5.45)$$

Here the coefficients A_m and A_n are given by the equations (5.46)-(5.47) below and the terms K_C, K_S and K_D are defined in equation (5.48).

$$A_m = \frac{\exp(2L_C K_C) - \exp(2Z_I K_C)}{\exp(2L_C K_C) - 1} \quad (5.46)$$

5.3 Double Interface Scattering Model

$$A_n = \frac{\exp(2Z_I K_C) - 1}{\exp(2L_C K_C) - 1} \quad (5.47)$$

$$K_C = \sqrt{\mathbf{q}_\perp^2 + k_C^2}; \quad K_S = \sqrt{\mathbf{q}_\perp^2 + k_S^2}; \quad K_D = \sqrt{\mathbf{q}_\perp^2 + k_D^2} \quad (5.48)$$

Taking the term for the scattering matrix element, $\mathbf{H}_{\mathbf{k}'\mathbf{k}}$, of equation (5.45) and completing the square of the magnitude to obtain

$$|\mathbf{H}_{\mathbf{k}'\mathbf{k}}|^2 = \left(\frac{eQ}{4\pi\epsilon_{Si}\epsilon_0} \right)^2 \frac{1}{\Omega^2} \left(\frac{4\pi}{\mathbf{q}_\perp^2 + q_z^2 + k_C^2} \right)^2 f_{dbl}(k_C, Z_I, L_C) \quad (5.49)$$

Here a new function defining the interaction with the source and drain regions, f_{dbl} , has been introduced and is given as

$$f_{dbl}(k_C, Z_I, L_C) = \frac{\exp(-2(L_C + Z_I)K_C)}{(\exp(2L_C K_C) - 1)^2} \left[\left(E_C - E_S \cos(q_z Z_I) - E_D \cos(q_z L_C) \right)^2 - \left(E_S \sin(q_z Z_I) + E_D \sin(q_z L_C) \right)^2 \right] \quad (5.50)$$

New coefficients have been formed to simplify this expression and are given by equations (5.51)-(5.53) below.

$$E_C = \exp((L_C + 2Z_I)K_C) (\exp(2(L_C - Z_I)K_C) - 1) \quad (5.51)$$

$$E_S = \exp((L_C + Z_I)K_C) (\exp(2L_C K_C) - 1) \quad (5.52)$$

$$E_D = \exp(2L_C K_C) (1 - \exp(2Z_I K_C)) \quad (5.53)$$

5.3.2 Scattering Rate

The double interface remotely screened impurity scattering model can now be developed using the scattering matrix element found in the previous section. The probability of scattering can be found using Fermi's Golden rule, substituting in the scattering matrix element gives

5.3 Double Interface Scattering Model

$$P(\mathbf{k}, \mathbf{k}') = \frac{2\pi}{\hbar} \left(\frac{eQ}{4\pi\epsilon_{Si}\epsilon_0} \right)^2 \frac{1}{\Omega^2} \left(\frac{4\pi}{\mathbf{q}_\perp^2 + q_z^2 + k_C^2} \right)^2 f_{dbl}(k_C, Z_I, L_C) \delta(E(\mathbf{k}') - E(\mathbf{k})) \quad (5.54)$$

The differential scattering cross-section can be calculated from this probability using equation (5.11) and defining the impurity charge to be $Q = Ze$, the number of unit charges of the impurity multiplied by the electronic charge.

$$\sigma = \left(\frac{Ze^2}{4\pi\epsilon_{Si}\epsilon_0} \right)^2 \frac{2^2 m_d^2}{\hbar^4} (1 + 2\alpha E)^2 \frac{1}{(\mathbf{q}^2 + k_C^2)^2} f_{dbl}(k_C, Z_I, L_C) \quad (5.55)$$

Substituting the scattering probability defined in equation (5.54) into the total scattering rate, equation (5.14) and completing the k' integral gives

$$\Gamma(\mathbf{k}) = \left(\frac{Ze^2}{4\pi\epsilon_{Si}\epsilon_0} \right)^2 N_I \frac{2^2 m_d k^*}{\hbar^3} (1 + 2\alpha E)^2 \int_0^{2\pi} d\varphi_{k'} \int_0^\pi d\theta_{k'} \frac{\sin \theta_{k'}}{(\mathbf{q}^2 + k_C^2)^2} f_{dbl}(k_C, Z_I, L_C) \quad (5.56)$$

Similar to the single interface model, the final integrals over the $\theta_{k'}$ and $\varphi_{k'}$ components will be discussed in the following section. The momentum relaxation rate for the scattering process can be simply defined by inserting the weighting term for the change in momentum into the theta integral of equation (5.56), yielding

$$\frac{1}{\tau_m(\mathbf{k})} = \left(\frac{Ze^2}{4\pi\epsilon_{Si}\epsilon_0} \right)^2 \frac{N_I 2^2 m_d k^*}{\hbar^3} (1 + 2\alpha E) \times \int_0^{2\pi} d\varphi_{k'} \int_0^\pi d\theta_{k'} \frac{\sin \theta_{k'} (1 - \cos \theta_s)}{(\mathbf{q}^2 + k_C^2)^2} f_{dbl}(k_C, Z_I, L_C) \quad (5.57)$$

5.3.3 Scattering Reference Frame

The double interface model will also employ the simplified scattering reference frame in an approach identical to that used with the single interface remote screening model. That is the incoming carrier will be aligned with the Z-axis of the scattering reference frame reducing the angular dependency of the scattering model. Following a similar analysis to that of section 5.2.3, this simplification will be tested for the double interface scattering model.

5.3 Double Interface Scattering Model

The fixed scattering reference frame given by Figure 5.1 and Figure 5.2 remains unchanged for the double interface model. The momentum transfer wave vector relations presented in section 5.2.3 for the full incoming carrier case, equations (5.25)-(5.27), and the Z-aligned simplified relations given by equations (5.30)-(5.32) are again used.

The scattering rate, momentum relaxation rate and the mobility analysis are completed for three impurity concentrations, $N_I = \{10^{14}, 10^{16}, 10^{18}\} \text{ cm}^{-3}$. Again as the potential assumes that the impurity is located at the origin of the radial axis, $R_I = 0$, there is rotational symmetry around the Z axis, the ϕ_k angle. The scattering and momentum relaxation rate plots assume an incoming carrier with average thermal energy given by equation (5.29) and the mobilities are calculated using the Kubo-Greenwood method of equation (5.34). To analyse the double interface model effectively the channel length, L_C , is varied with the impurity position located at exactly half the channel length, $Z_I = 0.5L_C$, in each of the cases below.

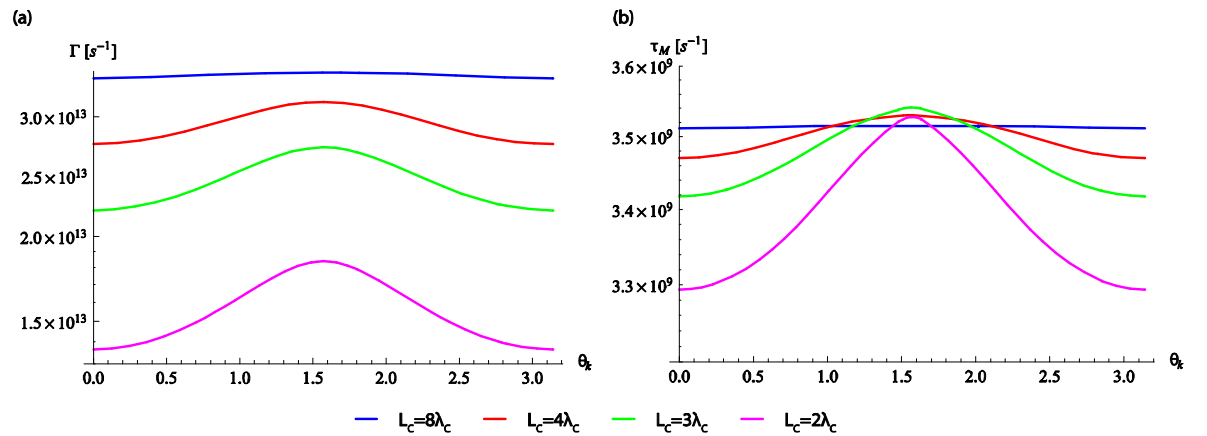


Figure 5.17: (a) Scattering and (b) momentum relaxation rates for an impurity concentration of $N_I = 10^{14} \text{ cm}^{-3}$ over a range of channel lengths for the incoming carrier dependent, remote screening model.

Starting with the lowest concentration of $N_I = 10^{14} \text{ cm}^{-3}$ in Figure 5.17 and Figure 5.18, the incoming carrier model clearly shows an increased scattering effect for carrier angles around $\theta_k = \pi/2$. This is very much consistent with the single interface model and can be again related to the momentum transfer in the Z-axis given by q_Z . For incoming carrier angles close to perpendicular to the Z axis there will be minimal momentum transfer in the Z plane and the q_Z component will become very small. Looking at the double interface coefficient in the scattering matrix element, equation (5.50), for small values of this momentum transfer component the coefficient will be large and hence the scattering will be increased.

5.3 Double Interface Scattering Model

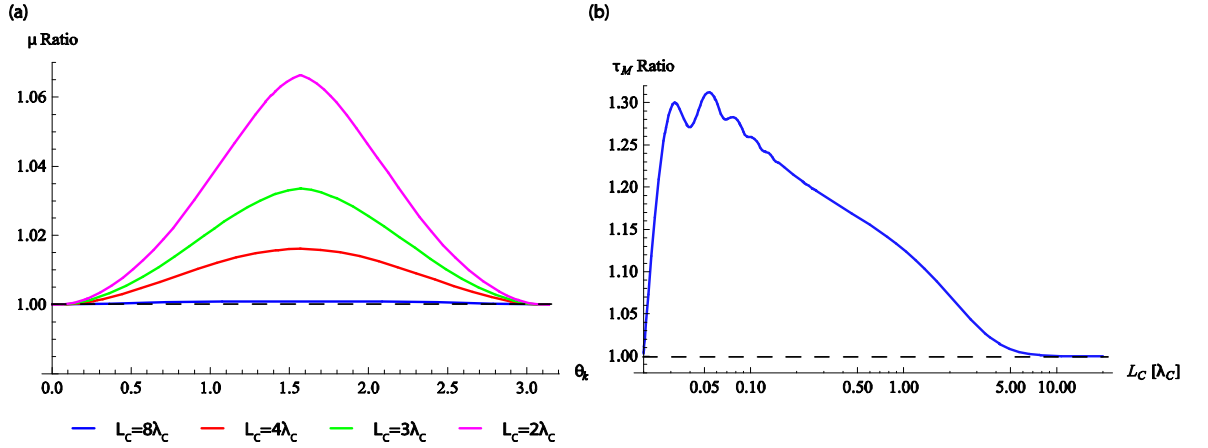


Figure 5.18: (a) Ratio of mobilities between the remote screening models over incoming carrier angle θ_k and (b) momentum relaxation ratios between models over channel length.

At this low density the simplified model overestimates the momentum relaxation over a wide range of channel lengths as shown in plot (b) of Figure 5.18. Completing an average over a wide range of channel lengths using the mean-value theorem for integrals given by equation (5.58) below, yields an average overestimation of around 1.8%.

$$\langle R_\mu \rangle = \frac{1}{(20\lambda_c - 10^{-5}\lambda_c)} \int_{10^{-5}\lambda_c}^{20\lambda_c} dL_c \frac{\mu_z}{\mu(\theta_k = \pi/2)} \quad (5.58)$$

For the double interface model it is not possible to complete the average value from an effective channel length of zero and instead a value of $10^{-5}\lambda_c$ is chosen as a non-zero channel length. The upper limit of $20\lambda_c$ coincides with the upper limit of the single interface case (given by equation (5.38)), allowing $10\lambda_c$ from each interface.

5.3 Double Interface Scattering Model

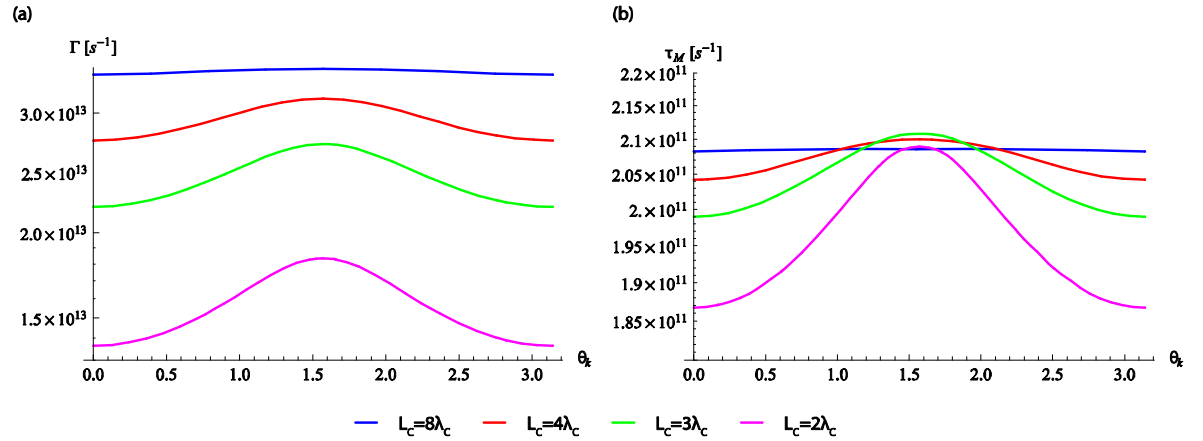


Figure 5.19: (a) Scattering and (b) momentum relaxation rates for an impurity concentration of $N_I = 10^{16} \text{ cm}^{-3}$ over a range of channel lengths for the incoming carrier dependent, remote screening model.

Examination of the intermediate impurity density of $N_I = 10^{16} \text{ cm}^{-3}$ in Figure 5.19 and Figure 5.20 shows that the simplified model overestimates the scattering for channel lengths greater than $L_c \approx 0.2\lambda_c$. At this density the momentum relaxation ratios plotted in part (b) of Figure 5.20 also demonstrate that underestimation occurs at small channel lengths. Completing the average mobility ratio using equation (5.58) for this density yields an average overestimation of around 2.4%.

The momentum relaxation ratio oscillates very much like the single interface model discussed in section 5.2.3 and shows the increased compression of this oscillation at higher screening concentration. Whereas in the single interface model the scattering matrix element has a single cosine function, here the double interface scattering matrix element coefficient, equation (5.50), has a set of cosine and sine functions all dependent on the Z directed momentum transfer, q_z .

5.3 Double Interface Scattering Model

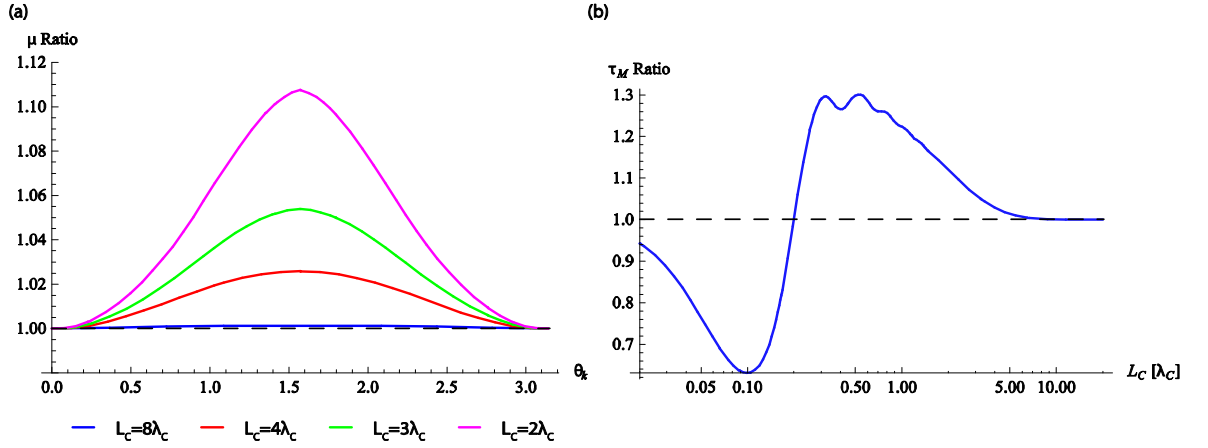


Figure 5.20: (a) Ratio of mobilities between the remote screening models over incoming carrier angle θ_k and (b) momentum relaxation ratios between models over channel length.

At the highest impurity concentration given by Figure 5.21 and Figure 5.22 the behaviour of the remotely screened double interface model differs to the behaviour seen this far. The scattering rate and momentum relaxation rate plots at a channel length of $L_C = 2\lambda_c$ show a double oscillation. This double oscillation has peaks at $\theta_k = \pi/4, 3\pi/4$ and a trough at $\theta_k = \pi/2$ for the momentum relaxation rate of plot (b) in Figure 5.21 with a much less understated double oscillation around the $\theta_k = \pi/2$ point in both the scattering rate and mobility ratio.

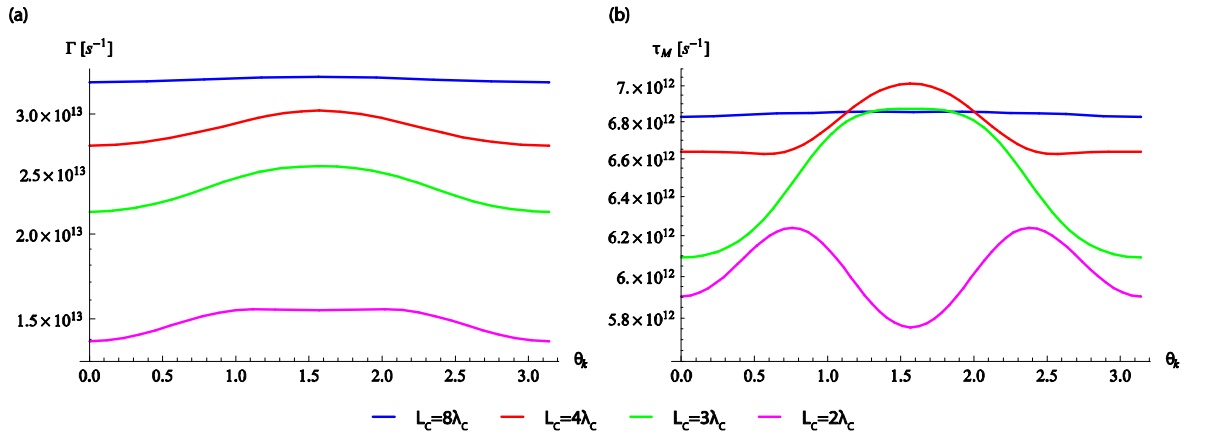


Figure 5.21: (a) Scattering and (b) momentum relaxation rates for an impurity concentration of $N_I = 10^{18} \text{ cm}^{-3}$ over a range of channel lengths for the incoming carrier dependent, remote screening model.

This double oscillation at small channel lengths is very much an effect brought on by the set of cosine and sine functions in the scattering matrix element. Examining the f_{dbl} coefficient of the scattering matrix element of equation (5.50), the cosine and sine functions both depend on the Z-directed momentum transfer q_z and either the impurity position, Z_I , or channel length, L_C .

5.3 Double Interface Scattering Model

As has been discussed previously the q_z component will tend to zero as the incoming carrier angle is close to perpendicular to the Z axis. This reduces the frequency of these angular functions which lead to the oscillatory behaviour. Here the angular functions will have two separate frequencies depending on the impurity position and channel length as q_z is reduced. In the cases plotted here the impurity position is taken to be always half the channel length, that is $Z_I = 0.5L_C$, but it will always be the case that $Z_I < L_C$.

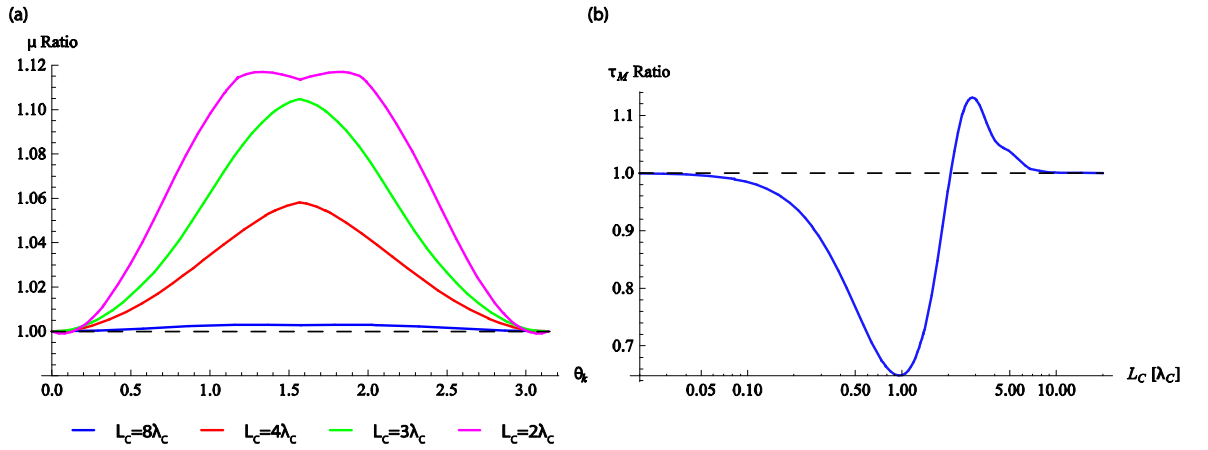


Figure 5.22: (a) Ratio of mobilities between the remote screening models over incoming carrier angle θ_k and (b) momentum relaxation ratios between models over channel length.

It can be seen that although this has a considerable effect on the momentum relaxation rate, the effect on the mobility is relatively minimised. This of course is due to the fact that the momentum relaxation rate is integrated over all energy in the mobility calculation. For this higher density the average mobility ratio is calculated to give an average underestimation of around 1%.

5.3.3.1 Z-Aligned Model

Using the Z-aligned momentum transfer wave-vector relations of equations (5.30)-(5.32) allows the integral over the angle $\phi_{k'}$ to be completed and yields the following final expressions for the double interface remotely screened scattering model.

$$\sigma = \left(\frac{Ze^2}{4\pi\epsilon_{Si}\epsilon_0} \right)^2 \frac{2^3\pi m_d^2}{\hbar^4} (1+2\alpha E)^2 \frac{1}{(\mathbf{q}^2 + k_C^2)^2} f_{dbl}(k_C, Z_I, L_C) \quad (5.59)$$

$$\Gamma(\mathbf{k}) = \left(\frac{Ze^2}{4\pi\epsilon_{Si}\epsilon_0} \right)^2 N_I \frac{2^3\pi m_d k^*}{\hbar^3} (1+2\alpha E) \int_0^\pi d\theta_{k'} \frac{\sin\theta_{k'}}{(\mathbf{q}^2 + k_C^2)^2} f_{dbl}(k_C, Z_I, L_C) \quad (5.60)$$

5.3 Double Interface Scattering Model

$$\frac{1}{\tau_m(\mathbf{k})} = \left(\frac{Ze^2}{4\pi\epsilon_{si}\epsilon_0} \right)^2 \frac{N_I 2^3 \pi m_d k^*}{\hbar^3} (1 + 2\alpha E) \times \int_0^\pi d\theta_{k'} \frac{\sin\theta_{k'} (1 - \cos\theta_s)}{(\mathbf{q}^2 + k_C^2)^2} f_{dbl}(k_C, Z_I, L_C) \quad (5.61)$$

5.3.4 Analysis of Scattering Rate

An analysis of the scattering model defined in section 5.3.2 will now be completed in a similar format to that completed for the single interface model. Here, the analysis of the double interface model will be centred around the effect that a small channel length has on the remotely screened impurity scattering model.

Starting with the differential scattering cross-section which has been plotted in Figure 5.23. For these plots the screening density is taken as (a) $n = N_I = 10^{16} \text{ cm}^{-3}$ and (b) $n = N_I = 10^{18} \text{ cm}^{-3}$ which leads to screening lengths of $\lambda_C = 39.95 \text{ nm}$ and $\lambda_C = 4.04 \text{ nm}$ respectively.

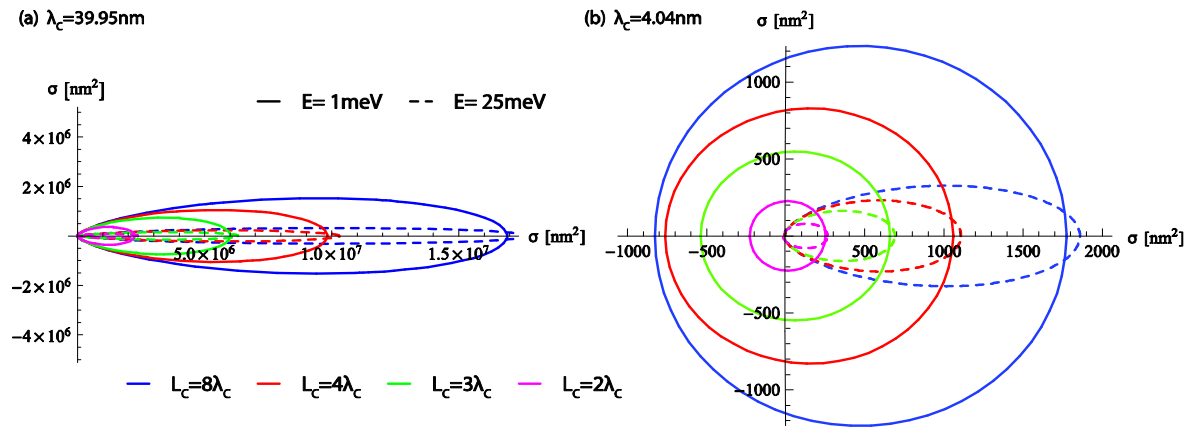


Figure 5.23: Polar plots of the double interface scattering cross-section for varying channel lengths with a single impurity located mid-channel, $Z_I = 0.5L_C$.

Similar to the behaviour of the single interface model, the low screening density differential scattering cross-section demonstrates mostly low-angle forward scattering. At high energies the differential scattering cross-section for this low density is restricted to a very small range of scattering angles around zero degrees. The momentum relaxing effect of such small scattering angles will be minimal.

The differential scattering cross-section for the low screening density, plot (a) of Figure 5.23 has an extremely large radius. As the channel length decreases, the remote screening effect reduces this radius and will reduce the scattering rate. The high screening density differential scattering cross-

5.3 Double Interface Scattering Model

section of plot (b) is somewhat more isotropic for low energy carriers than the low density plots. Plotted in Figure 5.25 are the scattering and momentum relaxation rates for the double interface remotely-screened impurity model with the low screening density conditions of the polar plots given above.

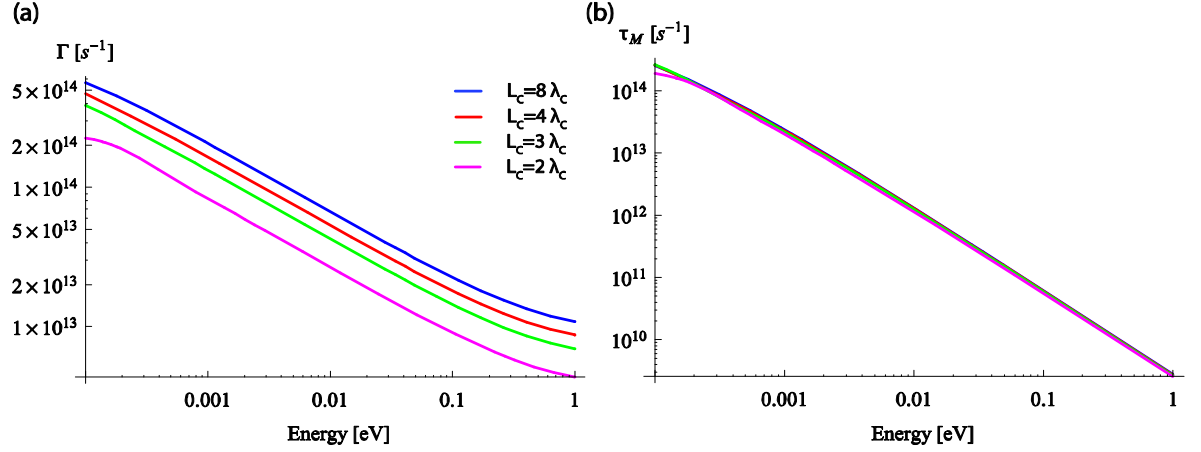


Figure 5.24: (a) Scattering and (b) momentum relaxation rates under the low screening conditions of $n = N_I = 10^{16} \text{ cm}^{-3}$ over a range of channel lengths with a single impurity located mid-channel, $Z_I = 0.5L_C$.

As the differential scattering cross section predicted, the scattering rate does decrease with the reducing distance between the source and drain interfaces but the momentum relaxation rate is largely unaffected. Plot (b) of Figure 5.24 shows a small difference between the different channel lengths at the very low energies around 0.1 meV which will have negligible effect in room temperature silicon. Nearly all the scattering at this low screening density is small angle forward scattering as seen by plot (a) of Figure 5.23, which is not altered by increasing the remote screening induced by the source and drain. Despite the small angle forward scattering, the momentum relaxation rate is high for low energy carriers but drops off very rapidly with energy.

5.3 Double Interface Scattering Model

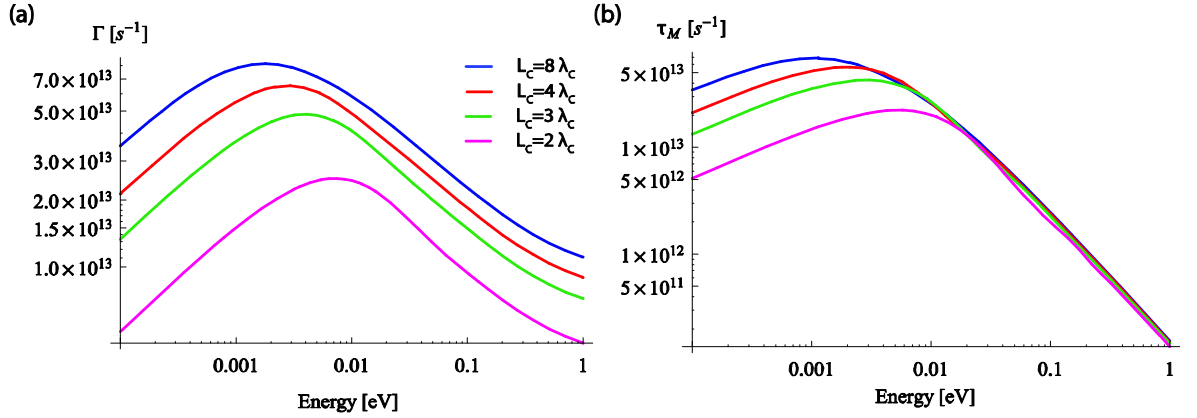


Figure 5.25: (a) Scattering and (b) momentum relaxation rates under the high screening conditions of $n = N_I = 10^{18} \text{ cm}^{-3}$ for varying channel lengths with a single impurity located mid-channel, $Z_I = 0.5L_c$.

Figure 5.25 shows (a) the scattering and (b) the momentum relaxation rates for the higher density. The scattering rate is clearly affected by the reduction in channel length as is the momentum relaxation rate for low energy carriers. Above approximately 20 meV the momentum relaxation rates becomes largely unaffected by the increase in the remote screening effect as the tendency to small angle scattering becomes more dominant.

The Kubo-Greenwood formula of equation (5.34) is used to plot a comparison of the double interface remotely screened impurity mobility against the BH model of equation (5.43). The BH model being the limit of $Z_I \gg 0$ and $L_c \rightarrow \infty$ of the double interface model. In plot (a) of Figure 5.26 the ratio of the remotely screened mobility to the BH mobility is given over a range of channel lengths which have been normalised to the respective channel screening lengths. For the three densities plotted here, $n = N_I = 10^{14} \text{ cm}^{-3}, 10^{16} \text{ cm}^{-3}, 10^{18} \text{ cm}^{-3}$, the screening lengths are calculated as $\lambda_c = 399.54 \text{ nm}, 39.95 \text{ nm}, 4.04 \text{ nm}$ respectively.

5.4 Sub-Threshold Impurity Scattering

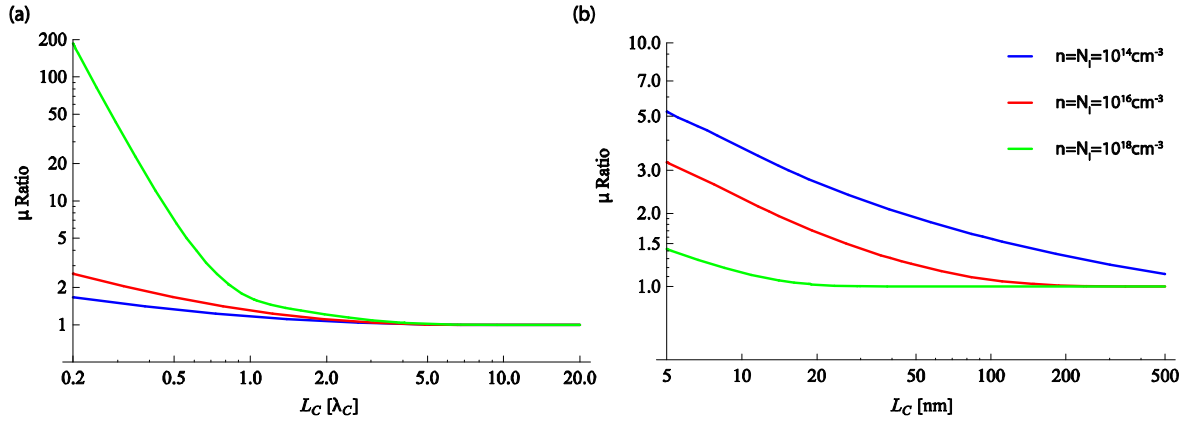


Figure 5.26: Ratio between the mobilities of the remotely screened and Brooks-Herring models. The channel length, L_C , is given in units of (a) the respective channel screening length, λ_C , and (b) nanometres where the impurity is always positioned at $Z_I = 0.5L_C$.

Plot (a) of Figure 5.26 clearly shows that beyond $L_C = 5\lambda_C$ the double interface remote screening has little effect on the impurity limited mobility. This plot also shows a large increase in the mobility at a channel lengths less than λ_C for the highest doped case represented by the green curve. This large increase in mobility is likely due to the strongly screened model over estimating the effect of remote screening and a quick calculation shows that at this point the impurity is located around $Z_I = 2nm$. It is around this distance that the strongly screened model is expected to overestimate the effect, as discussed in the previous chapter.

Plot (b) of Figure 5.26 gives the mobility comparison using a fixed reference for the channel length at each density. This figure highlights the strength of the interaction for low screening density channels where the screening length is extremely long. For the lowest density, given by the blue curve, the screening length is almost $400nm$ which for the remote screening interaction to dissipate, would require a channel length of $5\lambda_C \approx 2\mu m$.

5.4 Sub-Threshold Impurity Scattering

It is well known that scattering rates that are based on the Coulomb potential can diverge unless they are well bounded. In the BH approach the Coulomb potential is screened by the mobile charge density which generally provides a good bound on the Coulomb potential. There are other approaches which use half the average inter-ion distance to confine the effect of Coulomb scattering such as the CW model and Ridley's Third-Body Exclusion (TBE) technique [47, 55]. These models are discussed in detail in the literature review of II scattering in Chapter 2.

5.4 Sub-Threshold Impurity Scattering

The remotely screened impurity scattering model that has been developed in this chapter follows a similar approach to that of BH in that it uses the mobile charge density to restrict the range of scattering. This approach works well when the mobile charge or screening density is greater than or equal to the II density. Under certain conditions such as a MOS capacitor or a MOSFET device at low gate bias, the screening density can be much lower than the fixed charge density and can approach intrinsic silicon carrier densities. At such low carrier concentrations the scattering rates for the BH approach, and similarly the remote screening model, will tend to very high values.

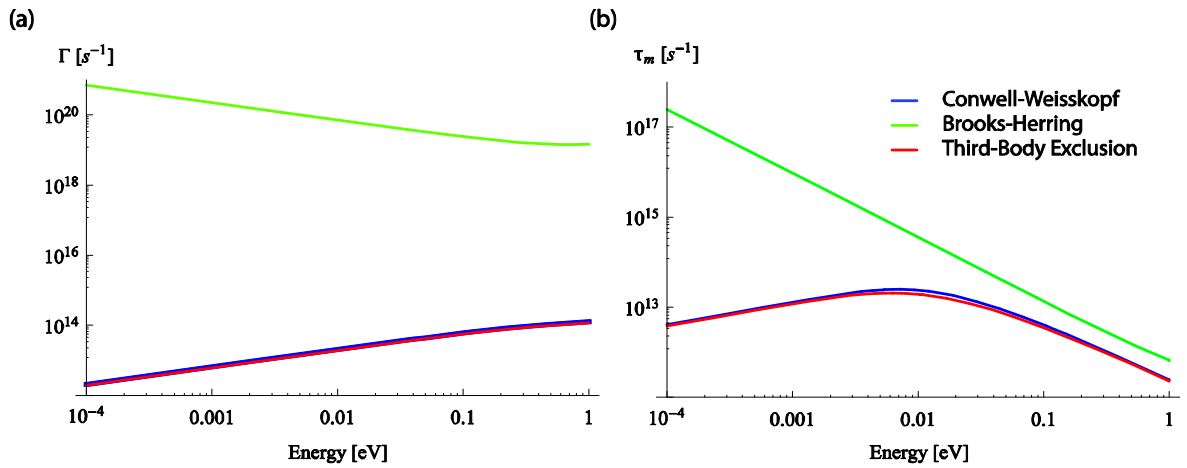


Figure 5.27: Plots of (a) the scattering rates and (b) the momentum relaxation rates for standard II scattering models at sub-threshold conditions with $N_I = 10^{18} \text{ cm}^{-3}$ and $n = 10^{12} \text{ cm}^{-3}$.

The three aforementioned II scattering models (CW, BH and TBE) are plotted in Figure 5.27 with high background impurity density and a low screening density, a typical sub-threshold case. In these plots the difference between using the the CW and TBE approaches of the inter-ion separation distance as a cut-off and using the BH approach of screening by mobile charge is clear to see. Plot (a) of this figure shows that with very low screening densities the BH model begins to diverge and results in a scattering rate of roughly $\Gamma_{BH} \approx 10^{20} \text{ s}^{-1}$. This is far too large for efficient numerical simulation considering that within a general bulk Monte Carlo simulation the timestep is around $\Delta t \approx 10^{-15} \text{ s}$ which leads to almost one hundred thousand events per timestep. Considering that it is typical to have only a few events per timestep, the processing overhead of using the BH model in these conditions becomes very large.

Looking at the momentum relaxation rates for the differing models in plot (b) of Figure 5.27 highlights the effect of limiting the scattering model through the average inter-ion separation. This difference in the momentum relaxation rates will alter the impurity limited mobility in device simulations directly. Therefore use of the TBE or CW approaches will lead to an underestimation of the effect that II scattering has on the mobility.

5.4 Sub-Threshold Impurity Scattering

The method for simulating II scattering in the Monte Carlo simulator used here is the TBE model as it overcomes the divergent scattering rate problem with low screening densities. It has traditionally been used in this Monte Carlo simulator and the loss of accuracy incurred is neglected in favour of efficient simulation. The loss of accuracy can be highlighted by examining the TBE approach applied to the remote screening model developed in this work.

The loss of accuracy lies with the cut-off used by the TBE model which utilises the impact parameter definition, given by equation (5.62). The scattering events which have an impact parameter beyond half the inter-ion separation distance are regarded as being more probable to scatter from another scattering centre and therefore are excluded.

$$\pi b(\theta)^2 = 2\pi \int_{\theta}^{\pi} \sin \theta_b \sigma(\theta_b) d\theta_b \quad (5.62)$$

To understand why this cut-off approach can be considered inaccurate it is necessary to examine the impact parameter, in particular for the case of remotely screened impurity scattering. Substituting the single interface differential scattering cross-section of equation (5.39) into the impact parameter definition above gives

$$\begin{aligned} \pi b(\theta)^2 = & \left(\frac{Ze^2}{4\pi\epsilon_{Si}\epsilon_0} \right)^2 \frac{2^4 \pi^2 m^{*2}}{\hbar^4} (1 + 2\alpha E)^2 \int_{\theta}^{\pi} d\theta_b \frac{\sin(\theta_b)}{(\mathbf{q}^2 + k_C^2)^2} \\ & \times \left[1 + \exp\left(-2Z_I \sqrt{\mathbf{q}_1^2 + k_C^2}\right) - 2\cos(q_Z Z_I) \exp\left(-Z_I \sqrt{\mathbf{q}_1^2 + k_C^2}\right) \right] \end{aligned} \quad (5.63)$$

In Figure 5.28 the impact parameter is plotted at various impurity positions for the sub-threshold conditions used in Figure 5.27. Also plotted is the average, half inter-ion separation distance given by $a = \frac{1}{2}(2\pi N_I)^{-\frac{1}{3}}$.

5.4 Sub-Threshold Impurity Scattering

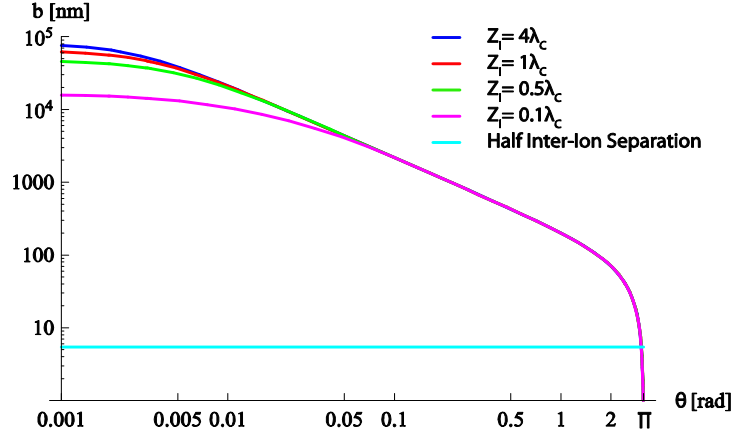


Figure 5.28: Impact parameter for single interface remotely screened impurity model against half the average inter-ion separation distance for sub-threshold conditions of $N_I = 10^{18} \text{ cm}^{-3}$ with a low carrier density of $n = 10^{12} \text{ cm}^{-3}$.

The plot highlights the large range of scattering events that will be excluded by the TBE model. In particular, the correction to the II scattering model introduced by the remote screening effect is excluded using this approach. Therefore in sub-threshold conditions the use of the TBE model will neglect a great deal of impurity scattering including the effect of remote screening. To properly account for all II scattering in sub-threshold conditions the full BH approach with remote screening must be modelled, thereby avoiding any underestimation of the importance of II scattering on the mobility.

In this work a new method has been developed to retain the accuracy of the BH approach to II scattering whilst controlling the behaviour in sub-threshold conditions where the scattering rate tends to large values. This new method restricts the scattering rate but maintains the original momentum relaxation rate, and is possible through the introduction of a simple numerical cap developed by Dr. Jeremy Watling [111]. This numerical cap will first be discussed for the BH model of scattering in section 5.4.1. In section 5.4.2 the application of this correction to the remotely screened models is presented. Finally in section 5.4.3 the model is tested with the Monte Carlo simulator used in this work.

5.4.1 Numerical Cap to II Scattering

This numerical cap to the II scattering process was designed to allow use of the complete BH formulation in Monte Carlo simulations without the drawback of large simulations times. Starting by defining the original BH scattering rate and momentum relaxation rate as Γ_{II}^{BH} and $1/\tau_m^{BH}$ respectively.

5.4 Sub-Threshold Impurity Scattering

$$\Gamma_{II}^{BH} = K_{II} \int_0^{\pi} P(\theta) d\theta \quad (5.64)$$

$$\frac{1}{\tau_m^{BH}} = K_{II} \int_0^{\pi} P(\theta) (1 - \cos(\theta)) d\theta \quad (5.65)$$

Here the term in front of the theta integral has been separated into K_{II} given by equation (5.66). The scattering angle probability, $P(\theta)$, has also been separated and is given by equation (5.67) below.

$$K_{II} = \left(\frac{Ze^2}{4\pi\kappa\epsilon_0} \right)^2 N_I \frac{8\pi m_d k^*}{\hbar^3} \quad (5.66)$$

$$P(\theta) = \frac{\sin(\theta)}{(2k^{*2} (1 - \cos(\theta)) + k_C^2)^2} \quad (5.67)$$

Now defining the conditions that the numerical correction must satisfy in equations (5.68) and (5.69) which state that the momentum relaxation rate of the numerically corrected scattering model must match the BH model but the scattering rate cannot increase beyond $\Gamma_{II}^{\max}$.

$$\frac{1}{\tau_m^{BH}} = \frac{1}{\tau_m^{new}} \quad (5.68)$$

$$\Gamma_{II}^{new} = \begin{cases} \Gamma_{II}^{BH} & \text{for } \Gamma_{II}^{BH} < \Gamma_{II}^{\max} \quad (a) \\ \Gamma_{II}^{\max} & \text{for } \Gamma_{II}^{BH} > \Gamma_{II}^{\max} \quad (b) \end{cases} \quad (5.69)$$

Here $\Gamma_{II}^{\max}$ is the fixed cap which for reasons discussed later must be at least greater than $1/2\tau_m^{BH}$. The solution to this problem is to introduce a minimum scattering angle to cap the scattering rate, $\theta_{\min}$, and to define a correction function, $G(\theta_{\min})$, to retain the momentum relaxation time.

$$\Gamma_{II}^{new} = K_{II} G(\theta_{\min}) \int_{\theta_{\min}}^{\pi} P(\theta) d\theta \quad (5.70)$$

$$\frac{1}{\tau_m^{new}} = K_{II} G(\theta_{\min}) \int_{\theta_{\min}}^{\pi} P(\theta) (1 - \cos(\theta)) d\theta \quad (5.71)$$

5.4 Sub-Threshold Impurity Scattering

The correction factor G can be expressed through use of the defining condition of equation (5.68) and after some basic manipulation yields

$$G(\theta_{\min}) = \frac{\int_0^\pi P(\theta)(1 - \cos(\theta))d\theta}{\int_{\theta_{\min}}^\pi P(\theta)(1 - \cos(\theta))d\theta} \quad (5.72)$$

It is clear that as $\theta_{\min} \rightarrow 0$ that this expression for G will tend to one which is the correct limit and ensures that the new scattering rate will adhere to the bounding condition (a) of equation (5.69). This leaves the minimum scattering angle, $\theta_{\min}$, which due to the self-consistency of the problem must be found numerically by a root-finding technique. Using the condition (b) of equation (5.69), the minimum scattering angle can be found by solving the following equation.

$$\Gamma_{II}^{\max} - \Gamma_{II}^{new} = 0$$

$$\Gamma_{II}^{\max} - K_{II} G(\theta_{\min}) \int_{\theta_{\min}}^\pi P(\theta)d\theta = 0 \quad (5.73)$$

This expression can be simplified by substituting in the expression for G given by equation (5.72) and dividing throughout by the original BH momentum relaxation rate.

$$\Gamma_{II}^{\max} \tau_m^{BH} - H(\theta_{\min}) = 0 \quad (5.74)$$

where the expression H is given by

$$H(\theta_{\min}) = \frac{\int_{\theta_{\min}}^\pi P(\theta)d\theta}{\int_{\theta_{\min}}^\pi P(\theta)(1 - \cos(\theta))d\theta} \quad (5.75)$$

This modification to the root-finding method by redefining the problem into a scaled maximum scattering rate, $\Gamma_{II}^{\max} \tau_m^{BH}$, and the function $H(\theta_{\min})$ also solves a secondary problem. Examining the $G(\theta_{\min})$ equation of (5.72), it is clear that as $\theta_{\min} \rightarrow \pi$ this function will tend to infinity. By re-arrangement of the final problem, it is now possible to define this limitation in more detail. Taking the limit $\lim_{\theta_{\min} \rightarrow \pi} H(\theta_{\min})$ it is found that the function tends to $\frac{1}{2}$. Therefore as long as the maximum scattering rate is $\Gamma_{II}^{\max} \tau_m^{BH} \geq 1/2$ (using equation (5.74)) the numerically corrected Π

5.4 Sub-Threshold Impurity Scattering

scattering model will provide the exact BH model at a reduced scattering rate. This is a considerable reduction in the scattering rate as the momentum relaxation rate can be many orders of magnitude smaller than the scattering rate [61].

5.4.2 Numerically Capped Single/Double Interface Models

The numerically corrected approach to II scattering outlined in the previous section can be applied to the newly developed remotely screened impurity models. The approach to the problem remains identical for the new models but the scattering angle probability, equation (5.67), for the new scattering models is changed appropriately. For the single interface model the angular probability dependence is simply the θ -integral of the scattering rate.

$$P(\theta) = \frac{\sin \theta}{(\mathbf{q}^2 + k_C^2)^2} \left(1 + \exp\left(-2Z_I \sqrt{\mathbf{q}_\perp^2 + k_C^2}\right) - 2 \cos(q_z Z_I) \exp\left(-Z_I \sqrt{\mathbf{q}_\perp^2 + k_C^2}\right) \right) \quad (5.76)$$

The probability for double interface model can be obtained in the same manner.

$$P(\theta) = \frac{\sin \theta}{(\mathbf{q}^2 + k_C^2)^2} f_{dbl}(k_C, Z_I, L_C) \quad (5.77)$$

Here the f_{dbl} expression is given by the equations (5.50)-(5.53).

For both the remotely screening II scattering models the limit of the $H(\theta_{\min})$ function is identical to that of the BH model, that is $\lim_{\theta_{\min} \rightarrow \pi} H(\theta_{\min}) = \frac{1}{2}$. This can be understood from the behaviour of the coefficients of the remotely screened models which simply scale the behaviour of the II scattering model.

5.4.3 Testing Numerical Capped II Scattering

The numerical correction reduces the scattering rate by restricting the range of angles through which the carrier can scatter. Introduction of a correcting coefficient $G(\theta_{\min})$ allows the new model to retain the original momentum relaxation rate by a self-consistent method of finding $\theta_{\min}$. As this method alters the dynamics of the carrier scattering process, it is important to ensure that the energy and velocity are being properly modelled. This can be tested by simulating the energy- and velocity-field data between the BH and the new numerical II model. With typical data for the

5.4 Sub-Threshold Impurity Scattering

energy- and velocity-field relations given for undoped silicon, it is not possible to compare this model directly with experiment as II scattering is obviously negligible in such samples. Here to induce II scattering the silicon has a donor doping concentration of $N_D = 10^{18} \text{ cm}^{-3}$.

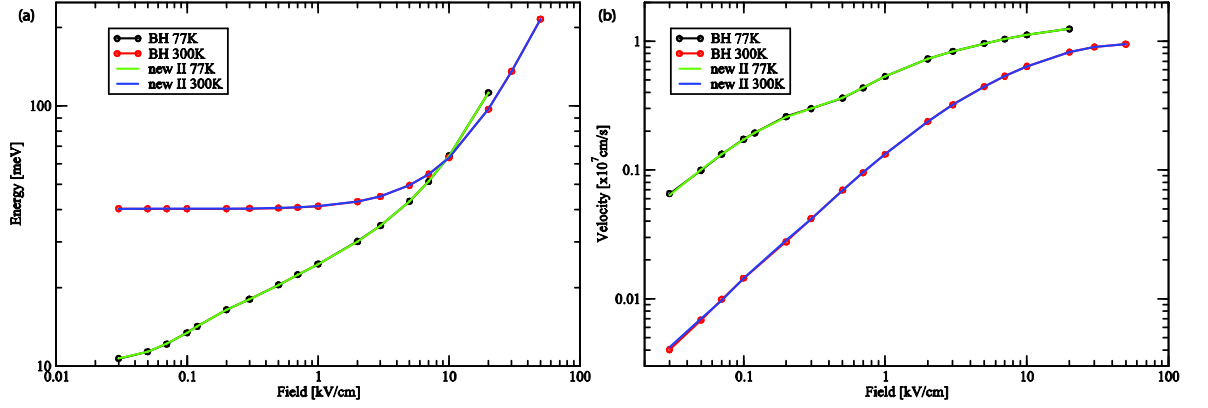


Figure 5.29: (a) Energy-field and (b) velocity-field curves for bulk silicon at a donor concentration of $N_D = 10^{18} \text{ cm}^{-3}$.

Figure 5.29 shows the energy-field relation and the velocity-field relation for the doped silicon. The new numerical corrected II model matches perfectly the BH model in both figures verifying that the energy and velocity of carriers is unaffected by numerically capping the scattering process.

Introduction of a new II scattering model may also affect the calibration of the simulator with other experimental data such as with the bulk and universal mobility. As the Monte Carlo simulator used in this work has been tested using Ridley's TBE model with the doping concentration dependent correction discussed in section 3.3.3 for impurity scattering, it is important to ensure that the new model doesn't negatively alter the calibration with experimental data.

The bulk or doping concentration dependent mobility has been tested for silicon with the original II model against the new numerical II approach in plot (a) of Figure 5.30. The doping-concentration dependent correction factor has not been modified for use with the new II model and remains identical to that used in the TBE approach discussed in section 3.3.3. Experimental data in this plot is from Thurber [29].

5.5 Simulator Implementation

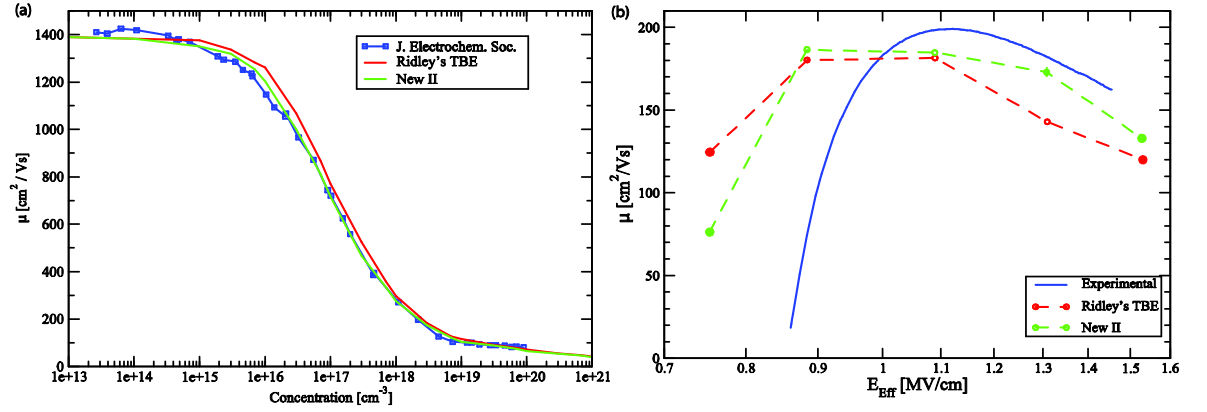


Figure 5.30: (a) Bulk mobility and (b) universal mobility for silicon at $N_A = 2 \times 10^{18} \text{ cm}^{-3}$ against experimental data at 300K.

The new II scattering model is a slightly better fit with the experimental bulk mobility than the TBE model. Between the concentrations of $10^{15} - 10^{18} \text{ cm}^{-3}$ the new model is a closer match to experimental data.

The above plots show that the numerical cap to the BH model doesn't alter the characteristics of the BH model in the energy/velocity plots whilst improving the calibration with experimental data over the TBE model with the bulk mobility. To demonstrate the validity of the new model in sub threshold conditions it is necessary to simulate a more advanced structure such as the MOS capacitor. Simulations of the MOS capacitor are used in Monte Carlo simulations to calibrate the universal mobility with experimental data [28] as discussed in chapter 3.5.2. In the device used here the substrate is doped to $N_A = 2 \times 10^{18} \text{ cm}^{-3}$ with a low horizontal field of $E = 0.5 \text{ kV/cm}$. The parameters for each of the scattering mechanisms are as detailed in chapter 3.3. In plot (b) of Figure 5.30 the universal mobility has been plotted showing the improved behaviour of the numerically capped BH model with the Ridley TBE model. Again, the new model is closer to experimental data than Ridley's TBE model and demonstrates the improved mobility of using the BH model.

5.5 Simulator Implementation

The implementation of the newly developed scattering processes into the numerical Monte Carlo simulation follows the typical method used for most scattering mechanisms [31, 75]. To briefly summarise, the maximum scattering rate of each mechanism is tabulated in the scattering table which is used to stochastically select a mechanism at each scattering event. Once a scattering mechanism is chosen, the appropriate scattering process is evaluated where the carrier is scattered.

5.5 Simulator Implementation

Within the scattering process, an out-scattering angle is stochastically selected for the carrier which, for elastic scattering, conserves the electron energy.

In this section a brief discussion of the details of the numerical method used will be given starting with the method for the calculation of the scattering rate in section 5.5.1. The scattering process and the method used to select the scattering angle is discussed in 5.5.2. Also discussed in section 5.5.3 is the numerical implementation of the double interface scattering model coefficient. Calculation of the coefficient during simulation can incur numerical floating point overflows under certain conditions. A solution has been found and this will be discussed in this final section.

5.5.1 Scattering Rate

The remotely-screened impurity scattering models have been developed as a correction to the existing BH scattering model. Remote screening has been shown to reduce the magnitude of II scattering and it is known that it will yield the BH model in the appropriate limit. Therefore in the numerical Monte Carlo simulation it is only necessary to tabulate the BH model for the scattering table as it will always be the upper limit on the scattering rate.

For the numerical II correction the remotely screened scattering and momentum relaxation rates must be evaluated which will require numerical integration of the θ integrals in equations (5.40), (5.41), (5.56) and (5.57). The Romberg integration method as discussed in Numerical Recipes for Fortran, section 4.3 [112] is used to evaluate the integral. It is also required to find the minimum scattering angle, $\theta_{\min}$, for the numerical II correction. This involves finding the root of equation (5.74) and must be found numerically. Referring to the methods in Numerical Recipes in Fortran [112], the Van Wijngaarden-Dekker-Brent method of section 9.3 has been employed. These numerical routines were chosen for both their simplicity in use and their efficiency as discussed in the Numerical Recipes book. The precision in the results is found to be sufficiently high and of course can be fine-tuned to suit the requirements.

5.5.2 Scattering Process

The scattering process for remotely screened impurity scattering is relatively typical for II scattering. There are some modifications to the standard II process which are outlined below, the most important of these is that of finding the carrier position. When this scattering event is chosen from the scattering table, the process must first determine the carrier position in relation to the source and drain interfaces. If the carrier is located in the source or drain the standard BH scattering process is invoked.

5.5 Simulator Implementation

In the case that the carrier is located in the channel, there is still the possibility that it is located in a region that remote screening has no effect. To combat this, the remote screening correction is only invoked if the carrier is within four screening lengths of the source interface in the single interface model and within four screening lengths of the source or drain in the double interface model. The value of four is chosen such that the difference between the scattering rate of the remotely screened model and the BH model is within a few percent, e.g. $1 - \exp(-4) \approx 0.98$.

For a carrier which is suitable for scattering with the remote screening correction, an out-scattering angle must be selected. The out-scattering angle can be selected from the probability distribution function for each model given by the equations (5.76) and (5.77). There are several methods available to select the scattering angle using random numbers which are discussed in appendix of the review paper by Jacoboni and Reggiani [75]. The BH model makes use of the direct technique which allows the scattering angle to be chosen directly from a single random number. As the probability distribution functions for the remotely screened impurity scattering models cannot be integrated analytically, the direct technique is of no use. Instead a rejection technique is chosen which unfortunately is less efficient than the direct technique as it requires repeated evaluation of the probability distribution function. To increase the efficiency of the rejection method, the probability distribution function (PDF) for the scattering is scaled to values between 0 and 1. Thereby allowing the upper value constant for the rejection method to be selected as the PDF maximum and ensuring a minimum number of rejections. To obtain the scaling factor requires finding the maximum value of the probability function which must be found numerically. Using Brent's method of section 10.2 in Numerical Recipes in Fortran the maximum value of this function can be easily evaluated.

5.5.3 Double Interface Coefficient Calculation

The f_{dbl} coefficient given by equations (5.50)-(5.53) contains many exponential terms whose components can be very large. This leads to numerical overflows during the numerical simulation. The solution to this problem is to use the approximation $\exp(x) - 1 \approx \exp(x)$ for large values of x . Within the IEEE double-precision format for floating-point numbers which is used in the numerical simulations in this work, the numerical precision for floating point numbers is $2^{\pm 53}$ with a range of $10^{\pm 308}$. The exponential function will overflow in this system for a power of roughly $x = \pm 308 \times \ln 10 = \pm 709.196$.

Rather than employing an approximation to the coefficient to all values of x or at values $x > 709$, it is best to introduce an approximation at the numerical precision. In other words, utilise an

5.6 Conclusion

approximation on the coefficient when the power is at the limit of numerical precision rather than the limit on range, therefore for $x = \pm 53 \times \ln 2 = \pm 36.7368$. Using this value with the IEEE double-precision system, the approximation that $\exp(x) - 1 \approx \exp(x)$ can be used and becomes exact when employed above powers of $|x| > 36.7368$.

The f_{dbl} coefficient given by equations (5.50)-(5.53) contains three different $\exp(x) - 1$ terms which can be simplified using the approximation discussed above. These three terms are

$$(\exp(2L_C K_C) - 1) \quad (5.78)$$

$$(\exp(2(L_C - Z_I)K_C) - 1) \quad (5.79)$$

$$(1 - \exp(2Z_I K_C)) \quad (5.80)$$

To attain the maximum accuracy it is important to approximate only the necessary terms to avoid overflow. It follows that with three conditions that there are $2^3 = 8$ cases which can easily be tested in the final program code and the suitably simplified expression for f_{dbl} chosen. As an example, the case where all three terms can be approximated is given here. Using the simplifying approximation on the equations (5.78)-(5.80), substitution back into the coefficient and re-arranging the terms yields

$$\begin{aligned} f_{dbl} = & 1 + \exp(-2Z_I K_C) - 2\cos(q_Z Z_I)\exp(-Z_I K_C) + 2\cos(q_Z L_C)\exp(-L_C K_C) \\ & - 2\cos(q_Z (Z_I - L_C))\exp((Z_I - L_C)K_C) + \exp(2(Z_I - L_C)K_C) \end{aligned} \quad (5.81)$$

This term is greatly simplified from the complete form and interestingly has some similarity with the single interface coefficient, the terms within the square brackets of equation (5.40). The first three terms of the above expression are identical to the single interface coefficient, which can be found exactly by allowing $L_C \rightarrow \infty$.

5.6 Conclusion

In this chapter a new scattering rate, entitled remotely screened impurity scattering, has been developed for numerical device simulation within the Monte Carlo technique. This newly developed scattering rate introduces polarisation charge effects induced from the highly doped source and drain regions on impurity scattering in the channel. Remotely screened impurity

5.6 Conclusion

scattering has been developed in two different forms, given as either the single or double interface case referring to the inclusion of one or two highly doped regions respectively. The single interface case allows the inclusion of a single polarisation charge on the screening of an impurity and the double interface case allowing multiple polarisation charges to be induced between the source and drain regions.

Remote screening of IIs has been shown to increase the II-limited mobility considerably when the II is located close to the highly-doped source and/or drain regions. The strength of remote screening becomes very strong when the impurity is located within one channel screening length of the highly-doped regions. In the context of real device channel lengths, the lower the impurity density in the channel leading to larger channel screening lengths, the stronger the effect of remote screening. In short channel length devices, taking into account remote screening from both the source and the drain, the II-limited mobility can be increased by up to 500%.

Due to the anisotropic nature of the scattering potential and the context of this work, a simplified approach has been utilised within the scattering model to reduce the complexity whilst allowing an analysis of the effect of remote screening. This simplification, here entitled the Z-aligned model, assumes that the incoming carrier is aligned with the Z-axis of the scattering reference frame thereby removing the anisotropy. Essentially the Z-aligned model assumes that the scattering potential is isotropic such that it can be used with the typical formulations of Monte Carlo scattering approach. The simplification was shown here using an analysis of incoming carrier angle to lead to an average (negligible) error of at most 2%. The average being taken over the domain where remote screening is effective and assuming that the incoming carrier is at the worst case alignment for anisotropy.

The developed scattering mechanism has been developed to fully replace the existing II scattering mechanism within the channel region of a MOSFET and although possible, for computational efficiency a transition has been introduced to merge with the classic BH approach. This transition is based on the roll-off of the polarisation charges at increasing distance from the source and drain interfaces. This transitional distance corresponds to roughly four channel screening lengths from the interface where the effect of polarisation charges on the screening is considered to be very small. Beyond this transitional distance, the II scattering model will revert to the classic BH approach, improving computational efficiency by removing the need to evaluate the complex remote screening expressions.

The existing approach to II scattering in the MC simulator used within this work made use of Ridley's TBE approach which has been shown to be non-ideal due to the removal of low screening density II scattering. The TBE approach is particularly bad when modelling low effective field

5.6 Conclusion

universal mobility where the screening density is much lower than the impurity density. To resolve this problem and allow a complete analysis of the effect of remote screening on II scattering, a new approach has been developed which allows low screening density II scattering to be modelled.

This new approach makes use of a numerical cap to II scattering which has been introduced to solve the problem of diverging scattering rates with very low screening densities. This problem exists with BH scattering and the approach used here for the remote screening model. Through restriction of the minimum scattering angle and use of a self-consistent correction function, the scattering rate can be numerically capped whilst still maintaining the momentum relaxation rate. Thereby all II scattering can be modelled efficiently and with scattering rates which are within reason for MC simulation.

Chapter 6 Results and Discussion

6.1 Introduction

The objective of this PhD research is to examine the remote screening effect that the highly doped source and drain regions have on channel ionized impurity (II) scattering. In Chapter 5 a scattering model suitable for Monte Carlo (MC) simulation has been developed which includes the remote screening effect. In this chapter this newly developed model has been applied to simulations of two n-type MOSFET devices.

Remote screening of channel dopants by the source and drain regions has been shown in the previous chapter to reduce the effect of II scattering. This reduction in II scattering is evident close to the source and drain interfaces and is considered negligible at a distance greater than four channel screening lengths from an interface. As the remote screening effect is heavily dependent on channel screening length, where larger screening lengths increase the strength of the remote screening, this effect will be more dominant at lower gate voltages. Lower gate voltages of course lead to lower screening densities in the channel region.

Hence, the remote screening of II scattering is expected to increase carrier transport performance through the channel region particularly near the source and drain interfaces. This increase in performance is expected to be greater at lower gate voltages and will be reduced as the gate voltage and channel screening concentration is increased. This increase in channel transport performance can also be described as reduction in the control that doping has on the channel. At low gate voltages II scattering helps to turn the device off by reducing the channel mobility. With the introduction of remote screening to the II scattering mechanism, the low gate voltage channel mobility may be increased leading to larger off-state currents.

The in-house MC simulator which was discussed in Chapter 3 is utilised for the device simulations. The scattering parameters and models remain identical to that of the calibrated simulator in chapter 3.3 with the exception of the II scattering model. For these device simulations the numerically capped Brooks-Herring (BH) model presented in section 5.4 is employed in place of the Third-Body Exclusion (TBE) II scattering model for the reasons discussed in the previous chapter.

A self-consistent MC simulation is completed for each of the two devices as discussed in Chapter 3. The simulation parameters for the two MC device simulations completed here are kept constant between the simulations with a timestep of $\Delta t = 10^{-17} \text{ s}$ and a total simulation period of 10 ps (at

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low gate voltages the simulation period is increased up to 20ps to reduce the statistical error). A transient period of 2ps is allowed before statistics are gathered and the non-linear Poisson solution is solved every 250 timesteps or 2.5fs . A total of 95000 particles are utilised in each MC simulation to represent the charge carriers.

The first of the devices to be simulated with the remotely screened impurity scattering model is a bulk MOSFET device. This bulk device was first developed and published by Toshiba in 2001 [113, 114] and is designed as a high-performance device for sub-50nm CMOS applications. This bulk MOSFET device is highly doped and has an advanced doping profile including a super-steep retrograde (SSR) doping profile and halo implants. This complex channel doping profile is implemented to reduce the short-channel effects that occur at this scale such as threshold voltage roll-off and punch-through. It has been used here to represent a typical current generation bulk MOSFET device which can be scaled successfully for use in future generations [115]. The industry roadmap, the International Technology Roadmap for Semiconductors (ITRS) 2008 update [1], predicts the bulk device structure to be continued in production until at least 2012.

The second device to be simulated is a device that is proposed for future technology generations. This device is a Ultra-Thin Body Double-Gate (UTB DG) MOSFET device which has been developed as part of the PullNano European project as a template device. The PullNano project used this template device to compare the a wide variety of different device simulation techniques used within the PullNano European consortium [116]. This device has been designed for a future low standby power technology (LSTP) generation and is constructed with a gate length of 22nm. The DG structure is currently predicted by the ITRS as the “ultimate MOSFET device” that can be scaled to the end of the roadmap [1].

The UTB DG device has highly doped source and drain region and unlike the bulk MOSFET, has a low doped channel which will increase channel screening lengths. Originally developed with a high- κ dielectric which has been replaced with the equivalent oxide thickness (EOT) in traditional silicon dioxide for the purposes of this simulation study. This allows the additional complex scattering mechanisms that need to be introduced with a high- κ dielectric to be neglected.

In these devices the effect of remote screening from the highly doped source and drain regions is considered but the remote screening from the highly doped or metal gate(s) has been left to research beyond the thesis. Within this work, the analysis of remote screening from the source and drain has been considered to be the more dominant component and has been studied first. Carriers travel through the source and drain remote screening regions to contribute to conduction and therefore are far more likely to feel the effect of remote screening. The effect of gate remote

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screening is still considered an important interaction and will be studied in the future. The gate remote screening effect will become stronger in future device such as the double gate device where gate oxides are become very thin and metal gates are commonplace.

The structure of the chapter will begin with the bulk MOSFET in section 6.2 followed by the UTB DG device in section 6.3 and finishing with the conclusions of the simulations in section 6.4. For the device simulation sections 6.2 & 6.3, the internal structure is repeated. The device simulation sections begin with an initial presentation of the device structure and calibration, followed by a brief study of the expected effect of remote screening. Next within the section, the numerical results of the MC simulations for the particular device are discussed in detail and finally the results are summarised.

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The 35nm bulk MOSFET device used here has been developed to replicate a published device structure from Toshiba [113, 114]. This device has been chosen as it represents a realistic device that is used within the industry in CMOS applications. The device structure has been reconstructed from published experimental data within the commercial TCAD software Sentaurus [117], and was completed as part of the PhD thesis of Fikru Ademu-Lema, a researcher from this group [118]. Full details of the calibration of the commercial tools along with the extraction of the device structure, doping profiles and characteristics are provided in [118]. The device has since been applied within the research group in Drift-Diffusion (DD) simulation. This required the device structure and doping profiles to be exported from Sentaurus for application with the in-house DD code. Another researcher from this group, Gareth Roy, completed this process and calibrated the DD simulator with Sentaurus as part of his PhD thesis [119].

Thankfully due to the construction of the Monte Carlo (MC) simulator used within this work, the device structure can be directly exported from the DD simulator and applied without difficulty to the MC simulator. As MC calibration is completed through non-device specific experimental data as discussed in Chapter 3, no further calibration is required.

This section will begin by presenting the device structure and doping profile for this bulk device along with the calibration data showing the match between the simulators in section 6.2.1. Following this in section 6.2.2 will be a brief analysis of the expected behaviour from the introduction of remote screening to ionized impurity scattering in simulation of this device. Finally the results of the MC simulation with remote screening will be analysed in detail within section 6.2.3.

6.2.1 Device Structure and Calibration

The structure and dimensions of the bulk device used with the MC simulator are given in Figure 6.1. It should be noted that this diagram is not drawn to scale but provides a generic overview of the structure. The remote screening plane is given in the upper-left corner of Figure 6.1 and the positions of the remote screening interfaces at $Z=0$ and $Z=L_c$ are marked at the edges of the source/drain regions.

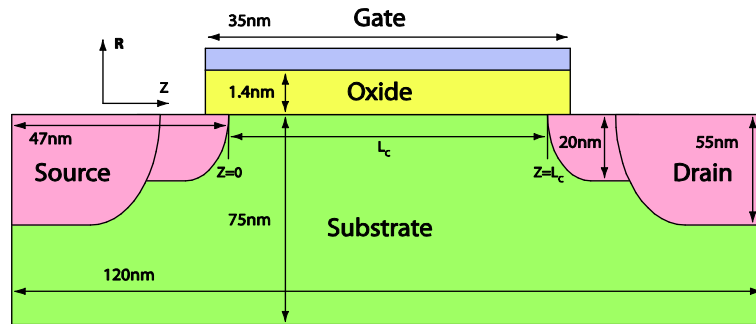


Figure 6.1: Structure of the bulk MOSFET device.

The printed gate length of 35nm defines the device scale and has a metallurgical channel length, measured from the net doping profile, of approximately 26nm. This device has been designed for the 45nm technology node and MOSFET's of this scale are already in production. The oxide thickness for this device is 1.4nm and is a silicon oxi-nitride dielectric with a dielectric constant of $\epsilon_r = 5.45$. The gate in the MOSFET device of Figure 6.1 used within the DD and MC simulators, is a metal gate with a work-function of $\phi_G = 3.945\text{eV}$. This deviates from the original specification of a poly-Si gate as discussed in the original paper [113, 114] and is shown below to have little effect on the calibration.

The net doping profile is given in Figure 6.2 for this bulk device which, as mentioned earlier, was produced in the commercial TCAD process tool Sentaurus [117] by Fikru Ademu-Lema [118]. Use of the commercial process tool has allowed the advanced doping profile to be accurately replicated from the published data of the Toshiba device.

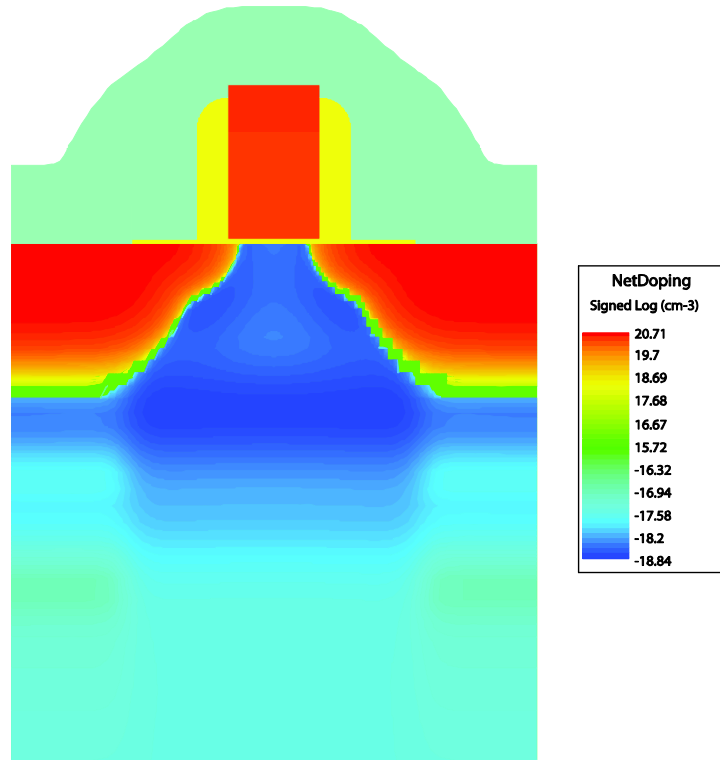


Figure 6.2: Density plot of bulk MOSFET net doping with the positive scale denoting donor doping and the negative acceptor doping.

In Figure 6.2 the advanced doping profile in the substrate can be clearly seen with n-type doping in red and p-type doping in blue. The device has an indium doped retrograde channel profile with the peak density just below the source/drain wells. This is coupled with boron Halo extensions in the channel to improve the punch through characteristics without heavily increasing the channel doping concentration. The source and drain wells are arsenic doped, with shallow extensions to reduce short-channel effects and deep junctions to reduce access resistance.

This channel doping profile has been directly imported into the DD simulation (and MC simulation) from Sentaurus and the technique is discussed within the PhD thesis of Gareth Roy [119]. It should be noted that this net doping profile figure, which is exported from Sentaurus, includes a poly-Si gate which has been neglected within the DD and MC simulations. Calibration of the commercial TCAD software with the in-house DD simulator is completed and discussed in detail within Gareth Roy's thesis and here the results are simply repeated. Calibration is completed through the I_D - V_G curves and is shown in Figure 6.3.

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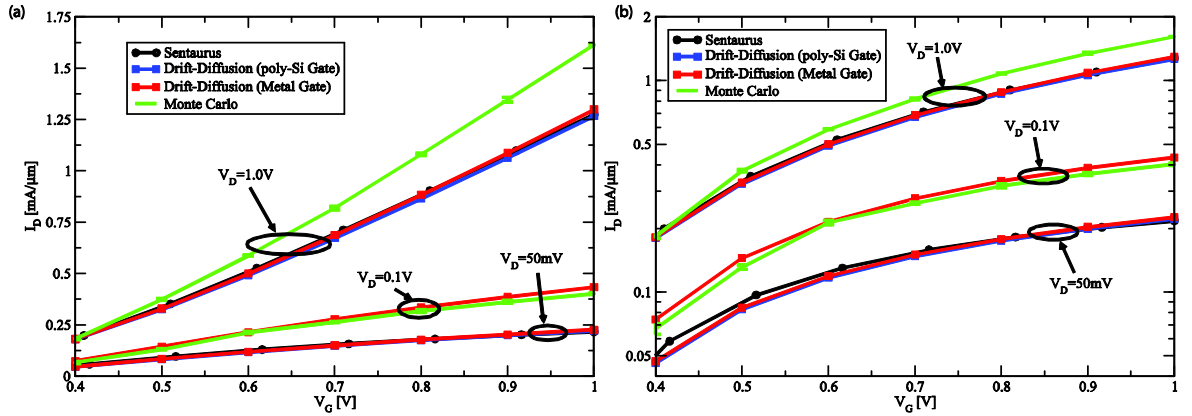


Figure 6.3: (a) Linear and (b) semi-log I_D - V_G curves for the bulk MOSFET device showing the comparison between Sentaurus, Drift-Diffusion and Monte Carlo simulation.

In plot (a) we see the excellent match between DD and the commercial Sentaurus software at both the low drain voltage, $V_D = 50\text{mV}$, and the high drain voltage of $V_D = 1\text{V}$. For reference the DD simulation has been completed with the original poly-Si gate and the metal gate to demonstrate the negligible difference between the results. Also shown is the comparison between the MC and DD simulation of the metal gate device at a low drain bias of $V_D = 0.1\text{V}$ and a high drain bias of $V_D = 1\text{V}$. As is expected, the MC simulation is very close to the DD results at low drain bias and shows an increase in the drain current at high drain bias. This increase is due to the non-equilibrium transport of carriers within the MC simulation.

As MC simulation is calibrated to other more generic experimental data such as energy-/velocity-field curves, bulk mobility and universal mobility, further calibration is not required. Although it is important to ensure that the MC results are similar to the DD simulation, it is indicative to check that the curves match in low-field conditions. This is easier to show in a semi-log plot of the I_D - V_G curves given in plot (b) of Figure 6.3. In plot (b) the match of the MC with the DD solution is clear at the low-field conditions given for $V_D = 0.1\text{V}$. The solutions between DD and MC also match well for low gate voltages at the high drain bias where the non-linear transport effects such as velocity overshoot are not important.

In both these plots for the I_D - V_G curves, the range of gate voltages was restricted to a minimum of $V_G = 0.4\text{V}$. This is the case as MC is unable to accurately model the device for lower gate voltages as the statistical noise in the data overcomes the results.

An important step in the use of the remote screening model for ionized impurity scattering is the position of the source and drain interfaces. In a device with a realistic doping profile this can

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become a complex decision as abrupt transitions in doping are not found. Instead a simple estimate has been made based on the net doping profile.

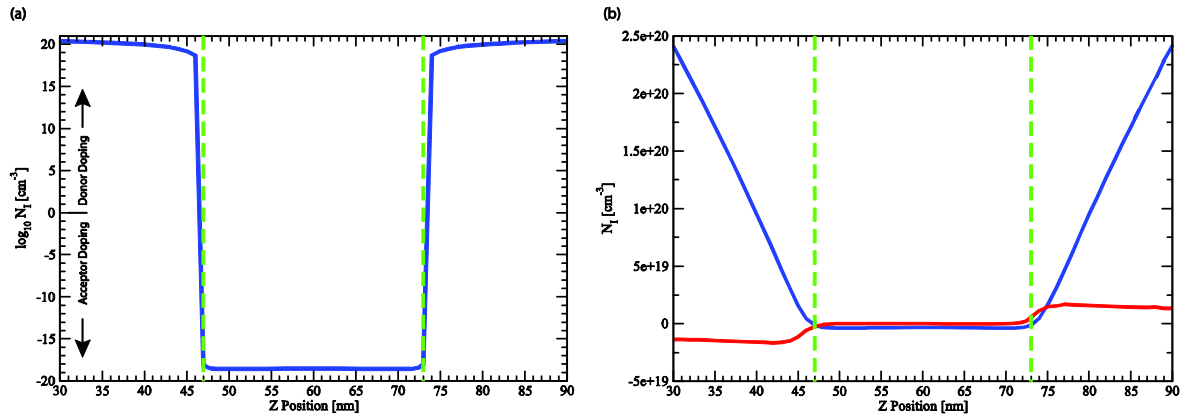


Figure 6.4: (a) Net doping profile with signed log scale and (b) net doping difference plot for the bulk MOSFET.

Plot (b) of Figure 6.4 demonstrates a difference plot of the net doping profile (given by the solid red line). In the channel of the bulk MOSFET the point at which the net doping is at the steepest gradient is chosen at the point that the source and drain interfaces are to be located. In Figure 6.4 the positions chosen for the source and drain interfaces are depicted by the dashed green lines, where the source interface is assigned at $Z = 47 \text{ nm}$ and the drain interface at $Z = 73 \text{ nm}$.

Plot (a) of Figure 6.4 also demonstrates a signed log plot of the net doping profile which highlights that the point at which the net doping is at the steepest gradient coincides with the metallurgical p-n junction. This strengthens the chosen positions of the source and drain interfaces as being closest to the original definition used in the scattering model calculation of abrupt interfaces.

6.2.2 Analytical Estimate of Remote Screening Effect

Before moving to MC simulations of the bulk MOSFET device it is important to examine what effect remotely screened ionized impurity scattering is expected to have on the device performance. A simple estimate is possible by using analytical calculation of the mobility in conjunction with data from DD simulation of the device. The DD data used within this mobility estimate is the same data used to initialise the MC simulation.

The mobility analysis completed here is not a typical mobility analysis, which normally might be completed to characterise uniformly doped silicon under various electric fields. Here the analysis of mobility is used to estimate the effect that the remotely screened II scattering mechanism has in the context of channel performance. In a channel of the device the mobility is spatially dependent

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on various factors such as doping density, carrier concentration and the electric field. Such spatial dependence makes definition of the mobility in a MOSFET channel extremely challenging. Here it must be stressed that this analysis is a simple, rough estimate for the channel mobility to allow greater insight into the behaviour of remote screening in a device context.

To compute the spatially dependent mobility, a 1D profile of the channel impurity and electron concentration data at each mesh point is obtained from the DD simulation data. The Kubo-Greenwood formula [33], given by equation (5.34), allows the mobility to be calculated at each mesh point along this channel profile for the scattering mechanisms considered. The total mobility can then be approximated through use of Mathiessen's rule [30], equation (6.1),

$$\frac{1}{\mu_{tot}} = \sum_i \frac{1}{\mu_i} \quad (6.1)$$

with μ_i denoting the i -th mobility mechanism. As mentioned above, the total mobility can be calculated at each mesh point along the channel. In this particular device the mesh points are evenly spaced at 0.5nm intervals.

Referring to the textbook definition of the mobility, it is defined as the proportionality of the carrier velocity gained by carriers in between scattering events to the electric field [15]. The average time between collisions is also known as the mean free time and can be expressed as the mean free path, $l = \tau v_{th}$, with the inclusion of the average thermal velocity of electrons. The use of the thermal velocity can only be considered a very rough estimation which although only applies at equilibrium has been used in literature to define an estimated mean free path (see [120]). Therefore, the mobility can be said to be a value defining the relation between carrier velocity and the electric field over a mean free path.

Taking the average thermal velocity as $v_{th} = (8k_B T / \pi m_C)^{1/2} = 0.9907 \times 10^7 \text{ cm/s}$ [51] and assuming the mesh spacing is the mean free path, the mean free time can be approximated as $\tau = 0.5 \times 10^{-9} / 0.9907 \times 10^5 \approx 5 \times 10^{-15} \text{ s}$. This mean free time is an order of magnitude smaller than has been reported in the literature [33] and highlights the problem that calculating the mobility on the mesh spacing interval will lead to overestimation. To combat this problem a moving median of the total mobility is taken with a span calculated from an estimate of the mean free path. A simple estimate for the mean free path can be obtained using the average ensemble momentum relaxation time, defined as equation (6.2) [121], for the mean free time between scattering events.

$$\langle \tau_m^{tot} \rangle = \frac{\int_0^\infty dE \tau_m^{tot}(E) E \frac{\partial f_0}{\partial E}}{\int_0^\infty dE E \frac{\partial f_0}{\partial E}} \quad (6.2)$$

where f_0 is the equilibrium Fermi distribution and τ_m^{tot} is given as

$$\frac{1}{\tau_m^{tot}(E)} = \sum_i \frac{1}{\tau_m^i(E)} \quad (6.3)$$

with τ_m^i denoting the i -th scattering mechanism.

Considering that the Kubo-Greenwood formula is valid for linear, low-field systems [122] and Mathiessen's rule is valid for independent scattering mechanisms [30], the use of this approach in bulk MOSFETs can only be regarded as an estimate [71]. Despite all this, the purpose of this analysis is to evaluate the remote screening effect on channel performance and the methodology discussed here is considered a reasonable approach.

The scattering mechanisms included in this mobility calculation include the acoustic and optical phonons along with II scattering. Three cases are presented, each case has a different II scattering model which will be either the BH model discussed in section 2.3, the single interface remotely screened II model from section 5.2.3.1, or the double interface remotely screened II model given in section 5.3.3.1. In all cases ellipsoidal, non-parabolic bands are assumed and for the purposes of a simple evaluation, only the first silicon band is included (the X valleys).

For the intra-valley acoustic phonon model, the approach discussed in section 3.3.1 is used here. The intervalley optical phonon scattering mechanisms presented in section 3.3.2 are also used here. This includes the scattering between equivalent X-valleys and the f- and g-type intervalley optical phonons. The material constants and transport parameters used in the phonon scattering calculations are those listed in Table 2 of Chapter 3.

As mentioned earlier the DD data is used to initialise the MC simulation and for the mobility calculations presented here, the impurity and electron density is all that is required. For this analysis, only the low drain solutions at three separate gate voltages will be analysed. At each gate voltage, the average ensemble momentum relaxation rate is calculated and the mean free path is estimated to obtain the span of the moving median.

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Presented in Figure 6.5 is (a) the carrier/impurity concentrations and (b) the calculated mobility for the different ionized impurity models with phonon scattering for $V_G = 0V$. The average ensemble momentum relaxation rate is calculated using equation (6.2) in conjunction with the sum of all momentum relaxing processes, equation (6.3), which for all the phonons and the BH model yields $\langle \tau_m^{tot} \rangle = 1.56 \times 10^{-14} s$. Hence the estimated mean free path is given as $l_{\tau_m} = 1.55 nm$.

For this the lowest gate voltage of $V_G = 0V$, the carrier concentration is very much lower than the impurity density in the channel. These are conditions where II scattering typically dominates [27] and will lead to a high II scattering rate.

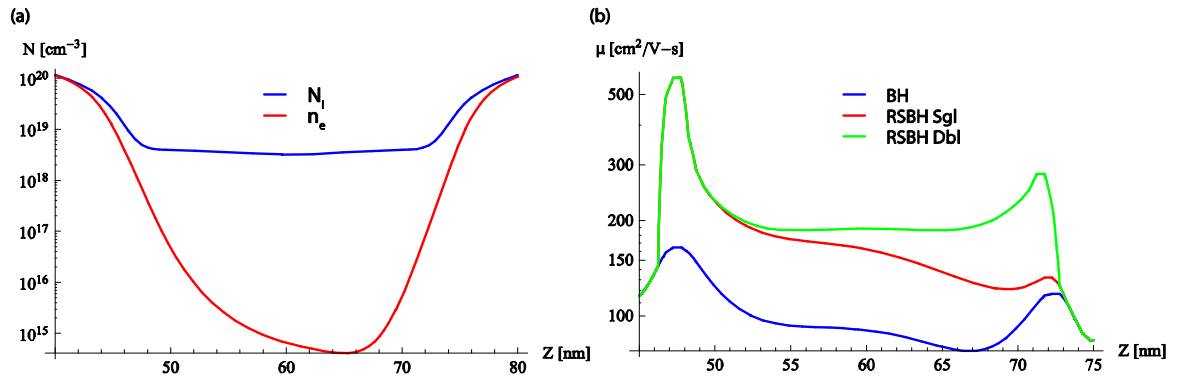


Figure 6.5: Plot of (a) the impurity and electron density, and (b) the impurity and phonon limited mobility at a gate voltage of $V_G = 0V$ and a drain voltage of $V_D = 0.1V$.

Plot (b) of Figure 6.5 shows a low mobility along the channel length consistent with the large II scattering for the BH case. It is clear in this plot that the remotely screened II models cause a large increase in the mobility over the entire length of the channel. At the source end of the channel both the single and double interface models corresponds to an increase of 196%, with an increase of 117% at the drain end of the channel for the double interface model.

The large increase in the channel mobility with the remotely screened models can be understood from the low carrier (screening) density in the channel as shown by the red line in plot (a) of Figure 6.5. The longer the screening length in the channel, the stronger the remote screening effect which reduces the momentum relaxing effect of II scattering.

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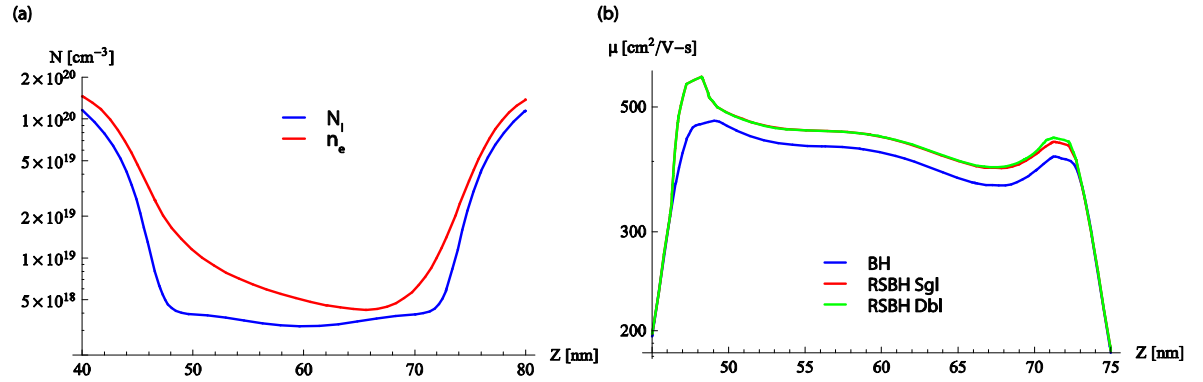


Figure 6.6: Plot of (a) the impurity and electron density, and (b) the impurity and phonon limited mobility at a gate voltage of $V_G = 0.4V$ and a drain voltage of $V_D = 0.1V$.

At a higher gate voltage of $V_G = 0.4V$, the average ensemble momentum relaxation rate is calculated as $\langle \tau_m^{tot} \rangle = 3.27 \times 10^{-14} \text{ s}$ which gives a estimated mean free path of $l_{\tau_m} = 3.24 \text{ nm}$. The electron concentration at this gate voltage, shown in plot (a) of Figure 6.6, is almost an order of magnitude larger than the impurity concentration. This will decrease the strength of the II scattering and the mobility will increase, clear from plot (b) which is approximately four times larger than that of $V_G = 0V$.

The increase in screening density at this higher gate voltage has the effect of reducing the strength of remote screening on II scattering. The effect on the channel mobility due to the remote screening models is consistently smaller, on the order of 20% at the source and 7-8% at the drain. There is still an increase in the mid channel mobility but it is reduced to $\sim 5\%$ improvement.

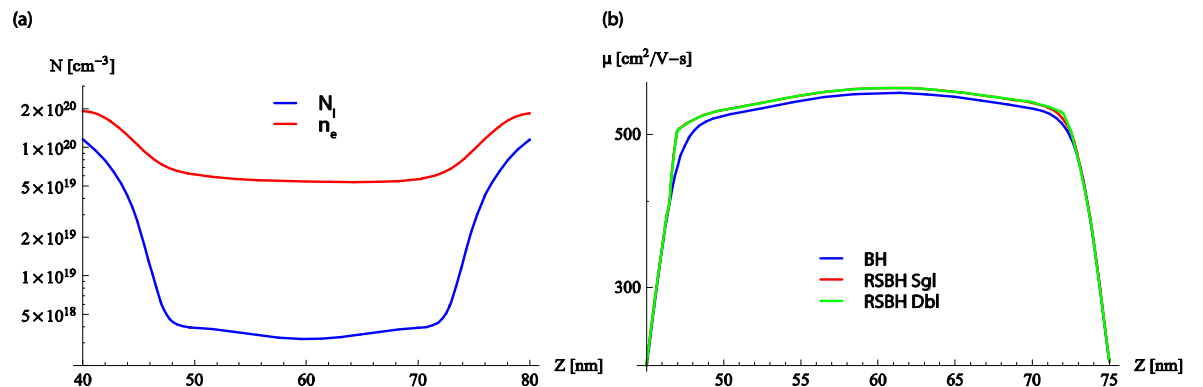


Figure 6.7: Plot of (a) the impurity and electron density, and (b) the impurity and phonon limited mobility at a gate voltage of $V_G = 1V$ and a drain voltage of $V_D = 0.1V$.

For the highest gate voltage of $V_G = 1V$ shown in Figure 6.7, the average momentum relaxation rate is $\langle \tau_m^{tot} \rangle = 5.59 \times 10^{-14} \text{ s}$ and the estimated mean free path is $l_{\tau_m} = 5.54 \text{ nm}$. At such a high gate

voltage the mobility here is dominated by phonon scattering as the electron concentration rises to well above the impurity concentration. The characteristic increase in mobility around the source and drain interface is still present although much less dramatic than at lower gate voltages. At the source end of the channel there is a peak increase due to remote screening of 10%, a consistent increase of 2% along the channel and a peak increase at the drain of 4%. This reduction in the effect of remote screening is expected at high gate voltages where the screening density is greatest.

From this analysis, the effect of remote screening on the device mobility will be larger at lower gate voltages where the carrier concentration is near to or lower than the impurity concentration. It predominantly has the largest effect in a region next to the source and/or drain interfaces, with the increase at the source interface less affected by the drain bias. As the gate voltage increases, the screening density increases and the effectiveness of remotely screened II scattering is reduced.

6.2.3 I_D - V_G Behaviour with Remote Screening

Implementing the remotely-screened impurity scattering rates developed in Chapter 5 into the MC simulator will allow the effect on device performance to be thoroughly analysed. MC simulations have been completed for the bulk MOSFET device using the newly developed, numerically capped methodology for II scattering, discussed in section 5.4.

The analytical analysis in the previous section suggests that the remote screening effect should increase the channel mobility for lower gate voltages. Ideally this increase in mobility should lead to an increase in the drain current at lower gate voltages with a decreasing effect as the gate voltage is increased. Given this evaluation of the remote screening effect, the bulk MOSFET device has been simulated for various voltage points to produce an $I_D - V_G$ curve. Such a curve can be used to assess the sub-threshold leakage current, the threshold voltage itself and the drive current. As mentioned previously, statistical noise means that simulations must have a gate voltage of $V_G \geq 0.4V$.

In Figure 6.8 the simulation data is plotted for four different cases of channel II scattering. The cases are: the numerically capped BH (Num BH) model throughout the device; no II scattering in the channel region with Num BH in the source/drain (No Chn II); single interface Remotely Screened Brooks Herring scattering (RSBH Sgl) in the channel with Num BH in source/drain; double interface remotely screened BH scattering (RSBH Dbl) in the channel and Num BH in source/drain.

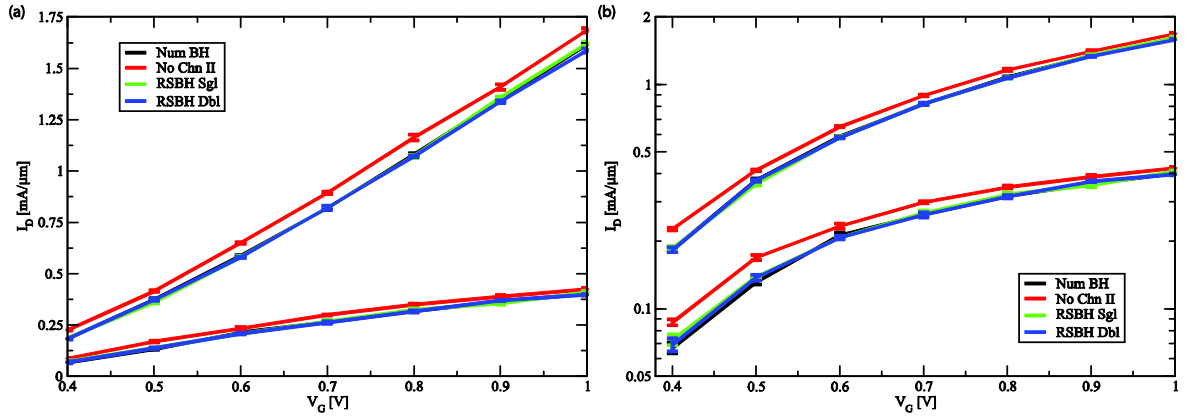


Figure 6.8: (a) Linear and (b) semi-log I_D - V_G curves for the bulk MOSFET with remotely screened impurity scattering.

The Num BH case is the baseline case with the *generic* II scattering model and is denoted by the solid black line in the two figures. As an upper limit on the effect of II scattering in the channel, simulations have been completed where II scattering has been neglected for the channel region and is shown in the figures as the red line.

The effect of neglecting the channel II scattering is clear, with a noticeable increase in the drain current. The increase at low drain bias is an almost constant increase at each gate voltage point, roughly $30\mu\text{A}/\mu\text{m}$. The increase in current at high drain bias increases slightly with gate voltage, roughly $40\mu\text{A}/\mu\text{m}$ at low gate voltage to $70\mu\text{A}/\mu\text{m}$ at high gate. Therefore in the bulk device the channel impurity scattering plays a role in characterising the device current drive and sub-threshold leakage.

The remotely screened models are also included in the figures for the single interface (green line) and the double interface (blue line) cases. The remote screening models clearly have negligible effect at any gate voltage. The small increases at low gate voltage of the low drain bias curve are within the error bars on the plot and therefore are not conclusive. In the following sub-sections the results will be analysed in more detail for the four different II cases discussed above. Initially, results of the low drain case of $V_D = 0.1\text{V}$ will be analysed followed by the high drain case of $V_D = 1\text{V}$.

6.2.3.1 Low Drain Bias

The results for $V_D = 0.1\text{V}$ will be examined in greater detail for two gate voltage points, one at a low gate voltage and one at the highest gate voltage of $V_G = 1\text{V}$. Given that MC simulation is prone to statistical noise at low gate voltages it is important to examine a low gate voltage data

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point where this noise is minimal. Examining the error bars at low gate voltage points of $V_G = 0.4V, 0.5V, 0.6V$ in more detail in Figure 6.9 will allow the data point with minimal noise to be chosen.

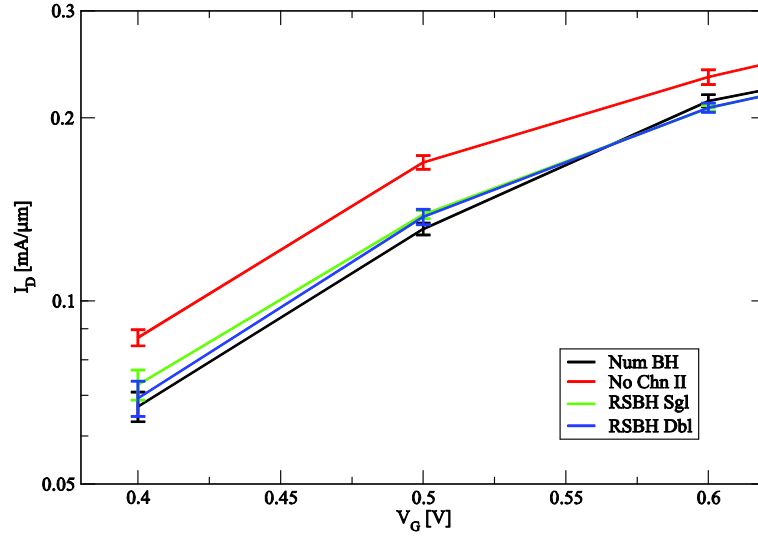


Figure 6.9: I_D - V_G characteristics for the bulk MOSFET with error bars for the low gate voltage points at $V_D = 0.1V$.

The error bars in the MC simulator are calculated from the standard deviation in the mean of the variable, the drain current in this case, where the statistical dependence has been included through an estimation of the correlation time [123]. The error is calculated using the following equation [124]

$$err = \sqrt{\frac{\sigma^2}{N} \left(1 + 2 \sum_{k=1}^{N-k} \left(1 - \frac{k}{N} \right) \rho_k \right)} \quad (6.4)$$

where σ is the standard deviation (σ^2 the variance), N is the number of steps in the simulation and ρ_k is the estimated k -th lag autocorrelation (which is dimensionless). The sum represents an estimation of the autocorrelation function. The k -th lag autocorrelation is estimated using the sample autocorrelation, $\rho_k = \gamma_k / \gamma_0$ where the autocovariance, γ_k , can be estimated by (γ_0 is the $k=0$ lag autocovariance, essentially the sample variance, σ^2)

$$\gamma_k = \frac{1}{N} \sum_{t=1}^{N-k} (z_t - \bar{z})(z_{t+k} - \bar{z}) \quad (6.5)$$

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Here z_t represents the variable at a time step t and $\bar{z}$ represents the sample mean over the entire time series. This method is discussed in more detail within the textbook by Box [124]. It should be noted that the error bars plotted are a 1σ case representing a confidence interval (assuming a normal distribution of error) of roughly 68%.

With a more detailed examination on the low gate voltage points in Figure 6.9, the remotely screened II scattering model appears to show a slight increase at $V_G = 0.4V, 0.5V$ and oddly a slight decrease at $V_G = 0.6V$. At a gate voltage of $0.4V$ the statistical noise, given by the error bars, make this result difficult to examine and validate. At the gate voltage point of $0.5V$ the remotely screened models are a close match, and slightly larger than the Num BH model. The error bars at this data point are also small enough to be considered not to dominate the results. It is this data point of $V_G = 0.5V$ which has been chosen to analyse the low gate voltage behaviour of the II models.

It is important to ensure that the remotely screened II models are operating correctly and that their behaviour is as expected. This is best shown by plotting a profile of the II scattering tally taken at each mesh point. That is, for each mesh square, the number of II scattering events was counted for each of the II scattering cases. This II scattering tally has been plotted in Figure 6.10 with the II scattering tally data given in arbitrary units.

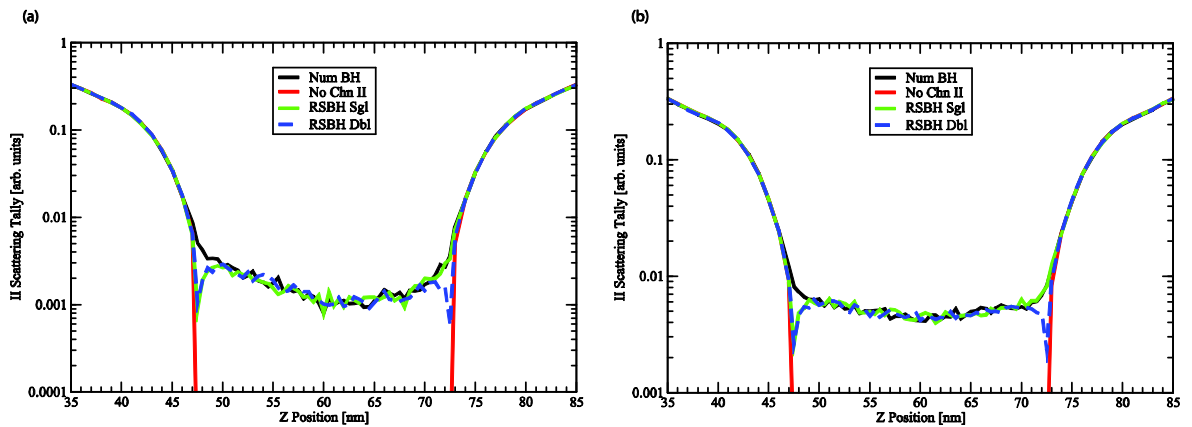


Figure 6.10: Ionized impurity scattering tally along the channel for the bulk MOSFET at (a) $V_G = 0.5V$ and (b) $V_G = 1V$ with $V_D = 0.1V$.

The plots in Figure 6.10 show that there is a finite number of II scattering events in the channel region which, away from the source and drain interfaces, is similar between the remotely screened and BH II models. For the case of no channel II scattering, the tally drops off abruptly at the source and drain interfaces as is expected. Also expected is the drop off in scattering events for the single and double interface RSBH model next to the source and drain interfaces respectively. As

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discussed in Chapter 4, the remotely screened II models reduces the II scattering rate located close to the interfaces which explains the reduced number of events seen above.

It is also interesting to note that at the higher gate voltage, plot (b) in Figure 6.10, the II scattering tally is larger in the channel than the lower gate voltage case, plot (a), for all channel II scattering models. This is contrary to the fact that at lower screening densities the II scattering rate will increase. This can be understood from the increased carrier density at the high gate voltage increasing the number of scattering carriers in the channel and consequently, the number of events.

Having established that the scattering models are operating correctly, it is now essential to examine what effect each model has on the carrier transport. This is best completed by examining the carrier velocity and density along the channel. Figure 6.11 presents (a) the electron velocity and (b) density for the gate voltage of 0.5V and Figure 6.12 the (a) velocity and (b) density for a gate voltage of 1V .

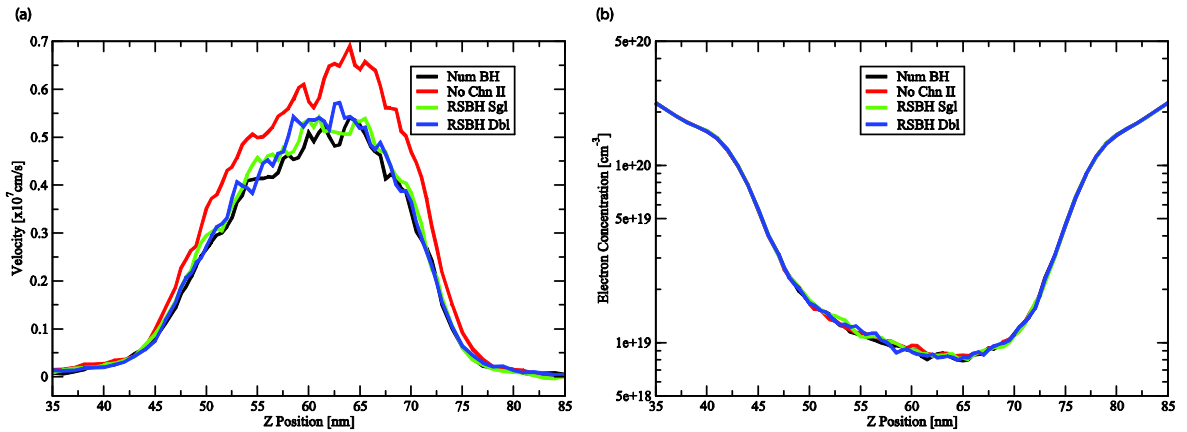


Figure 6.11: (a) Velocity profile and (b) electron density along channel of bulk MOSFET comparing standard and remotely screened ionized impurity scattering models at $V_G = 0.5V$ and $V_D = 0.1V$.

For $V_G = 0.5V$ the electron velocity along the channel in plot (a) of Figure 6.11 increases within the source region and is rapidly accelerating as it crosses the source interface at 47nm. At this point, the model which neglects channel II scattering (No Chn II, the red line) has an increased velocity which remains larger throughout the channel length and into the drain region at 73nm. The standard and remotely screened II scattering cases remain fairly close to each other throughout the channel region. There is a slight increase in carrier velocity mid channel, around the 55-60nm region, with remote screening but this is very much within the region suffering from statistical noise.

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Plot (b) of Figure 6.11 gives the corresponding electron density along the channel. The electron density is identical between all four cases of channel II scattering in the MC simulation. Hence, it can be said that the larger drain current of the No Chn II case is due simply to the increased electron velocity through the channel. It also explains the mild increase of the remote screening models drain current as the electron velocity in plot (a) of Figure 6.11 is very slightly higher over the standard case. This result is partially obscured by the noise in the data which, if we look at the electron density, can be understood. Given the channel electron density of roughly $n = 1 \times 10^{19} \text{ cm}^{-3}$ and multiplying this by a rough estimate of the channel volume, $26 \text{ nm} \times 10 \text{ nm} \times 1 \text{ nm} = 2.6 \times 10^{-19} \text{ cm}^3$, corresponds to around 2-3 electrons in the channel volume. With so few electrons in the channel contributing to the current density, noise in the results is unavoidable.

The electron velocity and density for the highest gate voltage of $V_G = 1 \text{ V}$ in Figure 6.12 demonstrates similar results for the different II scattering cases. Here the electron velocity in the channel for the case without II scattering is higher than the standard case, but is not as significant an increase as the lower gate voltage case. In fact, the peak velocity for this higher gate voltage is lower than the velocities shown in Figure 6.11 for the low gate voltage point.

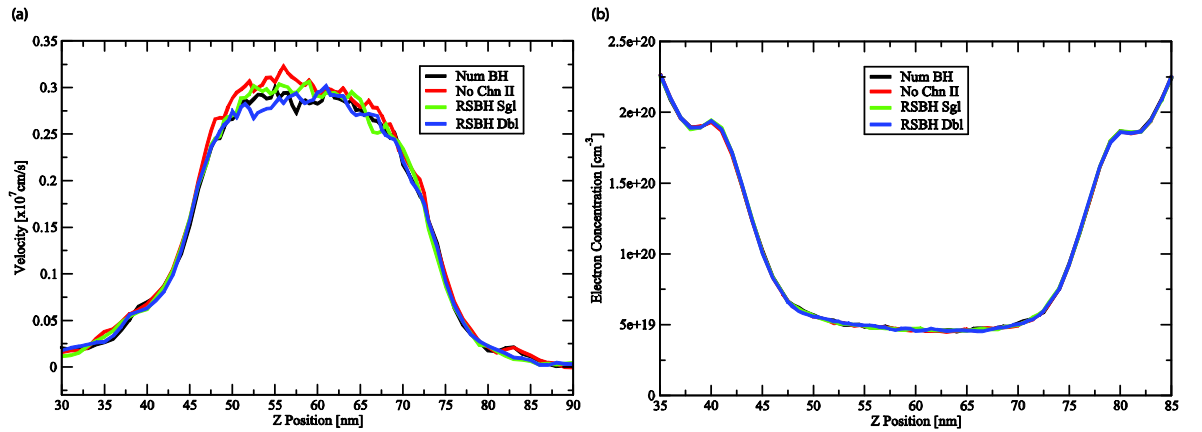


Figure 6.12: (a) Velocity profile and (b) electron density along channel of bulk MOSFET comparing standard and remotely screened ionized impurity scattering models at $V_G = 1 \text{ V}$ and $V_D = 0.1 \text{ V}$.

The relative decrease in velocity can be explained by the electron density given by plot (b) of Figure 6.12. At this higher gate voltage the electron density is around $n_e = 5 \times 10^{19} \text{ cm}^{-3}$ which is approximately five times the number of electrons present in the channel region. Referring to the simple expression for current density, which can be written

$$J = en_e v_d \quad (6.6)$$

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where e is the electronic charge, n_e the carrier density and v_d the drift velocity. Hence, given that the drain current at $V_G = 1V$ is roughly 2.5 times larger and the electron density is 5 times larger than the $V_G = 0.5V$ case, the velocity at high drain need only be half the magnitude of the low drain results. Examining the velocity of the low drain case given in Figure 6.11, the peak is roughly $v_d = 0.6 \times 10^7 \text{ cm/s}$ and for the high drain case the peak is roughly $v_d = 0.3 \times 10^7 \text{ cm/s}$ which coincides with this basic theory.

The energy profiles for the carriers are quite similar between the different channel II scattering cases. As II scattering is an elastic process, the carrier energies in the channel will not be directly modified by changes in this model. Although with the reduction in II scattering, other scattering processes could become more prominent such as inelastic phonon scattering which potentially could modify the carrier energies, this has not been the case here.

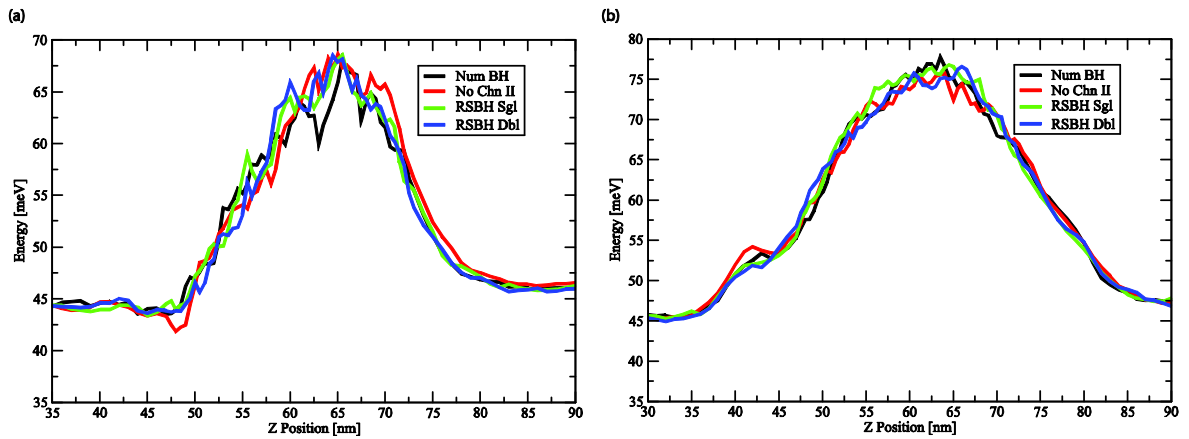


Figure 6.13: Energy profile along channel of bulk MOSFET comparing standard and remotely screened ionized impurity scattering at (a) $V_G = 0.5V$ and $V_D = 0.1V$ and (b) $V_G = 1V$ and $V_D = 0.1V$.

At low drain bias the remotely screened II scattering model has little effect on the drain current. Considering the analytical mobility analysis completed in section 6.2.2, the remotely screened models was expected to increase the channel performance, particularly at the source interface. Therefore examination must move to the final scattering mechanism, interface roughness (IR) scattering which was not considered in the analytical mobility analysis. IR scattering is found to have a strong performance defining factor in the bulk MOSFET device with the removal of this scattering mechanism from the device leads to a 52% increase in drain current at $V_G = 0.5V$, and a 88% increase at $V_G = 1V$.

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An estimate to the IR scattering mobility can be evaluated using the IR scattering model and estimating the effective vertical electric field, E_{eff} , in the channel of the device from the MC simulation results. Taking an estimate of the effective field in the middle of the channel, $Z = 60nm$, for both gate voltages gives $E_{eff} \approx 1.09MV/cm$ and $E_{eff} \approx 1.68MV/cm$ respectively. Using these values in the IR momentum relaxation rate, equation (6.7) below, it is possible to compute the corresponding mobility with the Kubo-Greenwood formula, equation (5.34).

$$\frac{1}{\tau_m^{IR}} = \frac{e^2 m_d}{2\hbar^3} (E_{eff} \Delta_{rms} L_e)^2 (1 + 2\alpha E) \int_0^{2\pi} d\varphi \frac{1 - \cos \varphi}{\left(1 + \frac{1}{2} L_e^2 \mathbf{q}^2\right)^{3/2}} \quad (6.7)$$

here $\Delta_{rms} = 0.35nm$ is the RMS amplitude of surface fluctuations and $L_e = 1.3nm$ is the correlation length. This IR scattering model is the Ando model with an exponential autocorrelation function [58] as discussed in section 3.3.4, here presented as a momentum relaxation rate. Numerical calculation gives an IR mobility of $\mu_{IR} = 275cm^2/Vs$ at $V_G = 0.5V$, and $\mu_{IR} = 92cm^2/Vs$ at $V_G = 1V$.

Referring to analytical mobility analysis, the remotely screened model was expected to provide a peak increase of mobility at the source end of the channel of 20% at $V_G = 0.4V$ and 10% at $V_G = 1V$ when considering only phonon and II scattering. Using Mathiessen's rule, given by equation (6.1), the IR mobility can be included in the estimate. The effect of remote screening at $Z = 48nm$ with IR scattering reduces from an increase of approximately 14% to 4.5% at low gate, and from approximately 4% to 0.5% at high gate (referring to the analytical mobility plots in Figure 6.6 and Figure 6.7). It is clear from this result that the inclusion of the IR scattering greatly reduces the effectiveness of remote screening on II scattering.

Further explanation for the negligible effect of remote screening can be understood from the regions over which remote screening has an effect on II scattering. This region is defined by the channel screening length which can be evaluated using the degenerate, non-parabolic Debye-Hückel model, equation (3.36). Examining plot (b) of Figure 6.11 and Figure 6.12, the electron densities in the channel can be approximated as $n = 2 \times 10^{19} cm^{-3}$ for $V_G = 0.5V$ and $n = 5 \times 10^{19} cm^{-3}$ for $V_G = 1V$ which gives screening lengths of $\lambda_c = 1.06nm$ and $\lambda_c = 0.79nm$ respectively. As discussed in the previous chapter (see Figure 5.16), the scattering model for remote screening has little effect beyond two channel screening lengths (and is negligible at $4\lambda_c$) which leads to a region of around 1.5-2nm from each interface where remote screening can be

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considered to have a strong effect. This is less than 10% of the metallurgical channel length, which is not an appreciable portion of the channel.

Taking a simple estimate on the number of probable scattering events in this small remote screening region is possible and will highlight the importance of II scattering. For both gate voltages, the carrier drift velocity is around $v_d = 0.25 \times 10^7 \text{ cm/s}$ which means the average carrier will traverse the remote screening region in approximately $\tau_{tr} \approx 2 \text{ nm} / 0.25 \times 10^7 \text{ cm/s} = 80 \text{ fs}$. Evaluating the BH scattering rate from section 3.3.3 and the remotely screened model (RSBH) from section 5.2.3.1 for the conditions outlined above, yields rates for both gate voltages on the order of $\Gamma_{BH} \approx 5 \times 10^{12} \text{ s}^{-1}$ and $\Gamma_{RSBH} \approx 2 \times 10^{11} \text{ s}^{-1}$ respectively. Taking these estimates for the scattering rate and transition time, the carriers travelling through the remotely screened region will have a probable number of scattering events of approximately $n_{\Gamma_{BH}} \approx \Gamma_{BH} \tau_{tr} = 0.4$ for the BH model and $n_{\Gamma_{RSBH}} \approx \Gamma_{RSBH} \tau_{tr} = 0.2$ for the RSBH model.

Therefore, within the remote screening region (here defined to be $\sim 2\lambda_c$ from either interface), the BH II model has a probability of scattering which is reduced by a factor of two in the RSBH II model. Although there is a factor of two reduction in probable scattering events, there are still relatively few events within the all important region of remote screening.

6.2.3.2 High Drain Bias

For the detailed analysis at high drain bias, the gate voltage points of $V_G = 0.4 \text{ V}$ and $V_G = 1 \text{ V}$ are chosen. At the higher drain voltage of $V_D = 1 \text{ V}$, the statistical noise in the MC simulation data is less of a factor. Examining the error bars for the high drain $I_D - V_G$ curves in Figure 6.14, this reduction in noise is clear.

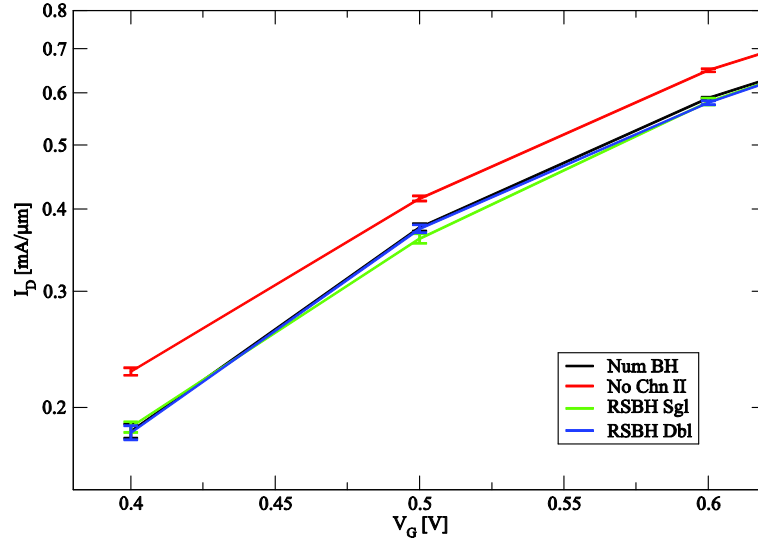


Figure 6.14: I_D - V_G characteristics for the bulk MOSFET with error bars for the low gate voltage points at $V_D = 1V$.

A similar procedure is followed for the presentation and discussion of the high drain results as was taken in the low drain bias analysis. The II scattering tally for both gate voltages is plotted in Figure 6.15. Following this the electron velocity and density are plotted in Figure 6.16 for the 0.4V gate voltage and in Figure 6.17 for the higher gate voltage of 1V.

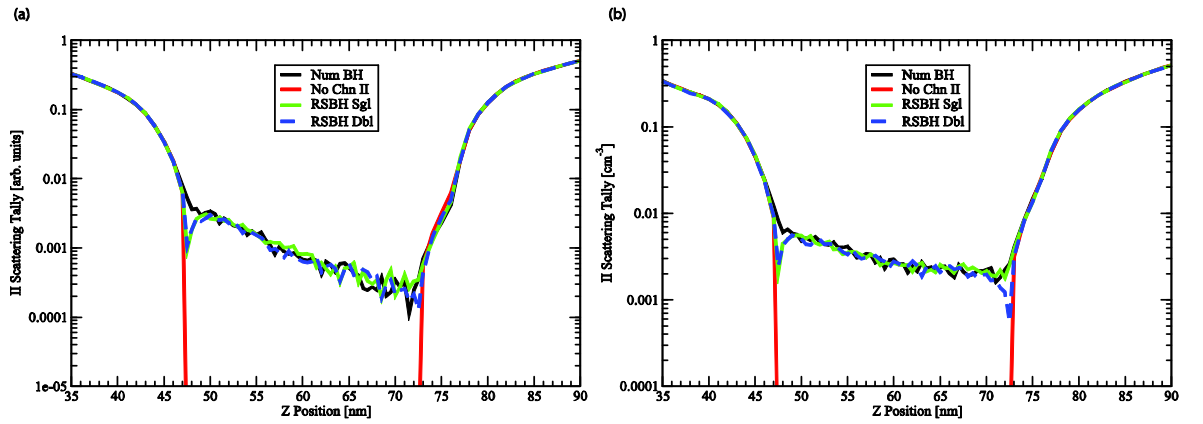


Figure 6.15: Ionized impurity scattering tally along the channel for bulk MOSFET at (a) $V_G = 0.4V$ and (b) $V_G = 1V$ with $V_D = 1V$.

Figure 6.15 shows that the inclusion of remote screening reduces the II scattering tally at the source and drain interfaces. Also evident is the effect of the high drain voltage which biases the channel and reduces the II scattering tally towards the drain. With the large bias across the channel, the electron concentration is very much reduced at the drain end of the channel (see Figure 6.16 and Figure 6.17), causing the reduction in the II scattering tally.

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The low gate voltage electron density, plot (b) in Figure 6.16, shows that the No Chn II case induces a higher density at the drain end of the channel. This is contrary to the behaviour of this scattering case at the lower drain voltage discussed in section 6.2.3.1, where increases in drain current could be explained solely by increases in channel velocity.

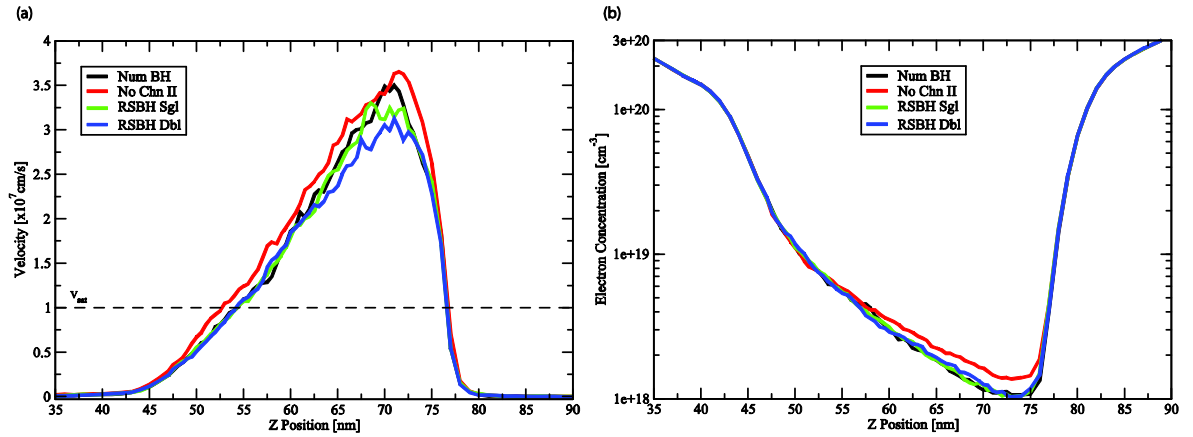


Figure 6.16: (a) Velocity profile and (b) electron density along channel of bulk MOSFET comparing standard and remotely screened ionized impurity scattering models at $V_G = 0.4V$ and $V_D = 1V$.

The increase in drain current of the No Chn II scattering case, as shown in Figure 6.14, is partly explained by the increased electron velocity in plot (a) of Figure 6.16, but more so by the significant increase in electron density in plot (b). With no II scattering in the channel region, the number of scattering events which can randomise the carrier trajectory will be smaller. This reduction in carrier trajectory randomisation will lead to a higher velocity of carriers traversing the channel from source to drain thereby altering the continuity balance and affecting the electron density.

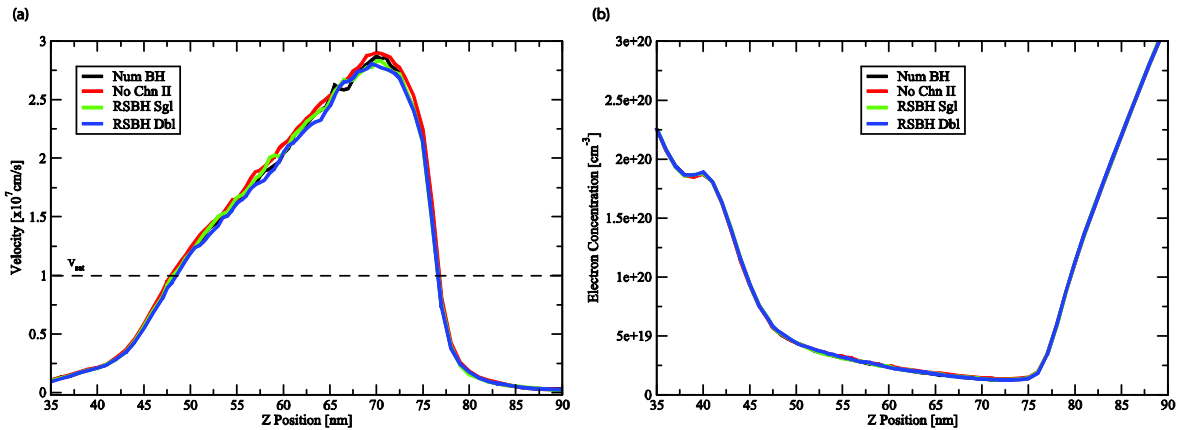


Figure 6.17: (a) Velocity profile and (b) electron density along channel of bulk MOSFET comparing standard and remotely screened ionized impurity scattering models at $V_G = 1V$ and $V_D = 1V$.

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At the highest gate voltage, shown in Figure 6.17, the electron densities are a close match for all the models. The velocity of the No Chn II case is marginally larger than the other models, especially at the peak velocity point at approximately 70nm. At this gate voltage and drain bias, the carriers are passing the source interface at the saturation velocity and continue to accelerate along the channel, that is velocity overshoot occurs over the entire channel length. This behaviour has a strong effect on controlling the drain current where the velocity at the source end of the channel is the dominant factor. Closer examination of the velocity at the source interface shows that the No Chn II case is approximately 4% higher than the Num BH case. Comparing drain currents from the linear $I_D - V_G$ curves of Figure 6.8 also shows a increase in the region of 4%.

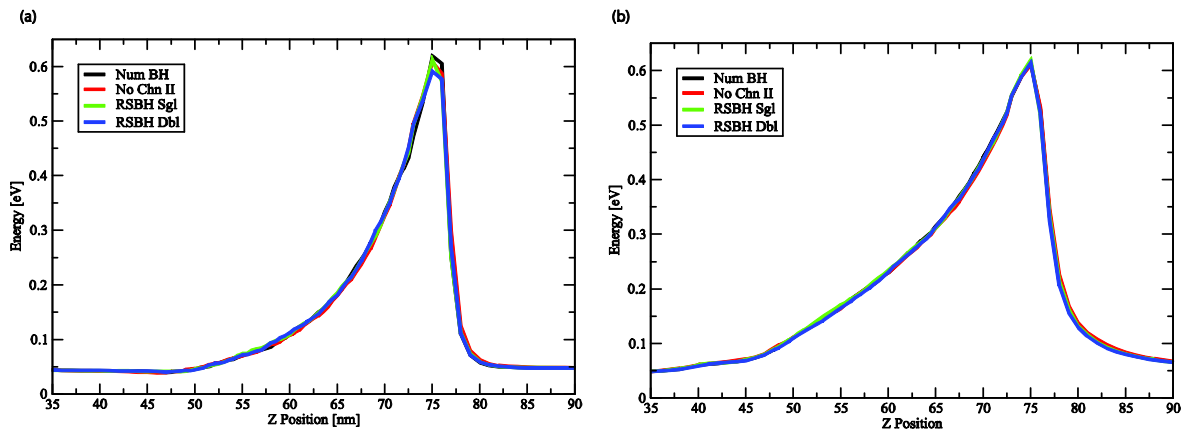


Figure 6.18: Energy profile along channel of bulk MOSFET comparing standard and remotely screened ionized impurity scattering at (a) $V_G = 0.4V$ and (b) $V_G = 1V$, for $V_D = 1V$.

Again the average carrier energies along the channel length remain very close to each other between the different channel II scattering cases. The average energy reached by the ensemble is considerably larger than the low drain bias. Near the drain end of the channel, the average carrier energy is around 600meV, an almost ten-fold increase on the low drain bias energies.

At high drain bias the remotely screened models again show negligible effect on the drain current. Interface roughness scattering continues to play a strong role in defining the channel performance. Removing IR scattering from the simulations provides a 22% increase at low gate voltage and a 28% increase at high gate. It is expected, from the analysis involving the analytical mobility estimate at low drain, that IR scattering will reduce the effectiveness of remote screening.

The region where remote screening can be considered strong can be approximated from evaluation of the screening length at the source and drain end of the channel, again making use of equation (3.36). Electron densities can be approximated from the plots of Figure 6.16 and Figure 6.17, but in this case it needs to be approximated for the both the source and drain end of the channel due to

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the high drain bias. For the lower gate voltage of $V_G = 0.4V$, the electron density is approximated at $n = 10^{19} \text{ cm}^{-3}$ for the source end and $n = 10^{18} \text{ cm}^{-3}$ for the drain end. Evaluating equation (3.36) yields the respective screening lengths of $\lambda_c = 1.4 \text{ nm}$ and $\lambda_c = 4 \text{ nm}$ for the source and drain ends of the channel. The source end of the channel will have a region in the order of $2\lambda_c \approx 3 \text{ nm}$ where remote screening is strongly effective. This corresponds well with the drop in the II scattering tally given in plot (a) of Figure 6.15. This region corresponds to just over 10% of the metallurgical channel length, yet there is no improved performance. At the drain end of the channel, the remote screening region is even larger and can be estimated at $2\lambda_c \approx 8 \text{ nm}$, which is over a third of the channel length.

This lack of performance improvement can be understood by examining the impurity scattering in the remote screening regions at the source and drain end of the channel. Starting by looking at the source end of the channel first, estimates will be made to gain insight into II scattering in the remote screening region. For the low gate bias, the electron velocity can be estimated from Figure 6.16, with a drift velocity of $v_d = 0.4 \times 10^7 \text{ cm/s}$ at the source interface. Given a remote screening region of approximately 3 nm , the transit time for the carrier through this region can be estimated as $\tau_{tr} \approx 3 \text{ nm} / 0.4 \times 10^7 \text{ cm/s} = 74 \text{ fs}$. The BH and RSBH scattering rates can be evaluated from equations (5.64) and (5.40) from Chapter 5, using the conditions outlined above, yielding rates of $\Gamma_{BH} \approx 10^{13} \text{ s}^{-1}$ and $\Gamma_{RSBH} \approx 6 \times 10^{12} \text{ s}^{-1}$ at the source interface. Therefore a carrier has approximately $n_{\Gamma_{BH}} = \Gamma_{BH} \times \tau_{tr} = 0.75$ and $n_{\Gamma_{RSBH}} = \Gamma_{RSBH} \times \tau_{tr} = 0.42$ probable scattering events for the BH and RSBH models respectively, in the remote screening region at the source interface. The relative number of probable II scattering events is almost a factor of two decrease in number of events, but due to the few II events in this small remote screening region the effect is almost negligible.

At the drain interface the scenario is quite different due to the high drain voltage. The drift velocity from Figure 6.16 is $v_d = 3.3 \times 10^7 \text{ cm/s}$ at the drain interface with a corresponding transit time through the 8 nm remote screening region of $\tau_{tr} \approx 24 \text{ fs}$. The average carrier energy, plotted in plot (a) of Figure 6.18, is around 0.45 eV which is very large. Evaluating the BH and RSBH scattering rates gives $\Gamma_{BH} \approx 6 \times 10^{13} \text{ s}^{-1}$ and $\Gamma_{RSBH} \approx 9 \times 10^{12} \text{ s}^{-1}$ at the drain interface. Estimating the probable number of scattering events at the drain end of the channel from this data, $n_{\Gamma_{BH}} = \Gamma_{BH} \times \tau_{tr} = 1.44$ and $n_{\Gamma_{RSBH}} = \Gamma_{RSBH} \times \tau_{tr} = 0.2$, shows a greater difference between the models. Despite this large difference between probable number of scattering events, there is still no noticeable change in the channel performance characteristics. This negligible shift in channel performance at the drain end is due to the very high carrier energy. Evaluation of the differential scattering cross section

highlights the dominance of small angle, forward scattering at these high carrier energies. Such scattering events typically have only a small effect on the momentum relaxing effect of scattering.

At high gate voltages, the increased screening of the high carrier density reduces the remote screening regions to around $1.6nm$ at the source interface ($\lambda_c = 0.79nm$) and $2.5nm$ at the drain interface ($\lambda_c = 1.25nm$). This in conjunction with the high carrier velocity and increased energy greatly reduces the effectiveness of II scattering. The number of probable scattering events for each electron in either the source or drain remote screening region becomes very small, on the order of $n_T \approx 0.02 - 0.04$ per electron. This behaviour is expected at this high gate, high drain condition where the carrier density and average energy are at peak levels.

6.2.4 Summary

The bulk MOSFET device has an advanced channel doping profile, demonstrated in Figure 6.2, that includes a retrograde channel with halo implants which help to reduce short-channel effects. The channel is very highly doped at around $N_I \approx 10^{18} cm^{-3}$ (with source/drain wells at $N_I \approx 10^{20} cm^{-3}$) which will lead to a large amount of channel impurity scattering.

In this device the source and drain interface position have been simply chosen as the point of steepest gradient of the net doping, shown in Figure 6.4. This choice of position happens to coincide with the metallurgical p-n junction and gives the source interface at $Z = 47nm$ and the drain interface at $Z = 73nm$.

Using initial DD simulation data, an analytical analysis of the phonon and impurity limited mobility was completed for low drain voltage conditions. This analysis provides insight into the effect that remote screening has on impurity scattering in a device context, and highlights the expected effect of remote screening on the channel performance. At very low gate voltages when the channel carrier density is low, remote screening leads to a large increase in carrier mobility. For $V_G = 0V$, the analysis predicts a channel mobility increase of over 100% along the channel. As the carrier density increases with gate voltage, the effect of remote screening is minimised.

At the minimum MC simulation gate voltage of $V_G = 0.4V$, the analytical mobility analysis predicts a peak increase of 20% at the source end of the channel and 10% at the drain end of the channel. Due to the high screening, this region of increased mobility is restricted to a few important nanometre's at each interface. At the highest gate voltage simulated, $V_G = 1V$, the effect

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of remote screening is very small with a maximum increase of 10% at the source interface and a consistent 2% increase along the channel length.

MC simulation of the bulk MOSFET with the remotely screened II model demonstrated results that are much less dramatic than predicted with the analytical mobility analysis. The simulation of the newly developed II scattering model proved to offer negligible difference to the carrier transport in the channel region. Results are also obtained which removes the II scattering entirely from the channel to obtain an upper limit. These results show that in the bulk MOSFET, the II scattering process has a role in determining the channel performance and drain current.

Not considered in the analytical mobility estimate is the effect of IR scattering on the channel performance, which is found to strongly affect the bulk MOSFET device. At low drain bias, removal of IR scattering from the device increases the drain current by up to 88% at a gate voltage of $V_G = 1V$. A simple estimate for the IR limited mobility is made at low drain voltage to evaluate the effect on the remote screening. Through use of Mathiessen's rule, the IR limited mobility was added to the analytical mobility and found to reduce the effectiveness of remote screening from 14% to 4.5% at low gate and from 4% to 0.5% at high gate. IR scattering is shown from this simple estimate to be a dominant mechanism in the bulk MOSFET device and reduces any appreciable effect of remote screening.

The region in a device channel where remote screening is effective was also analysed and found to be around 2-3nm at the source end, but could be as much as 8nm at the drain end of the channel. For the metallurgical channel length of 26nm in this device, these remote screening regions can be an appreciable portion of the channel length. Examining the II scattering in these remote screening regions, it was shown that for the source end of the channel, probable II scattering events are quite low. Typically there is a probability of less than one II scattering event per carrier travelling through the remote screening region.

At low drain bias, the carriers have approximately $n_{\Gamma_{BH}} \approx 0.4$ probable scattering events with the BH model which halves to $n_{\Gamma_{RSBH}} \approx 0.2$ with remote screening. At high drain bias and low gate voltage conditions, the probability of II scattering is slightly higher with $n_{\Gamma_{BH}} \approx 0.75$ for BH which drops to $n_{\Gamma_{RSBH}} \approx 0.42$. Despite the consistent drop with the use of remote screening of II scattering, the number of events is too low to affect the channel performance characteristics.

At the drain end of the channel for high drain voltages, where the remote screening region is large and can be up to 8nm, the carrier energy is so large that II scattering has little effect. For high

energy carriers, the scattering is dominated by small angle forward scattering events which have little momentum relaxing effect on the carriers.

6.3 22nm Double-Gate Device

The ultra-thin body double gate (UTB DG) device has been developed as a template device for the PullNano European research project. It was developed originally to compare device simulations amongst a consortium of European research groups [116]. Here this device has been reconstructed and calibrated using the commercial Sentaurus software to the original specification, then exported for use with the in-house DD simulator. As discussed before, the MC simulation uses the DD solution output as a starting point and requires no further calibration.

Repeating a similar analysis for the UTB DG device as for the bulk MOSFET, the section will start with a brief discussion of the device structure and the calibration between simulations in section 6.3.1. Using initial DD data, an analytical calculation of the carrier mobility with and without remote screening has been completed with discussion in section 6.3.2. Section 6.3.3 presents and examines the MC simulation data for the device with the newly developed II scattering mechanisms.

6.3.1 Device Structure and Calibration

The UTB DG device has been developed and optimised for low standby power (LSTP) applications for the 22nm technology node. The device has a 22nm metal gate (a work function of $\phi_G = 4.8eV$) with a 1.1nm silicon-dioxide insulator layer and a 10nm silicon body thickness as depicted in Figure 6.19. The remote screening plane definition is given in the lower-left corner of Figure 6.19 and the positions of the remote screening interfaces at $Z=0$ and $Z=L_C$ are marked.

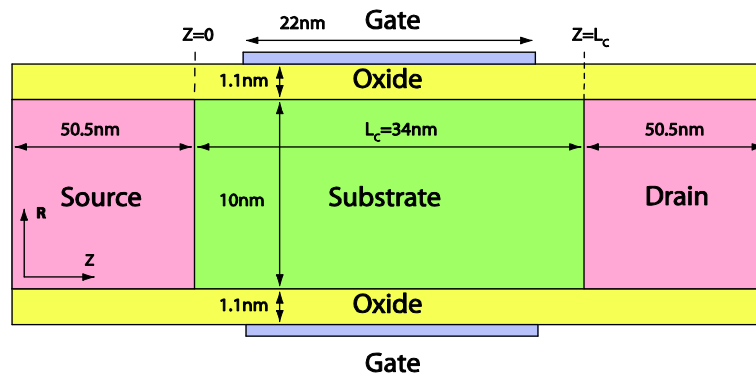


Figure 6.19: Structure of the Ultra-Thin-Body Double-Gate device.

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This device was originally developed with a high- κ dielectric with effective oxide thickness (EOT) of 1.1nm but this has been disregarded here as the high- κ dielectric requires additional scattering mechanisms for accurate simulation. Instead, the oxide layer is replaced with silicon dioxide of 1.1nm so that the electrostatic nature of the insulator is retained without the additional overhead of dealing with the advanced gate stack of a high- κ dielectric.

The net doping profile for the structure is shown in Figure 6.20. The DG device has a low doped p-type channel with $N_A = 1.2 \times 10^{15} \text{ cm}^{-3}$ and highly doped source/drain regions at $N_D = 5.2 \times 10^{19} \text{ cm}^{-3}$.

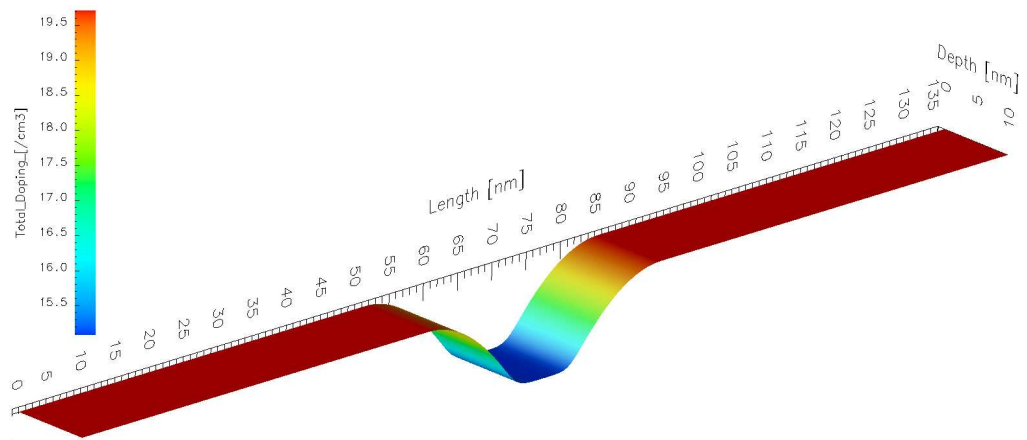


Figure 6.20: Net doping concentration for the Ultra-Thin-Body Double-Gate device.

The source and drain doping is a constant doping level from the edges of the device up to 50.5nm and 84.5nm respectively, with a Gaussian function roll-off of the doping into the channel region. This gives a gate underlap of 6nm from the region of constant doping of the source and drain to the metal gate.

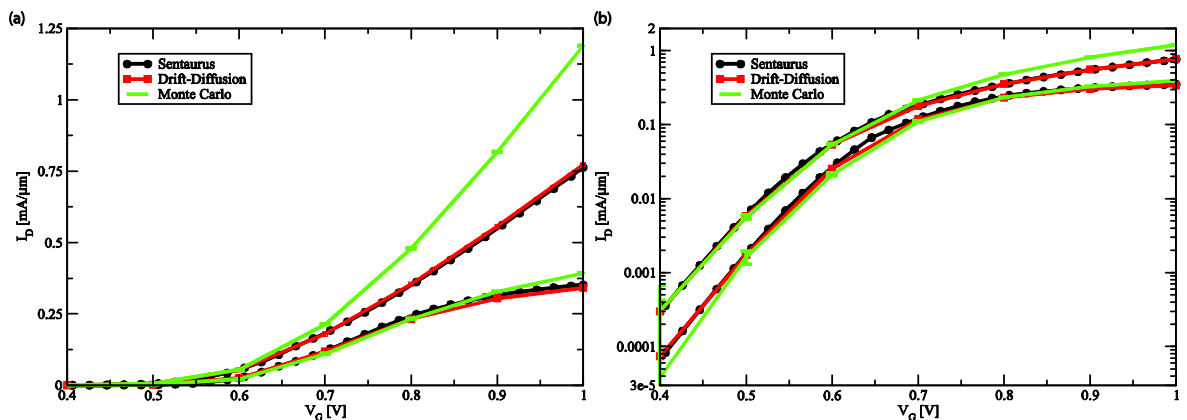


Figure 6.21: (a) Linear and (b) semi-log I_D - V_G calibration plots showing the comparison between Sentaurus, Drift-Diffusion and Monte Carlo simulation.

6.3 22nm Double-Gate Device

The DD simulation was calibrated against the commercial TCAD tool, Sentaurus [117] at both low and high drain voltages of $V_D = 0.1V, 1V$. The calibrated $I_D - V_G$ characteristics for both drain voltages are shown in Figure 6.21 along with the MC simulation output. The MC simulation is a close match with the DD simulation when non-equilibrium carrier transport effects are minimal, that is at low drain and/or low gate voltage. The effects of non-equilibrium transport are clear for the MC results for high drain at high gate voltage.

The source and drain interfaces must also be selected for the remotely screened II models and again the choice of interface position is taken here solely through the use of the difference plot of the net doping profile, plot (b) of Figure 6.22.

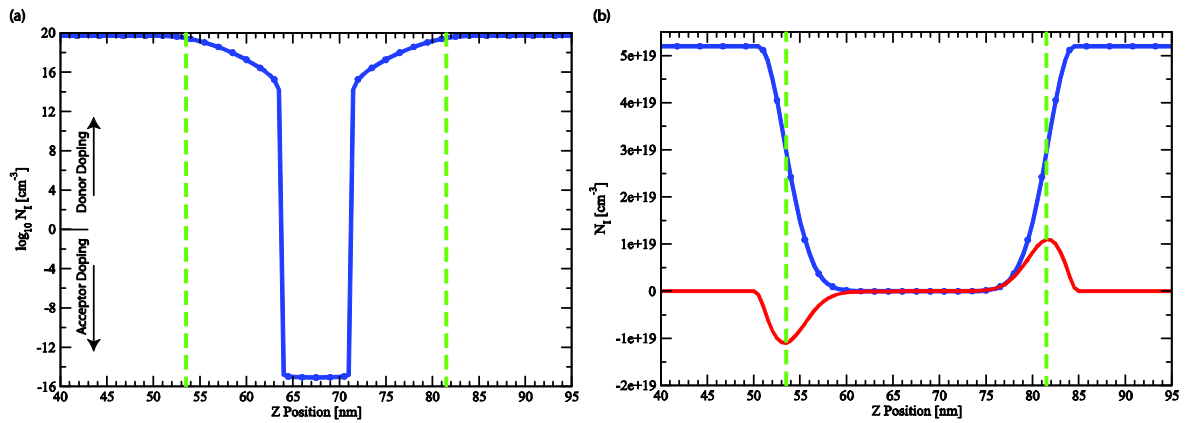


Figure 6.22: (a) Net doping profile with signed log scale and (b) net doping difference plot for the Ultra-Thin-Body Double-Gate device.

The position where the net doping is at its maximum gradient, highlighted by the difference plot, is chosen here as the position of the interface and is considered to be closest to the original definition of the interface as the point where the doping density changes abruptly from source/drain to channel concentrations. The source and drain interfaces, depicted in Figure 6.22 as the green dashed lines, are at 53.5nm and 81.5nm giving a novel channel length of around 28nm.

6.3.2 Analytical Estimate of Remote Screening Effect

An estimate of the remote screening effect on carrier transport through the channel of the DG device can be calculated using the Kubo-Greenwood formula for mobility [33]. The spatially varying channel mobility can be estimated using the momentum relaxation rates for phonons and BH and RSBH II models along with DD simulation data for impurity and electron concentrations.

The method used to obtain the channel mobility here is identical to that explained and utilised in section 6.2.2. To recap, Mathiessen's rule is used to sum the individual scattering mechanisms

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along with an ensemble averaged momentum relaxation length to take a moving median of the spatially varying total mobility. The phonon relaxation rates presented in section 3.3.2 are used to calculate phonon mobilities independently. The II scattering models are calculated from expressions given in the previous chapter, Chapter 5, and include the BH, single interface RSBH and double interface RSBH models. The analysis has been completed for three gate voltages, $V_G = \{0V, 0.4V, 1V\}$, at the low drain voltage of $V_D = 0.1V$.

In Figure 6.23 the plots of (a) electron and impurity concentration and (b) phonon and impurity limited mobility are given for the lowest gate voltage of $V_G = 0V$. The ensemble average momentum relaxation rate is calculated using equation (6.2) to be $\langle \tau_m^{tot} \rangle \approx 5.6 \times 10^{-14} s$, giving a mean free path as $l_{\tau_m} \approx 5.6nm$.

The effect of the minimal impurity density in the channel region is shown in plot (b) of Figure 6.23, where the mobility is entirely phonon controlled between roughly 63-72nm. It is within this phonon controlled region that impurity concentration is just above $N_I = 10^{15} cm^{-3}$. At this low density the II limited mobility is extremely high and can be considered to have negligible effect. For example, for an impurity density of $N_I = 10^{15} cm^{-3}$ with an electron concentration of $n_e = 10^{10} cm^{-3}$, the impurity limited mobility is roughly $\mu_{II} \approx 150\,000 cm^2 / Vs$.

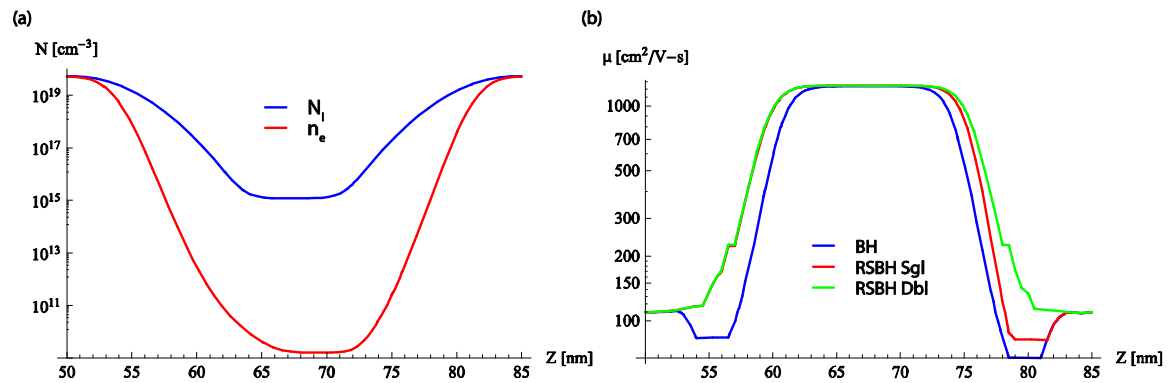


Figure 6.23: Plot of (a) the impurity and electron density, and (b) the impurity limited mobility for the UTB DG MOSFET at a gate voltage of $V_G = 0V$ and a drain voltage of $V_D = 0.1V$.

II scattering in the channel has only an effect within the region of the Gaussian roll-off of the source/drain doping at the edges of the channel. This region of II scattering controlled transport is clearly shown in plot (b) of Figure 6.23. The II controlled region constitutes approximately a 9nm region at each end of the channel where remote screening affects the channel performance.

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At this low gate voltage where the electron density in the channel is very low, remote screening has a large effect in the mobility. At the source end of the channel both remotely screened models provide in the region of a 150% increase in mobility, and around 200% for the double interface model at the drain end of the channel.

The analytical mobility estimate for the gate voltage $V_G = 0.4V$, is plotted in Figure 6.24. The average ensemble momentum relaxation rate is calculated as $\langle \tau_m^{tot} \rangle = 6.2 \times 10^{-14} s$ giving a mean free path of $l_{\tau_m} = 6.1nm$.

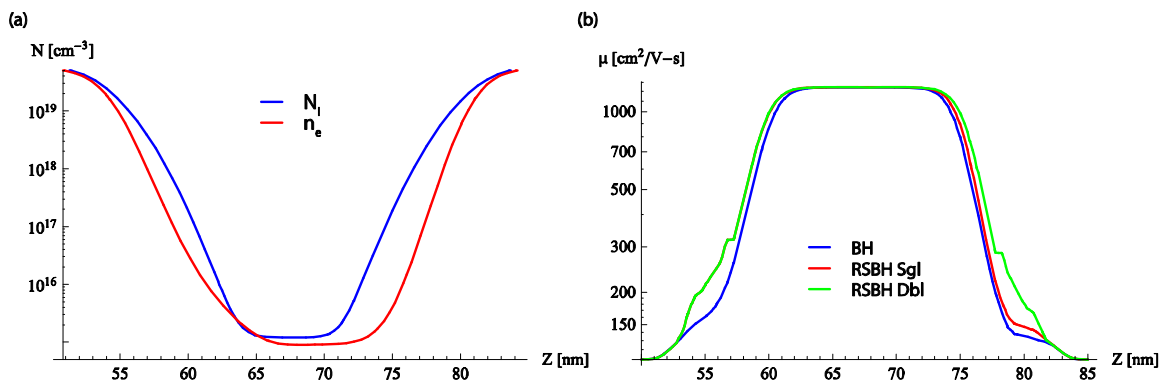


Figure 6.24: Plot of (a) the impurity and electron density, and (b) the impurity limited mobility for the UTB DG MOSFET at a gate voltage of $V_G = 0.4V$ and a drain voltage of $V_D = 0.1V$.

Increasing the gate voltage to $V_G = 0.4V$, the electron concentration in the channel of the device has increased by several orders of magnitude, as plotted in (a) of Figure 6.24. This increase in the screening concentration leads to a reduction in the strength of II scattering to control the mobility, as shown in the mobility, plot (b). This of course has the roll on effect of reducing the strength of remote screening on the II scattering. Despite the large increase in the screening within the channel, there is a peak increase of channel mobility of approximately 40% at the source and 60% at the drain for the single and double interface models, respectively.

Increasing the gate voltage to the highest simulated, $V_G = 1V$, increases further the channel electron concentration which is now several orders of magnitude bigger than the impurity concentration. At this gate voltage, the ensemble momentum relaxation rate is found to be $\langle \tau_m^{tot} \rangle = 7.8 \times 10^{-14} s$, leading to a mean free path of $l_{\tau_m} = 7.8nm$.

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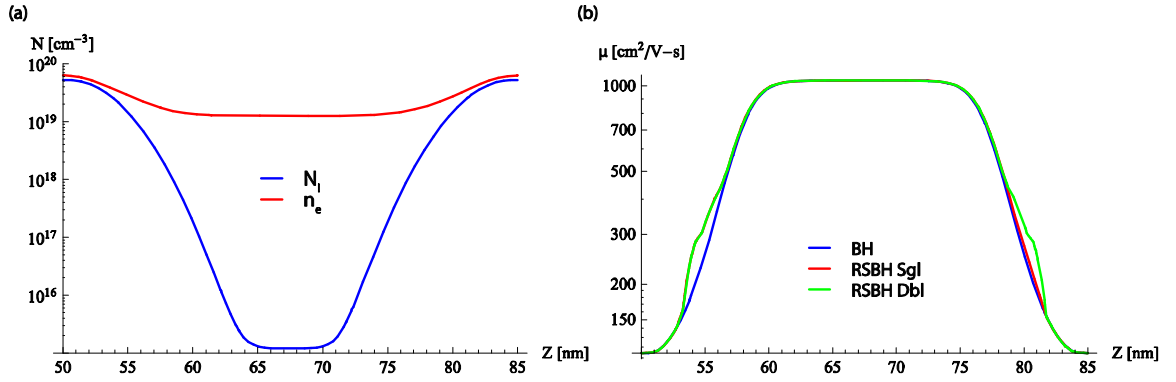


Figure 6.25: Plot of (a) the impurity and electron density, and (b) the impurity limited mobility for the UTB DG MOSFET at a gate voltage of $V_G = 1\text{V}$ and a drain voltage of $V_D = 0.1\text{V}$.

The increase in screening will further reduce the effectiveness of remote screening in increasing the channel mobility, which is expected at high gate voltages. Although the effect of remote screening is minimised, it still leads to approximately a 40% increase in the mobility at either end of the channel (drain increase due to double interface model).

Summarising this simple analysis of the phonon and impurity limited mobility for the DG device, it is clear that the low doped channel region is significantly less controlled by impurity scattering than in the case of a typical bulk MOSFET. Impurity scattering plays a negligible role within the 9nm metallurgical p-n junction region in the centre of the device, although there is still significant II scattering surrounding the source and drain interfaces. Remote screening is shown to have a very large increase at the low gate voltage of $V_G = 0\text{V}$, in the region of 150-200%. This large increase in mobility at low gate voltages is predicted to increase the sub-threshold leakage of this MOSFET device. As the device has been developed to fulfil the LSTP requirements, the effect of remote screening could play a strongly detrimental role in the device performance.

As the screening strength increases, the strength of remote screening reduces, as is expected. At $V_G = 0.4\text{V}$, the new II scattering model is expected to increase the channel mobility near the interfaces by up to 40% at the source and 60% at the drain. Even at the highest gate voltage, there is an expected 40% increase in channel mobility within the region of II controlled mobility near the interfaces.

6.3.3 I_D - V_G Behaviour with Remote Screening

The UTB DG device has been simulated in the MC code with four different channel II scattering cases, identical to the bulk MOSFET simulation discussed previously in this chapter. These cases

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are: Num BH – numerically capped Brooks-Herring scattering in the channel region as presented in section 5.4.1; No Chn II – all channel II scattering is removed; RSBH Sgl – remotely screened BH model for the single (source) interface case; RSBH Dbl – remotely screened BH model for the double interface case.

Simulations have been completed to obtain the $I_D - V_G$ characteristics for a range of gate voltages of $V_G = \{0.4V, \dots, 1V\}$ and drain conditions $V_D = 0.1V, 1V$. The restricted range of gate voltages is again due to the statistical noise in MC simulation at low gate voltages, when the majority carrier concentration in the channel region becomes extremely low. Here Figure 6.26 present the results of the MC simulations for all four II scattering cases with error bars at each data point giving the statistical error due to noise.

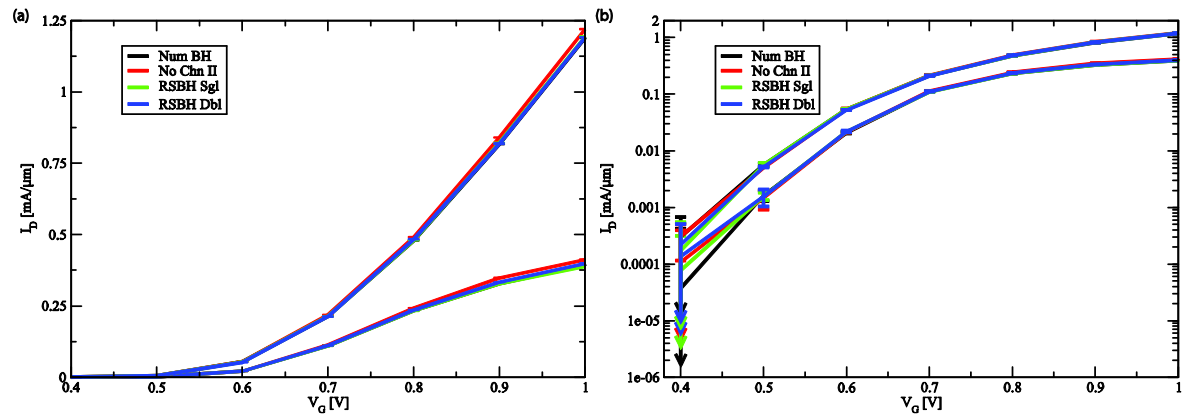


Figure 6.26: (a) Linear and (b) semi-log $I_D - V_G$ characteristics for the UTB DG MOSFET with remotely screened impurity scattering.

Examining the linear plot of the $I_D - V_G$ characteristics of plot (a) in Figure 6.26 show that II scattering plays a very minor role in determining the channel performance. Simulations with the channel II scattering turned off show that there is a very small increase in the drain current at high gate voltages. This increase in drain current corresponds approximately to a maximum increase of around $20 - 30 \mu\text{A}/\mu\text{m}$ at the peak gate voltage.

The logarithmic plot of the drain current, plot (b) of Figure 6.26, further demonstrates the lack of impurity scattering in controlling the device performance. At the lowest gate voltage point, $V_G = 0.4V$, the statistical noise is dominant and examination of the results are not reliable due to this. At the higher voltage of $V_G = 0.5V$, the noise is still considerable but the results seem to corroborate the minimal affect of impurity scattering. These results strongly demonstrate that impurity scattering in the channel region of this particular device is very much a negligible effect in determining the device performance. Remote screening clearly has negligible effect in defining the

drain current. A brief analysis of several data points at low and high drain will be completed in the following sub-sections to confirm the behaviour seen in the $I_D - V_G$ plots.

6.3.3.1 Low Drain Bias

The low drain voltage analysis will examine two gate voltage points to confirm the behaviour shown in the $I_D - V_G$ characteristics. A low gate voltage point will be chosen below with the aid of the error bars in the $I_D - V_G$ plots, Figure 6.27. The high gate voltage will be the $V_G = 1V$ point which can be selected without error bar consideration as statistical noise is not a factor at high fields.

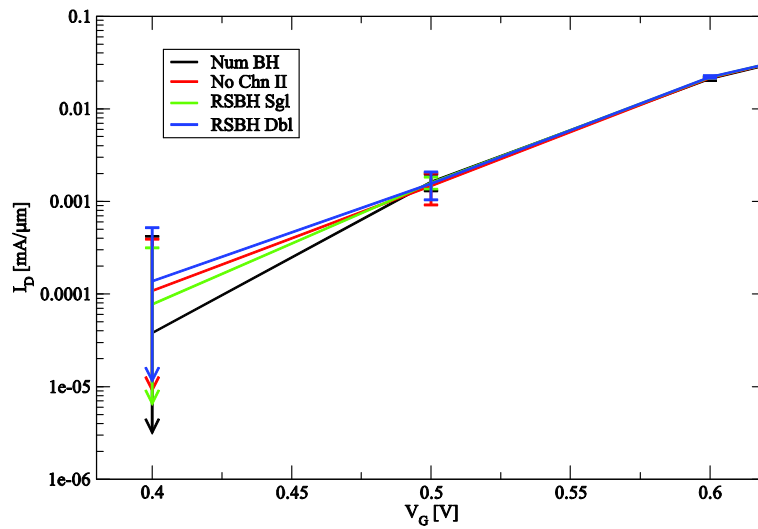


Figure 6.27: Semi-log plot of the low gate voltage $I_D - V_G$ characteristics with error bars for the UTB DG MOSFET at $V_D = 0.1V$.

Figure 6.27 gives the low gate voltage drain currents in more detail with their corresponding error bars. The error bars at the lowest gate voltage of $V_G = 0.4V$ are particularly large and have been clipped to fit them on the plot, hence the arrow as the bottom cap. Considering the magnitude of the noise at this voltage this point is not analysed here. At the higher gate voltage of $V_G = 0.5V$ the error bars are still quite large despite the corroboration between the drain currents, and for this reason it also will not be analysed here. Instead, the data point at $V_G = 0.6V$ will be analysed given that results appear stable, given the small error bars.

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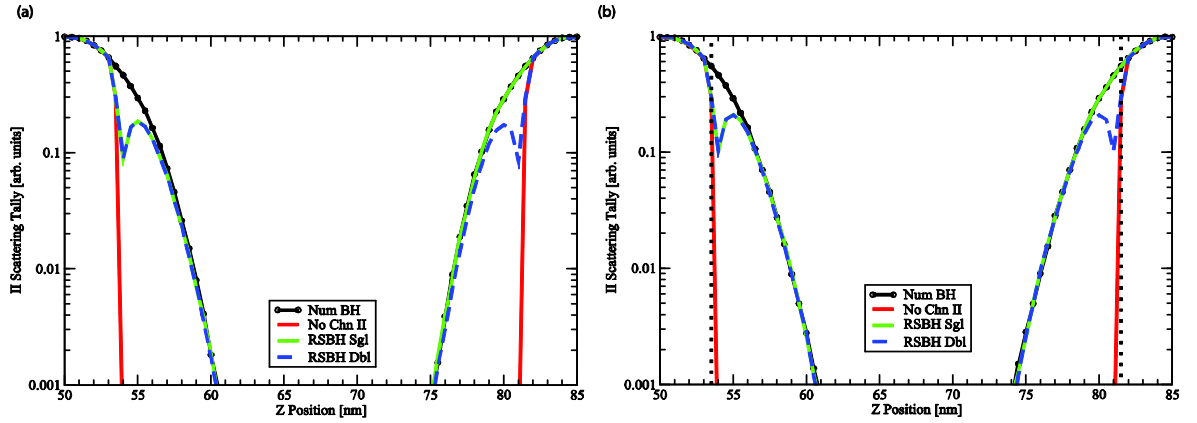


Figure 6.28: Ionized impurity scattering tally along the channel for UTB DG MOSFET at (a) $V_G = 0.6V$ and (b) $V_G = 1V$ with $V_D = 0.1V$.

Starting by looking at the II scattering tally for both gate voltage points in Figure 6.28 (note that the II scattering tally is given with arbitrary units). Here the II scattering tally is extremely low in the centre of the channel of the device which, referring to Figure 6.22, is expected as the dopant density is very low. In both plot (a) and (b) of Figure 6.28 the effect of remote screening on the II scattering tally is evident. There is a distinct reduction in the number of events at both of the interfaces, considering either the single or double interface model. This is consistent with the expectation of a reduced scattering rate with remotely screened II scattering.

Given the close match between the drain currents at low gate voltages of each of the II cases considered here (Figure 6.26), the velocities and carrier densities are expected to be almost identical between the models. At high gate voltages only the case that removes channel II scattering, No Chn II, is expected to demonstrate any shift in velocity/carrier density.

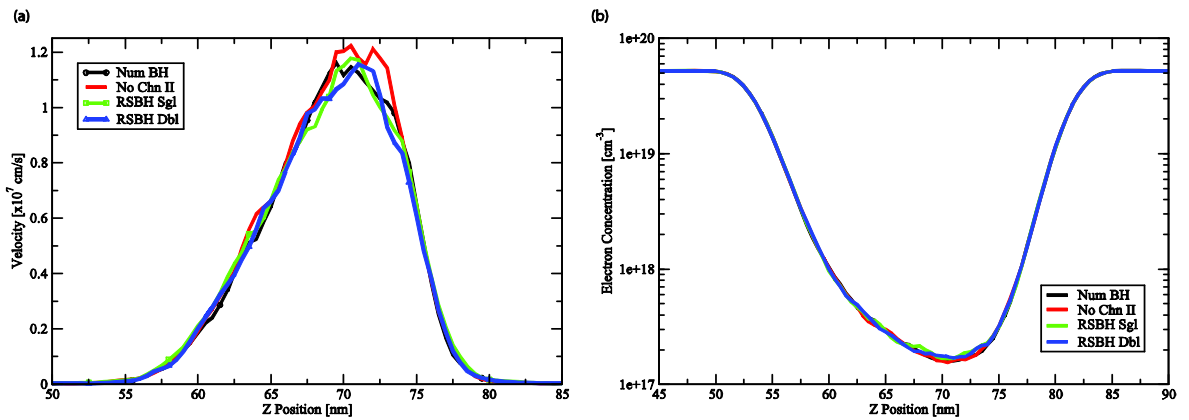


Figure 6.29: (a) Velocity profile and (b) electron density along channel of UTB DG device with $V_G = 0.6V$ and $V_D = 0.1V$.

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The electron velocity and density for the low gate voltage point are shown in Figure 6.29. As expected, given that the drain currents match, the carrier densities and velocities are very close along the length of the channel for all four cases.

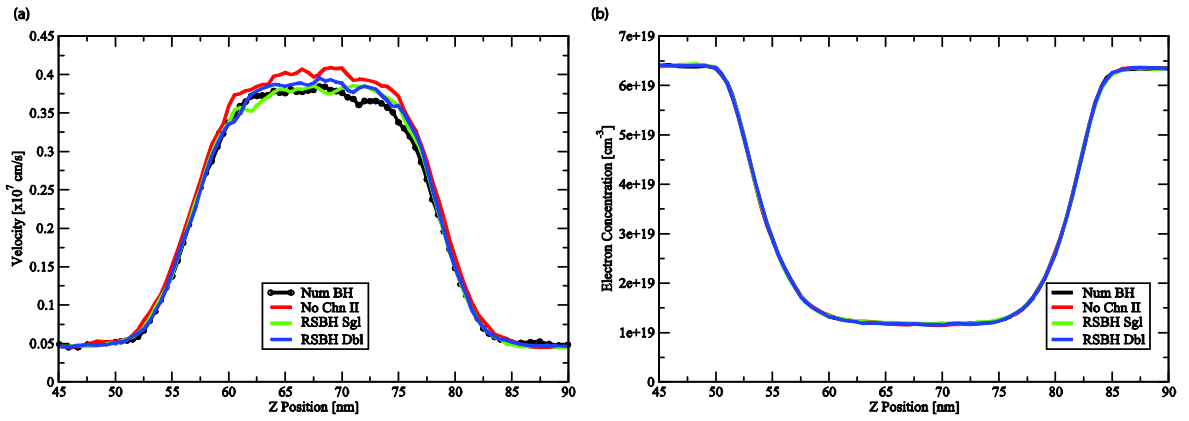


Figure 6.30: (a) Velocity profile and (b) electron density along channel of UTB DG device with $V_G = 1V$ and $V_D = 0.1V$.

At a gate voltage of $V_G = 1V$ the electron densities of plot (b), Figure 6.30 are identical. As expected the No Chn II case demonstrates an increase in electron velocity over an appreciable length of the channel, approximately a 5% increase in velocity over the Num BH case. This explains the increase in drain current at this data point displayed in the drain current plot of Figure 6.26.

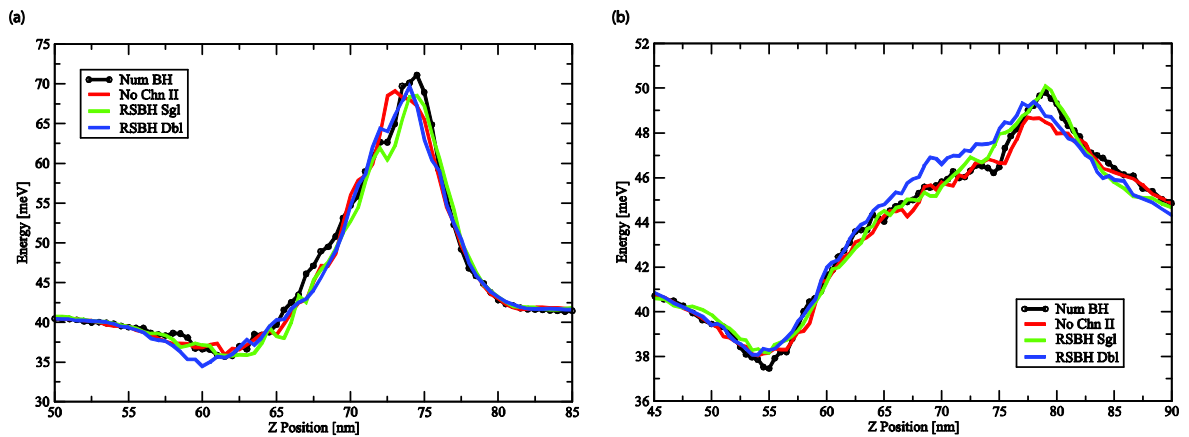


Figure 6.31: Energy profile along channel of UTB DG device with (a) $V_G = 0.6V$ and (b) $V_G = 1V$ for $V_D = 0.1V$.

The UTB DG device shows negligible difference with the inclusion of remotely screened impurity scattering at low drain bias. This is explained by the low doped channel, which due to the small impurity concentration has minimal channel II scattering. This is highlighted by the very small

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shift in drain current when channel II scattering is removed from the simulation. The small amount of impurity scattering at the source and drain end of the channel account for the modest increase in drain current at very high gate voltage. Of course, with high gate voltages the screening density in the channel is large and remote screening is minimised. For $V_G = 1V$ the electron density in the channel can be approximated at $n = 10^{19} cm^{-3}$ and evaluating equation (3.36) gives a screening length of $\lambda_c = 0.92nm$.

The role of IR scattering has been studied in this device and is found to have a small effect in defining the channel performance. Removal of IR scattering in the device causes around a 2-4% increase in drain current. This lack of IR scattering is an advantage of the UTB DG device as the channel enters the volume inversion regime [125]. That is, for silicon body thicknesses between $3nm < t_{si} < 20nm$, the channel region becomes almost fully inverted at high gate voltage causing the conducting channel to be located in the middle of the body. This is known to reduce the influence of surface scattering events including IR scattering [125-127].

6.3.3.2 High Drain Bias

With the high drain bias the statistical noise in the results is reduced considerably, as shown in Figure 6.32. Again, analysis of the results will be undertaken for two gate voltages. The low gate voltage point will be $V_G = 0.5V$ and the high gate voltage at $V_G = 1V$. Here the results are expected to be close to each other except for the No Chn II case at high gate voltages, similar to the low drain results.

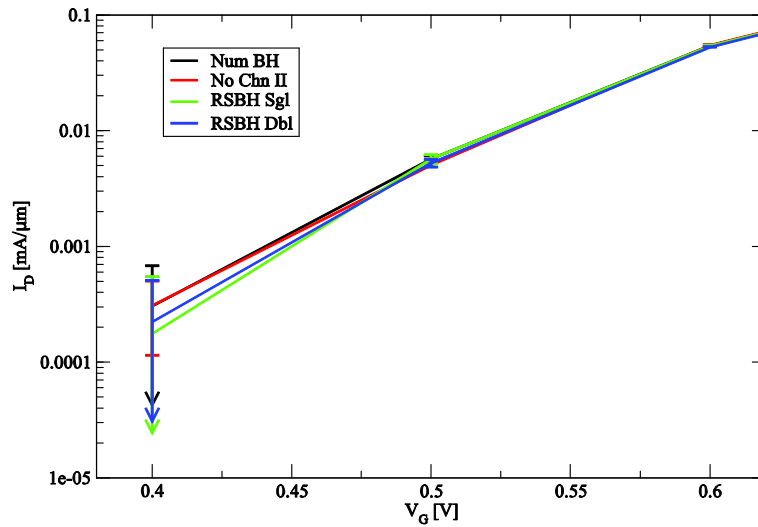


Figure 6.32: Semi-log plot of the low gate voltage I_D - V_G characteristics with error bars for the UTB DG MOSFET at $V_D = 1V$.

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The II scattering tally is plotted for both gate voltage points in Figure 6.33. The distinctive behaviour of the remote screening models is evident at the source interface where the II scattering tally drops abruptly at the interface and at the drain in the high gate voltage plot of (b). At the drain interface of the low gate voltage in plot (a), this distinctive behaviour is not present and all the II scattering cases drop off rapidly.

A closer examination of plot (a) in Figure 6.33 shows that the numerically capped BH model (Num BH) matches with the remotely screened single interface model (RSBH Sgl) as is expected at the drain interface. The remotely screened double interface model (RSBH Dbl) follows the no channel II scattering case (No Chn II) which demonstrates that the II scattering at the drain is being correctly remotely screened.

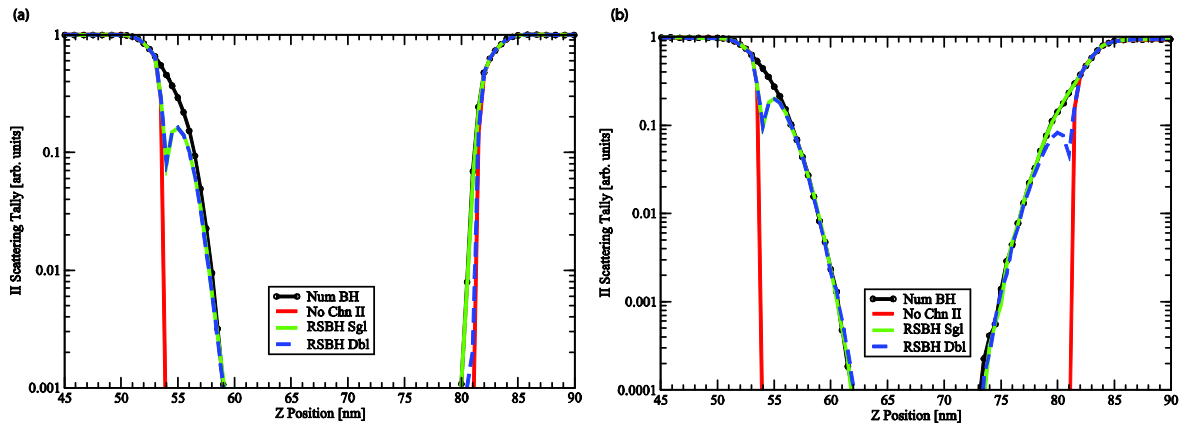


Figure 6.33: Ionized impurity scattering tally along the channel for UTB DG MOSFET at (a) $V_G = 0.5V$ and (b) $V_G = 1V$ with $V_D = 1V$.

This change in behaviour at the drain in plot (a) of Figure 6.33 is obviously due to a reduction in II scattering at the drain end of the channel. Given the high drain bias of $V_D = 1V$, the channel inversion layer will be biased such that the carrier density at the drain end of the channel will be lower. Combined with the increased carrier energy due to the drain bias, plot (a) of Figure 6.36, this results in a reduced II scattering tally at the drain end of the channel. This behaviour is also shown to a lesser effect in plot (b) of Figure 6.33.

To confirm this justification a simple calculation can be completed, through use of equation (6.8), to obtain an estimate on the number of carriers present in the drain end of the channel.

$$n_e^{vol} = V \times n_e \quad (6.8)$$

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Here n_e^{vol} is the number of electrons in a volume given by V with an electron density of n_e . Referring to Figure 6.19 the volume of the channel is given as $V = 34nm \times 10nm \times 1nm = 3.4 \times 10^{-19} cm^3$ (for the MC simulations completed here the device width is 1nm), but considering only the drain end of the channel this becomes $1.7 \times 10^{-19} cm^3$. The electron density is given in plot (b) of Figure 6.34 and for the drain end of the channel will be estimated at $1.5 \times 10^{16} cm^{-3}$. Evaluating equation (6.8) gives an electron number of 2.55×10^{-3} in the drain end of the channel which relates to roughly 4 superparticles (1 superparticle $\approx 5.7325 \times 10^{-4}$ electrons).

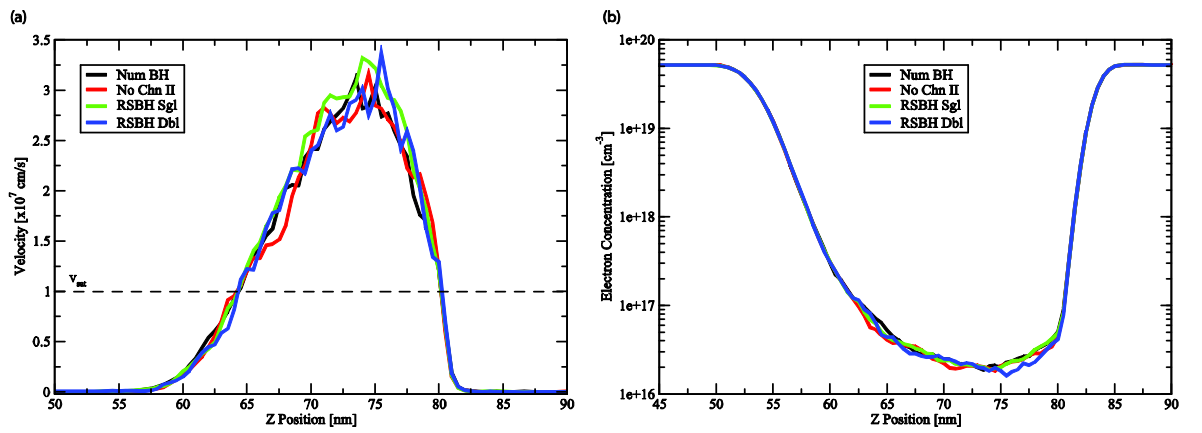


Figure 6.34: (a) Velocity profile and (b) electron density profile along channel of UTB DG device with $V_G = 0.5V$ and $V_D = 1V$.

The velocities of each of the four channel II scattering cases for the low gate voltage, plot (a) of Figure 6.34, are comparable given the relatively few electrons (or superparticles) that travel through the channel region. At the high gate voltage shown in Figure 6.35, the velocities are again very close to each other with the No Chn II case being the largest by a small margin. This increased velocity explains the drain current increase shown in Figure 6.26.

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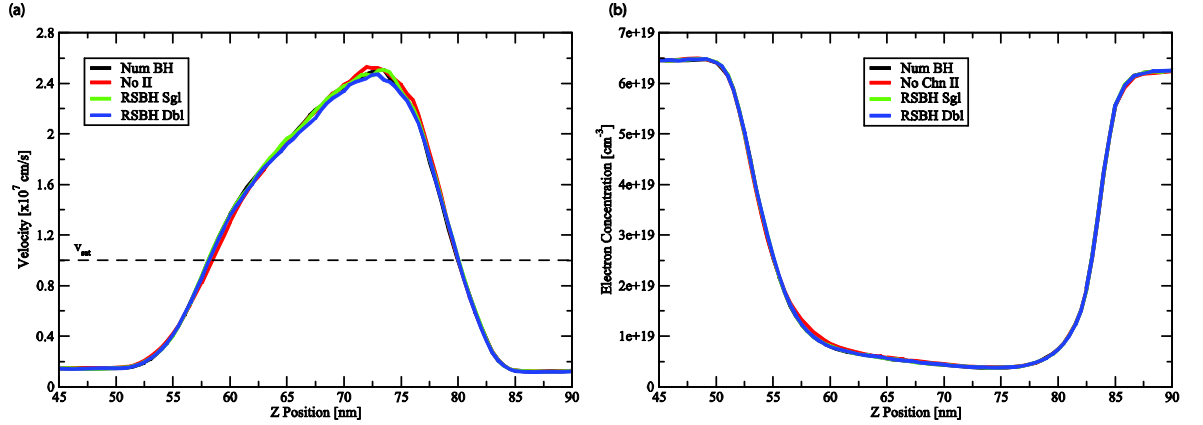


Figure 6.35: (a) Velocity profile and (b) electron density profile along channel of UTB DG device with $V_G = 1V$ and $V_D = 1V$.

Plot (a) of Figure 6.35 shows that the electrons are above the saturation velocity over a large proportion of the channel. This phenomenon, which is a feature of non-linear transport in MC simulations, provides an increase in drain current beyond the velocity saturated value [15]. An interesting point demonstrated in these figures is that the peak velocity and energy of the carriers at low gate voltage is much larger than that at high gate voltage. This can be explained through the density of carriers that traverse the channel at low or high gate voltage.

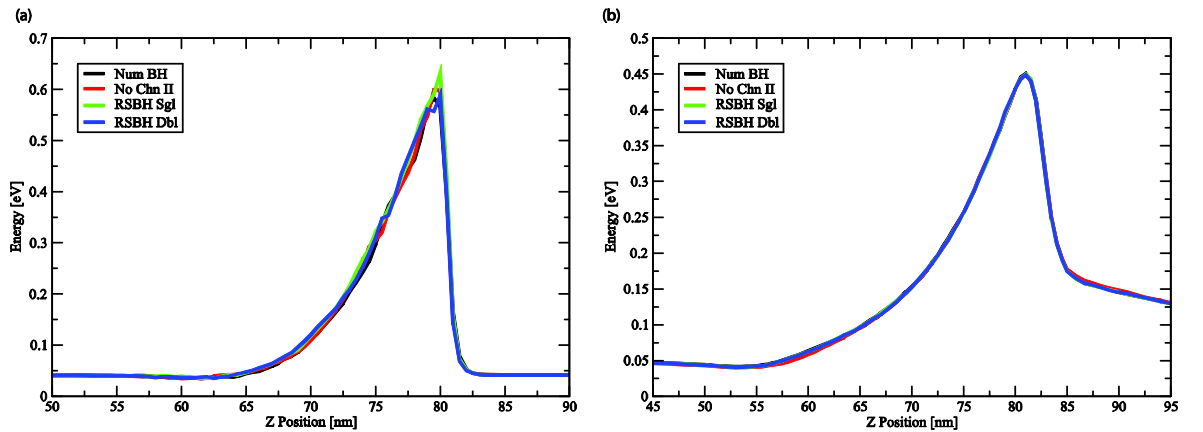


Figure 6.36: Energy profile along channel of UTB DG device with (a) $V_G = 0.5V$ and (b) $V_G = 1V$ for $V_D = 1V$.

At low gate voltage the potential barrier in the channel between the source and drain is high and only high energy carriers are able to make it into the channel. These high energy carriers that make it into the channel will encounter a large field accelerating them into the drain. It is these few carriers from the high energy tail of the carrier distribution that are being averaged to obtain the velocity plot in Figure 6.34. This is corroborated by the high average energy of the carriers in the channel shown in plot (a) of Figure 6.36.

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In the high gate voltage case the potential barrier is much lower and a larger fraction of the carrier distribution can traverse the channel to the drain. As carriers with lower energy are able to contribute to the drain current, the average energy in the channel will decrease along with the average carrier velocity.

At high drain the overall effect of remote screening is negligible which again is due to the low impurity density in the channel. The effect of the impurity scattering in the small regions at each of the channel provide only a small factor in defining channel performance at high gate voltage. Due to the new models inherent dependence on low screening, the high gate voltage cancels the effect that remote screening has in this device.

6.3.4 Summary

The 22nm template UTB DG device was originally developed as a template device to allow a comparison to be made between a large set of different simulators from the European device modelling community [116]. The device structure consists of a 10nm thick silicon body with a 1.1nm EOT oxide layer, here modified to be silicon dioxide from the original specification of a high- κ material.

With highly doped source and drain contact regions and a low doped channel region, the definition of source and drain interface positions for the remotely screened models is again chosen as the point of steepest gradient in the roll-off of the source and drain doping into the channel. This gives the source and drain interfaces at positions of $Z=53.5\text{nm}$ and $Z=81.5\text{nm}$ respectively.

An initial estimate on the effect of remote screening has been completed by analytically computing the phonon and II limited mobility from initial DD simulation. This examination showed that II scattering in the centre of the channel plays little role in determining the channel performance where dopant concentration is at its lowest. Channel II scattering has a controlling factor in the device performance near the interfaces where the source and drain doping is still evident and coincides with the region that remote screening is active. Within these small regions at the interfaces, the analysis demonstrated that remote screening will increase the channel mobility between 40-60% at gate voltages greater than $V_G = 0.4\text{V}$.

The MC simulation of this device includes simulation of four different cases of channel II scattering that include the BH scattering model, no channel II scattering and the remotely screened models. Simulations were completed to produce $I_D - V_G$ curves for low and high drain biases for each of the four cases. The drain current curves established that channel II scattering in this device

is not a strongly controlling factor on the device performance. This is made particularly clear by the No Chn II case which removes all II scattering from the channel and had little effect on the drain current. Given this conclusion, the new remote screening models for II scattering have an understandably negligible effect on the device characteristics.

6.4 Conclusion

This chapter has taken the newly developed remote screening II scattering models presented in Chapter 5 and applied them in a fully self-consistent MC device simulator. The objective of this simulation study is to analyse what effect that remote screening has in the modern MOSFETs where the distance between the highly-doped source and drain regions is small. The MC device simulator has been employed to simulate two distinct MOSFET devices, one with a highly doped channel typical of the current generation MOSFETs and the second device a future generation MOSFET with low doping in the channel.

The first device is a bulk MOSFET which is forecast to continue in the industrial roadmap until at least 2012 [1]. Originally developed by Toshiba as a future device for the high-performance technology [113, 114], it has been reconstructed from published data by fellow researchers in the Device Modelling Group [118]. This device has been constructed with a metal gate, a 1.4nm thick silicon oxi-nitride insulator and a highly doped, advanced channel doping profile design. Calibration of the bulk MOSFET is completed between the industrial TCAD tool, Sentaurus [117], the in-house DD simulator and the MC simulator.

Although MC simulation incorporates non-equilibrium transport that is not present in DD, it suffers from the problems of statistical noise inherent to such a stochastic particle based approach. Due to this limitation, the bulk MOSFET device can only be accurately simulated for gate voltages greater than $V_G = 0.4V$. This is an important restriction to analysis of remotely screened II scattering as very low screening conditions, where remote screening is expected to be strongest, cannot be simulated. This is a limitation of using the MC methodology which can only be worked around by moving to a different simulation approach that doesn't suffer from stochastic noise.

An important step in the modelling of remote screening is the choice of position for the interfaces between the source and the drain. Abrupt doping transitions don't occur in realistic doping profiles and therefore in this work the gradient of the doping profile is used to select the position. The point at which the doping is changing most rapidly between the highly doped source/drain and the channel is selected as the remote screening interface.

6.4 Conclusion

An analytical analysis of the phonon and II limited mobility has been completed using the Kubo-Greenwood formula in conjunction with channel profile data from the DD solution of the bulk MOSFET. This analysis allows the effect of remote screening to be estimated at low screening conditions (low gate voltages) and provides a picture of the region that remote screening is effective in the device. The analysis highlights that remote screening will have a larger effect at low gate voltages where the screening density in the channel is low, as is expected. As the gate voltage is increased, so does the screening density and the effect of remotely screened II scattering is reduced to smaller regions at the edge of the interfaces. At very low gate voltages in particular, the II and phonon limited mobility in the channel region is increased by almost a factor of two.

Simulations of the bulk MOSFET in the MC simulator have been completed with and without the remotely screening impurity scattering, and also for the case of no impurity scattering in the channel. Results without II scattering in the channel of the bulk MOSFET show that in this device that the II scattering mechanism plays an important role in defining the channel performance. The drain current is substantially increased when no channel II scattering is included. However when the remotely screened II model is included, the simulation shows negligible effect at any particular gate voltage or drain bias.

This lack of improvement in channel performance with remotely screened II scattering can be explained partly by the strong role that interface roughness scattering has in defining channel performance. The analytical estimate using DD data for the phonon and II limited mobility suggested that remote screening may have up to a 20% increase in channel mobility within the remote screening regions at either end of the channel. It was discussed that the inclusion of IR scattering reduces this analytical estimate of the channel mobility to less than 5%. Secondly, the region over which remote screening is effective in the bulk MOSFET device is small with few II scattering events. Typically, the number of scattering events that occur within the remote screening region was found to be less than one per carrier. Therefore, the combination of strong IR scattering with a small region where remote screening is effective leads to a negligible effect for the bulk MOSFET.

The second device to be simulated was the PullNano UTB DG device which is expected to be the device that allows scaling to the end of the industrial roadmap [1]. The UTB DG device has an low doped channel region with a 10nm thick silicon body and 1.1nm oxide layer. A difference plot of the net doping profile has again been used to find the source and drain interface positions.

An analytical estimate on the channel mobility has been completed and demonstrates the effect that remote screening has on the channel performance. At the lowest gate voltage, remote screening is shown to have an increase in channel mobility within the remote screening region at either end of

6.4 Conclusion

the channel. Predictably, as the gate voltage increases the effect of remote screening is reduced. At the minimum MC simulation gate voltage, $V_G = 0.4V$, it was shown that remote screening can increase the mobility close to the interfaces by up to 60% and at the highest gate voltage this is reduced slightly to 40%. Despite this increase the remote screening region is limited to a small regions at either end of the channel with the centre of the channel dominated by phonon scattering.

MC simulation of the device with the remote screening models doesn't provide the expected increase in channel performance as was estimated by the mobility analysis. It is shown that impurity scattering in the channel plays an almost negligible role in defining the channel performance. This lack of II scattering effect can be understood from the channel doping profile, which is very low, on the order of $N_I \approx 10^{15} cm^{-3}$. At this low doping, II scattering is negligible and the phonon scattering is dominant.

In conclusion, it has been shown by extensive simulation of two distinct MOSFET devices, that remote screening plays no role in defining the channel performance in these devices at the simulated gate voltages. In the bulk device, the dominant IR scattering combined with high screening strongly reduces the effect of remote screening. With the UTB DG device, it is explained by the low dopant density in the channel removing the dependence of II scattering in the channel characteristics.

In sub-threshold conditions the remote screening model has been shown to have a considerable effect on channel mobility and is predicted to increase the leakage current when the device is off (at low gate voltages). The restriction introduced by MC simulations on the allowable gate voltages means that simulations cannot be completed to examine this effect on leakage current. Further work is required to study the effect of this new scattering model at lower gate voltages using a different simulation methodology which doesn't suffer from the statistical noise of MC.

Chapter 7 Conclusions

The aim of this work was to develop and test an advanced Coulomb scattering model that includes the effect of the highly-doped source and drain regions on channel ionized impurity (II) scattering for the simulation of nanoscale MOSFET devices. The highly-doped source and drain regions introduce additional screening of the channel IIs through polarisation charge effects, the aptly named remote screening within this work, which as channel lengths are scaled in MOSFETs will increase and strongly affect II scattering in the channel region.

Here scattering potentials are developed which represent a single channel II located next to one or two highly doped regions, the source and drain, for the single and double interface cases respectively. An exact analytical solution to the Linearized Thomas-Fermi (LTF) form of Poisson's equation for the system has been calculated and is shown to be an excellent match with a fully self-consistent numerical Poisson solution. These scattering potentials include the important polarisation charge effects induced from the source and drain regions which increase the screening of channel IIs, hence the descriptive title of remote screening.

It has also been demonstrated that the remote screening scattering potential will return to the Brooks-Herring (BH) scattering potential in the limit that the II is located a large distance from the highly-doped regions. This is an important limit to obtain as it ensures that the newly developed scattering potential not only returns to the classic solution, but that it will also work alongside existing II scattering approaches. This is of importance for integration into Monte Carlo (MC) simulation.

For the purposes of this work which is to undertake a study on the strength of remote screening in MOSFET devices using a MC simulation methodology, a simplified model of remote screening has been employed. The simplified model is obtained using the aptly named strong-screening limit which assumes the source and drain regions become metallic-like. This simplification is shown to be almost exact for IIs located greater than 1nm from an interface and represents a worst-case scenario for remote-screening interactions. This worst-case scenario providing an upper limit on the remote screening interaction and is suitable for the context of this work.

Utilising the strongly screened scattering potentials, a MC suitable scattering model has been calculated using Fermi's Golden Rule approach. Again, as the context of this work is to explore the strength of remote screening in device simulations, an assumption on the scattering potential has been made to reduce the complexity of the problem. The remotely screened scattering potential

7. Conclusions

is anisotropic in nature but the typical approach to the calculation of scattering rates in MC is for isotropic scattering potentials. In this work the scattering potential is assumed to be isotropic such that the scattering carrier always approaches the II aligned with the Z-axis of the scattering frame. Use of the Z-aligned simplification is shown to lead to a less than 2% error over the region where remote screening is effective.

An analysis of the remotely screened scattering models has shown that remote screening reduces the strength of II scattering near to the highly-doped source and drain regions. For impurities within 1-2 channel screening lengths of either interface, the effect of remote screening can reduce the scattering rate by up to several orders of magnitude. As channel lengths shrink, the remote screening effect induced from the source and drain increases, particularly when the channel screening length becomes larger than the channel length. In such cases, the II limited mobility can increase up to 300% over the standard model for channel lengths less than 20nm.

The existing approach for II scattering utilised in the MC simulation in this work made use of Ridley's Third-Body Exclusion (TBE) model which is far from ideal as it neglects the vast majority of II scattering events when screening densities are low. This becomes a distinct problem for the accurate modelling of MOSFET devices as channel screening densities can be several orders of magnitude lower than II density leading to an underestimation of the scattering effect. In this work a new approach has been developed which allows the full complement of II scattering to be modelled. This new approach utilises a self-consistent model that allows the scattering rate to be capped whilst maintaining the full momentum relaxation rate. This allows II scattering to be fully modelled improving the low screening density simulations whilst ensuring that the simulation analysis of remote screening is accurate.

The remotely screened II scattering model has been used to complete a simulation study of two MOSFET devices which are chosen to represent a the state of the art technology and possible future technology. The first device being a bulk MOSFET that is typical of those currently in production with high channel doping, and the second device is an low channel doped Ultra-Thin Body Double Gate (UTB DG) MOSFET that is a proposed structure for future technological generations. These two devices are chosen to represent the trends in channel doping design, that is the highly doped bulk MOSFET or the relatively undoped channel design of the DG design.

The bulk MOSFET device has a strong dependence on II scattering which was demonstrated by the clear improvement in drain current when this scattering mechanism was removed from the channel region. An analytical mobility analysis due to phonon and II scattering suggested that remote screening in this device will greatly improve the channel mobility at low gate voltages. This increase in low gate voltage channel mobility would lead to a detrimental affect on device

7. Conclusions

performance by increasing the off-state current of the MOSFET. MC simulation of the device with remote screening of channel IIs demonstrated that for gate voltages above 0.4V, the effect is negligible. This negligible result was shown to be due to a combination of the high Interface Roughness (IR) scattering in the device which damped any effect of remote screening and the small remote screening region at the respective gate voltages.

The UTB DG MOSFET device was demonstrated to have a minimal dependence on II scattering due to the low doping in the channel region. The analytical analysis highlighted the phonon scattering dominance in the channel which was reinforced by the minimal shift in drain current with the removal of channel II scattering. Again, MC analysis of remote screening has a negligible effect on the device performance which can be understood from the lack of II scattering in the channel.

To conclude, the remote screening for II scattering has been shown for higher gate voltages to have negligible effect in current generation and low channel doped devices. Remote screening of channel IIs is expected to have a large effect at very low gate voltages where screening densities are low. Unfortunately the MC simulation approach is not suitable to simulate such conditions and future work should aim to simulate such low screening conditions perhaps through a direct solution of the Boltzmann equation using spherical harmonics expansions [73, 128, 129].

7.1 Future Work

The study of remote screening with sub-threshold MOSFET conditions should be completed to fully understand the role of this effect. This will involve moving to a simulation methodology that doesn't suffer from statistical noise. An approach which is suitable is that of the spherical harmonics expansion of the distribution function enabling a deterministic solution of the Boltzmann Transport Equation [73, 128, 129]. This would allow the low gate voltage simulations of MOSFETs to be completed whilst including the remote screening scattering mechanism.

Further studies of MOSFET devices with smaller dimensions are required to confirm the effect of remote screening and could be completed using the simulator and remote screening scattering approach developed here. Example devices include the final scaled devices of each particular architecture such as a 14nm physical channel length bulk MOSFET, a 10.7nm physical channel length Silicon-On-Insulator MOSFET and a 8.1nm physical channel length DG device [1]. This would provide a comprehensive study on the effect of remote screening in nanoscale devices by extending the study to the end of roadmap scaled devices.

7.1 Future Work

The full anisotropic scattering potential should also be studied in simulations of MOSFETs which would allow the full scattering effect of the remotely screened II to be analysed. There are several approaches which could be used including the radial wave expansion of the Schrödinger equation [105] or perhaps use of a linear Boltzmann expansion to obtain scattering expressions [108]. It would also be beneficial for an exact description of the remote screening effect to remove the strong-screening limit from the scattering models. In this work an upper limit or worst-case condition for remote screening was sufficient to be able to examine the effect but could be extended to provide a more detailed study. This may be required for the ultra-small channel length devices predicted for the end of the ITRS roadmap.

Finally, the remote screening of channel ionized impurities from the gate region should also be studied. The gate contact in future generation MOSFETs will become a metal and in conjunction with oxide thickness scaling, will lead to strong remote screening of channel IIs. This interaction will be evident along the entire length of the channel, extending the remote screening regions to a larger portion of the device and possibly leading to a stronger effect. In particular, this should be studied for possible future multiple gate MOSFET architectures where the channel can be surrounded by metallic gate regions.

Appendix A Single Interface Potential Calculation

This appendix will provide a detailed outline of the single interface potential calculation discussed in section 4.2.1. An exact solution to the potential of a single ionized impurity located close to highly-doped region has been obtained by solving Poisson's equation. This is a complex problem which has been simplified through use of the linear Thomas-Fermi (LTF) approximation to allow an analytical solution to be found.

A.1 Linearized Poisson's Equation

Starting with the LTF form of the Poisson equation, equations (4.4)-(4.5) from section 4.2.1 which define the system depicted in Figure 4.1.

$$\nabla^2 \varphi_s - k_s^2 \varphi_s = 0 \quad \text{for } Z < 0 \quad (\text{A.1})$$

$$\nabla^2 \varphi_c - k_c^2 \varphi_c = -\frac{Q}{\epsilon_{si} \epsilon_0} \delta(\mathbf{r} - \mathbf{r}_1) \quad \text{for } Z > 0 \quad (\text{A.2})$$

where φ_s is the potential in the source region, $Z < 0$, and φ_c is the potential in the channel, $Z > 0$. The $k_s = \lambda_s^{-1}$ and $k_c = \lambda_c^{-1}$ terms represent the inverse screening lengths in the source and drain regions respectively and the ionized impurity is located at position $\mathbf{r}_1$ in the channel region.

As discussed in section 4.2.1, the potential solution will use cylindrical co-ordinates throughout. For this model we neglect any radial dependence on impurity position by assuming the impurity is located at the origin of the radial axis. This reduces the complexity of the model by allowing radial symmetry around the Z axis. Expanding the Dirac delta function of equation (A.2) in cylindrical co-ordinates, assuming that $\mathbf{R}_1 = 0$

$$\nabla^2 \varphi_c - k_c^2 \varphi_c = -\frac{Q}{2\pi \epsilon_{si} \epsilon_0} \frac{\delta(\mathbf{R})}{R} \delta(Z - Z_1) \quad \text{for } Z > 0 \quad (\text{A.3})$$

Considering the channel potential initially, the solution will involve finding the general (homogenous) solution and the particular solution. This can be written as

$$\varphi_c = \varphi_c^G + \varphi_c^P \quad (\text{A.4})$$

A.2 General Solution

where φ_C^G is the general solution and φ_C^P the particular. The general solution for the channel potential can be found by allowing $Z \neq Z_I$ for which the RHS of equation (A.3) becomes

$$\nabla^2 \varphi_C - k_C^2 \varphi_C = 0 \quad (\text{A.5})$$

This is identical to the source term given by equation (A.1) and will only differ in the behaviour of the solution.

In Figure 7.1 the expected behaviour of the Z components of the potential is given. For the general solutions the expected behaviour is depicted by the red curves and the particular solution by the blue curves. The behaviour is defined by the boundary condition at large distance, Z , which is presented in more detail later in this appendix.

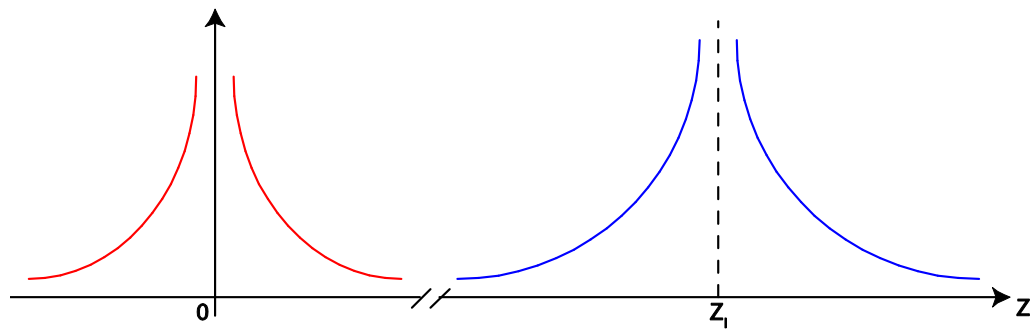


Figure 7.1: Expected behaviour of the Z dependent component of the potentials.

For the general solution, the potential is expected to decrease with distance from the source-channel interface. The particular solution will model the point charge with an increasing potential moving towards the impurity location at $Z = Z_I$.

A.2 General Solution

First solving the general (homogeneous) solution for the source and channel regions given by equations (A.1) and (A.5). Generalising between the source and channel forms, the equation can be written as

$$\nabla^2 \varphi_x - k_x^2 \varphi_x = 0 \quad (\text{A.6})$$

A.2 General Solution

with x denoting either the source (S) and channel (C) region. Using the separation of variables technique [96] the potential solution can be expressed in cylindrical co-ordinates using a known form.

$$\varphi(R, Z) = F(R)\zeta(Z) \quad (\text{A.7})$$

Here due to the cylindrical symmetry of this problem around the Z axis there will be no θ dependence in the solution and this component is a constant. Substituting this form of the potential back into equation (A.6) gives

$$\nabla^2 F\zeta - k_x^2 F\zeta = 0 \quad (\text{A.8})$$

Expanding the Laplacian operator in cylindrical co-ordinates, again neglecting the term involving θ as there is no dependence on this in the solution gives

$$\left[\frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial}{\partial R} \right) + \frac{\partial^2}{\partial Z^2} \right] F\zeta - k_x^2 F\zeta = 0 \quad (\text{A.9})$$

Rearranging this solution into separable components

$$\begin{aligned} \left[\frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial}{\partial R} \right) \right] F\zeta &= \zeta \left[\frac{1}{R} \frac{\partial F}{\partial R} + \frac{\partial^2 F}{\partial R^2} \right] \\ &= F\zeta \left[\frac{1}{FR} \frac{\partial F}{\partial R} + \frac{1}{F} \frac{\partial^2 F}{\partial R^2} \right] \end{aligned} \quad (\text{A.10})$$

$$\left[\frac{\partial^2}{\partial Z^2} \right] F\zeta = F\zeta \left[\frac{1}{\zeta} \frac{\partial^2 \zeta}{\partial Z^2} \right] \quad (\text{A.11})$$

Substituting these back into equation (A.9) and dividing throughout by $F\zeta$ gives

$$\frac{1}{FR} \frac{\partial F}{\partial R} + \frac{1}{F} \frac{\partial^2 F}{\partial R^2} + \frac{1}{\zeta} \frac{\partial^2 \zeta}{\partial Z^2} - k_x^2 = 0 \quad (\text{A.12})$$

Having now got a form of the equation in terms of R and Z only, the equation can be separated introducing a separation constant $-k^2$.

A.2 General Solution

$$\frac{1}{FR} \frac{\partial F}{\partial R} + \frac{1}{F} \frac{\partial^2 F}{\partial R^2} = -k^2 \quad (\text{A.13})$$

$$\frac{1}{\zeta} \frac{\partial^2 \zeta}{\partial Z^2} - k_x^2 = k^2 \quad (\text{A.14})$$

Rearranging these equations

$$R^2 \frac{\partial^2 F}{\partial R^2} + R \frac{\partial F}{\partial R} + k^2 R^2 F = 0 \quad (\text{A.15})$$

$$\frac{\partial^2 \zeta}{\partial Z^2} = (k^2 + k_x^2) \zeta \quad (\text{A.16})$$

A general form of Bessel's differential equation [96]

$$\rho^2 \frac{\partial^2 y}{\partial \rho^2} + \rho \frac{\partial y}{\partial \rho} + (k^2 \rho^2 - n^2) y = 0 \quad (\text{A.17})$$

and its solution is

$$y = AJ_n(k\rho) + BN_n(k\rho) \quad (\text{A.18})$$

Using this general form gives a solution to equation (A.15) of

$$F = AJ_0(kR) + BN_0(kR) \quad (\text{A.19})$$

Solving the Z dependence from (A.16) which takes the form of a standard exponential solution

$$\zeta = \exp\left(-Z\sqrt{k^2 + k_x^2}\right) + \exp\left(Z\sqrt{k^2 + k_x^2}\right) \quad (\text{A.20})$$

Substituting these solutions back into equation (A.7) using linear superposition of Bessel functions to obtain the final potential gives

$$\varphi_x = \int_0^\infty dk \, a(k) \left(AJ_0(kR) + BN_0(kR) \right) \left(\exp\left(-Z\sqrt{k^2 + k_x^2}\right) + \exp\left(Z\sqrt{k^2 + k_x^2}\right) \right) \quad (\text{A.21})$$

A.3 Particular Solution

Boundary conditions (BC) define the exact form of this solution for the source and channel regions. For the Bessel solution of the radial dependence, $F(kR)$, the solution must be finite as $kR \rightarrow 0$. This means the Neumann function coefficient must be zero, $B=0$, to satisfy this BC where the coefficient A will be solved later.

$$F = AJ_0(kR) \quad (\text{A.22})$$

The expected behaviour of the Z dependence of this solution is given in Figure 7.1, which is defined from the BC that the potential must tend to zero as $Z \rightarrow \pm\infty$. Therefore for the source region $\zeta(Z \rightarrow -\infty) = 0$ and for the channel region must be $\zeta(Z \rightarrow \infty) = 0$. This yields the following solution for the source and channel

$$\zeta_s(Z) = \exp\left(Z\sqrt{k^2 + k_s^2}\right) \text{ for } Z < 0 \quad (\text{A.23})$$

$$\zeta_c(Z) = \exp\left(-Z\sqrt{k^2 + k_c^2}\right) \text{ for } Z > 0 \quad (\text{A.24})$$

The general solution to equation (A.6) can now be defined for the source and channel regions. Substituting equations (A.22)-(A.24) into equation (A.21) gives

$$\varphi_s = \int_0^\infty dk A_s(k) J_0(kR) \exp\left(Z\sqrt{k^2 + k_s^2}\right) \text{ for } Z < 0 \quad (\text{A.25})$$

for the source region and

$$\varphi_c^G = \int_0^\infty dk A_c(k) J_0(kR) \exp\left(-Z\sqrt{k^2 + k_c^2}\right) \text{ for } Z > 0 \quad (\text{A.26})$$

for the channel region where the coefficients $A_s(k) = a_s(k)A_s$ and $A_c(k) = a_c(k)A_c$ include the coefficient of the radial Bessel function and are yet to be obtained.

A.3 Particular Solution

The particular solution for the channel potential can be found by solving equation (A.3). Simplifying the RHS of the potential equation using the following theorem, which can be found using equation (6.512.8) of Gradshteyn & Ryzhiks book [130],

A.3 Particular Solution

$$\frac{\delta(R)}{R} = \int_0^{\infty} dk \, k J_0(kR) \quad (\text{A.27})$$

the equation becomes

$$\nabla^2 \phi_C - k_C^2 \phi_C = -\frac{Q}{2\pi\epsilon_{si}\epsilon_0} \int_0^{\infty} dk \, k J_0(kR) \delta(Z - Z_I) \quad (\text{A.28})$$

Using a known form of the solution from the separation of variables method and using the general solution for the R dependence, the potential can be defined as

$$\phi_C^p = \int_0^{\infty} dk \, k J_0(kR) \zeta(Z) \quad (\text{A.29})$$

Taking the LHS of equation (A.28) separately, expanding the Laplacian operator and substituting equation (A.29) gives

$$\left[\frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial}{\partial R} \right) + \frac{\partial^2}{\partial Z^2} - k_C^2 \right] \int_0^{\infty} dk \, k J_0(kR) \zeta(Z) \quad (\text{A.30})$$

Here we neglect the angular term as before due to the cylindrical symmetry around the Z axis. Attempting to factorise equation (A.30) into separable components yields

$$\int_0^{\infty} dk \, k \left[\left(\frac{\partial^2 J_0(kR)}{\partial R^2} + \frac{1}{R} \frac{\partial J_0(kR)}{\partial R} \right) \zeta + J_0(kR) \left(\frac{\partial^2 \zeta}{\partial Z^2} - k_C^2 \zeta \right) \right] \quad (\text{A.31})$$

To separate the variables of this equation the terms must be independent of each other. The problem here is that we cannot factor out the Bessel function due to the first term within the square brackets. Thankfully this problem has been solved earlier. Referring to equation (A.15) of the general solution which can be re-written here, assuming that equation (A.22) still holds, as

$$\frac{\partial^2 J_0(kR)}{\partial R^2} + \frac{1}{R} \frac{\partial J_0(kR)}{\partial R} = -k^2 J_0(kR) \quad (\text{A.32})$$

Using this solution in equation (A.31) and factorising gives

A.3 Particular Solution

$$\int_0^{\infty} dk \, k \, J_0(kR) \left\{ \frac{\partial^2 \zeta}{\partial Z^2} - \zeta(k^2 + k_C^2) \right\} \quad (\text{A.33})$$

Substituting this back into equation (A.28) yields

$$\int_0^{\infty} dk \, k \, J_0(kR) \left\{ \frac{\partial^2 \zeta}{\partial Z^2} - \zeta(k^2 + k_C^2) \right\} = \frac{-Q}{2\pi\epsilon_{Si}\epsilon_0} \int_0^{\infty} dk \, k \, J_0(kR) \delta(Z - Z_I) \quad (\text{A.34})$$

Simplifying this equation by removing the common terms,

$$\frac{\partial^2 \zeta}{\partial Z^2} - \zeta(k_C^2 + k^2) + \frac{Q}{2\pi\epsilon_{Si}\epsilon_0} \delta(Z - Z_I) = 0 \quad (\text{A.35})$$

which provides a form which is dependent on Z only. The solution to this equation is challenging due to the singularity of the Dirac delta function at $Z = Z_I$. To work around this it is necessary to take limits around Z_I , allowing the delta function to be integrated. Integrating around $Z = Z_I - \eta$ to $Z = Z_I + \eta$ for $\eta \rightarrow 0$

$$\int_{Z_I - \eta}^{Z_I + \eta} \frac{\partial^2 \zeta}{\partial Z^2} dZ - (k_C^2 + k^2) \int_{Z_I - \eta}^{Z_I + \eta} \zeta dZ + \frac{Q}{2\pi\epsilon_{Si}\epsilon_0} \int_{Z_I - \eta}^{Z_I + \eta} \delta(Z - Z_I) dZ = 0 \quad (\text{A.36})$$

The first integral can be completed to give

$$\int_{Z_I - \eta}^{Z_I + \eta} \frac{\partial^2 \zeta}{\partial Z^2} dZ = \left[\frac{\partial \zeta(Z)}{\partial Z} \right]_{Z_I - \eta}^{Z_I + \eta} = \frac{\partial \zeta(Z_I + \eta)}{\partial Z} - \frac{\partial \zeta(Z_I - \eta)}{\partial Z} \quad (\text{A.37})$$

The second integral can be completed using the limit on η

$$\begin{aligned} -(k_C^2 + k^2) \int_{Z_I - \eta}^{Z_I + \eta} \zeta dZ &= -(k_C^2 + k^2) [\zeta(Z)]_{Z_I - \eta}^{Z_I + \eta} \\ \lim_{\eta \rightarrow 0} &\approx -(k_C^2 + k^2) 2\eta \zeta(Z_I) = 0 \end{aligned} \quad (\text{A.38})$$

Taking the third integral and using $\int_a^b \delta(Z - Z_I) dZ = 1$ when $a < Z_I < b$

A.3 Particular Solution

$$\frac{Q}{2\pi\epsilon_{Si}\epsilon_0} \int_{Z_I-\eta}^{Z_I+\eta} \delta(Z-Z_I) dZ = \lim_{\eta \rightarrow 0} \frac{Q}{2\pi\epsilon_{Si}\epsilon_0} \quad (\text{A.39})$$

Rewriting equation (A.36) with the result of these integrals

$$\frac{\partial \zeta(Z_I + \eta)}{\partial Z} - \frac{\partial \zeta(Z_I - \eta)}{\partial Z} = -\frac{Q}{2\pi\epsilon_{Si}\epsilon_0} \quad \text{for } Z \approx Z_I \quad (\text{A.40})$$

For a correct solution of the particular case it is important to ensure that the solution is consistent for both $Z \approx Z_I$ and $Z \neq Z_I$. Looking at equation (A.35) for the case of $Z \neq Z_I$

$$\frac{\partial^2 \zeta}{\partial Z^2} = (k_C^2 + k^2) \zeta \quad \text{for } Z \neq Z_I \quad (\text{A.41})$$

which the solution is already known (see equation (A.20)). This result for $Z \approx Z_I$, equation (A.40), suggests that there is a difference in the gradients of the solution around the impurity position, Z_I . Referring to the expected behaviour of the solution depicted in Figure 7.1, the potential is expected to change gradient around Z_I . The boundary conditions state that for $Z < Z_I$ the potential must tend to zero at $Z \rightarrow -\infty$ and for $Z > Z_I$ the potential must tend to zero at $Z \rightarrow \infty$. Using the solution to equation (A.41) with the BC's, the solution to the Z dependence of the particular solution can be found as

$$\zeta_a(Z) = \alpha \exp\left((Z - Z_I)\sqrt{k^2 + k_C^2}\right) \quad \text{for } Z < Z_I \quad (\text{A.42})$$

$$\zeta_b(Z) = \beta \exp\left(-(Z - Z_I)\sqrt{k^2 + k_C^2}\right) \quad \text{for } Z > Z_I \quad (\text{A.43})$$

To ensure continuity of the solution, the gradients of the potential must match at $Z = Z_I$. Setting equations (A.42)-(A.43) equal to each other and solving for the coefficients gives

$$\begin{aligned} \zeta_a(Z_I - \eta) &= \zeta_b(Z_I + \eta) \\ \alpha \exp\left(-\eta\sqrt{k^2 + k_C^2}\right) &= \beta \exp\left(-\eta\sqrt{k^2 + k_C^2}\right) \\ \lim_{\eta \rightarrow 0} \alpha &= \beta \end{aligned} \quad (\text{A.44})$$

A.3 Particular Solution

Using equation (A.40) to find a value for α by calculating the gradients of equations (A.42) & (A.43).

$$\frac{d\zeta_a(Z_I - \eta)}{dZ} = \sqrt{k^2 + k_C^2} \alpha \exp(-\eta \sqrt{k^2 + k_C^2}) = \lim_{\eta \rightarrow 0} \sqrt{k^2 + k_C^2} \alpha \quad (\text{A.45})$$

$$\frac{d\zeta_b(Z_I + \eta)}{dZ} = -\sqrt{k^2 + k_C^2} \alpha \exp(-\eta \sqrt{k^2 + k_C^2}) = \lim_{\eta \rightarrow 0} -\sqrt{k^2 + k_C^2} \alpha \quad (\text{A.46})$$

Substituting this into equation (A.40) yields the value for the α coefficient.

$$\begin{aligned} -\sqrt{k^2 + k_C^2} \alpha - \sqrt{k^2 + k_C^2} \alpha &= -\frac{Q}{2\pi\epsilon_{Si}\epsilon_0} \\ \alpha &= \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} \frac{1}{\sqrt{k^2 + k_C^2}} \end{aligned} \quad (\text{A.47})$$

Completing the solution for the ζ function

$$\zeta(Z) = \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} \frac{1}{\sqrt{k^2 + k_C^2}} \exp(-|Z - Z_I| \sqrt{k^2 + k_C^2}) \quad (\text{A.48})$$

and substituting this into equation (A.29) will provide the final particular solution of the channel potential.

$$\phi_C^p = \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} \int_0^\infty dk J_0(kR) \frac{k}{\sqrt{k^2 + k_C^2}} \exp(-|Z - Z_I| \sqrt{k^2 + k_C^2}) \quad (\text{A.49})$$

The channel potential can then be found by substituting the general and particular solutions into equation (A.4) to give

$$\begin{aligned} \phi_C &= \int_0^\infty dk J_0(kR) \left\{ A_C(k) \exp(-Z \sqrt{k^2 + k_C^2}) \right. \\ &\quad \left. + \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} \frac{k}{\sqrt{k^2 + k_C^2}} \exp(-|Z - Z_I| \sqrt{k^2 + k_C^2}) \right\} \end{aligned} \quad (\text{A.50})$$

A.4 Coefficients

The coefficients A_s and A_c of equations (A.25) and (A.50) can be found by defining the boundary conditions at $Z = 0$, the source – channel interface. The static electric field boundary conditions apply at this interface, defining that the electric field must be continuous perpendicular to the interface and that the normal electric flux be continuous across the interface.

$$\frac{\partial \varphi_s(Z=0)}{\partial R} = \frac{\partial \varphi_c(Z=0)}{\partial R} \quad (\text{A.51})$$

$$\epsilon_{si}\epsilon_0 \frac{\partial \varphi_s(Z=0)}{\partial Z} = \epsilon_{si}\epsilon_0 \frac{\partial \varphi_c(Z=0)}{\partial Z} \quad (\text{A.52})$$

Finding the derivate of the potentials for the first boundary condition

$$\frac{\partial \varphi_s}{\partial R} = \int_0^\infty dk A_s (-kJ_1(kR)) \quad (\text{A.53})$$

$$\frac{\partial \varphi_c}{\partial R} = \int_0^\infty dk (-kJ_1(kR)) \left\{ A_c + \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \frac{k}{\sqrt{k^2 + k_c^2}} \exp\left(-Z_I \sqrt{k^2 + k_c^2}\right) \right\} \quad (\text{A.54})$$

Setting equation (A.53) equal to equation (A.54) and re-arranging gives

$$A_s - A_c = \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \frac{k}{\sqrt{k^2 + k_c^2}} \exp\left(-Z_I \sqrt{k^2 + k_c^2}\right) \quad (\text{A.55})$$

The derivates for the second boundary condition, equation (A.52) are

$$\frac{\partial \varphi_s}{\partial Z} = \int_0^\infty dk A_s J_0(kR) \sqrt{k^2 + k_s^2} \quad (\text{A.56})$$

$$\frac{\partial \varphi_c}{\partial Z} = \int_0^\infty dk J_0(kR) \left\{ A_c \left(-\sqrt{k^2 + k_c^2}\right) + \frac{Q}{4\pi\epsilon_{si}\epsilon_0} k \exp\left(-Z_I \sqrt{k^2 + k_c^2}\right) \right\} \quad (\text{A.57})$$

Substituting these into the boundary condition and after some manipulation yields

A.5 Single Interface Solution

$$A_s \frac{\sqrt{k^2 + k_s^2}}{\sqrt{k^2 + k_c^2}} + A_c = \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \frac{k}{\sqrt{k^2 + k_c^2}} \exp\left(-Z_I \sqrt{k^2 + k_c^2}\right) \quad (\text{A.58})$$

It is now a matter of solving the two simultaneous equations to find the values for the coefficients. The source coefficient can be easily found by adding equation (A.55) to (A.58) giving

$$A_s = \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \frac{2k}{\sqrt{k^2 + k_c^2} + \sqrt{k^2 + k_s^2}} \exp\left(-Z_I \sqrt{k^2 + k_c^2}\right) \quad (\text{A.59})$$

To find the channel coefficient, the two equations must be subtracted

$$A_c = \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \frac{k}{\sqrt{k^2 + k_c^2}} \exp\left(-Z_I \sqrt{k^2 + k_c^2}\right) \frac{\sqrt{k^2 + k_c^2} - \sqrt{k^2 + k_s^2}}{\sqrt{k^2 + k_c^2} + \sqrt{k^2 + k_s^2}} \quad (\text{A.60})$$

A.5 Single Interface Solution

Substituting the coefficients back into the solutions for the potential gives the final form for the source and channel potentials.

$$\varphi_s = \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \int_0^\infty dk J_0(kR) \frac{2k}{K_c + K_s} \exp(-Z_I K_c) \exp(Z K_s) \quad (\text{A.61})$$

$$\begin{aligned} \varphi_c = \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \int_0^\infty dk J_0(kR) \frac{k}{K_c} \left\{ \exp(-|Z - Z_I| K_c) \right. \\ \left. + \frac{K_c - K_s}{K_c + K_s} \exp(-(Z + Z_I) K_c) \right\} \end{aligned} \quad (\text{A.62})$$

where

$$K_c = \sqrt{k^2 + k_c^2} \quad (\text{A.63})$$

$$K_s = \sqrt{k^2 + k_s^2} \quad (\text{A.64})$$

A.5 Single Interface Solution

Remembering here that the variable k is purely a separation constant introduced in the solution of the partial differential equation and should not be confused with the carrier wave vector variable of the same letter.

Appendix B Double Interface Potential Calculation

In this appendix the double interface potential solution will be presented in more detail than is provided in chapter 4.3.1. Due to the similarities in the procedure and the solution, the previous appendix will be referenced for part of the solution method. Here a potential solution is found for a single ionized impurity between two highly-doped regions.

B.1 Linearized Poisson's Equation

Starting with Poisson's equation for the source, channel and drain regions which has been linearized using the Thomas-Fermi approximation in section 4.3.1

$$\nabla^2 \varphi_s - k_s^2 \varphi_s = 0 \text{ for } Z < 0 \quad (\text{B.1})$$

$$\nabla^2 \varphi_c - k_c^2 \varphi_c = -\frac{Q}{\epsilon_{si} \epsilon_0} \delta(\mathbf{r} - \mathbf{r}_1) \text{ for } 0 < Z < L_c \quad (\text{B.2})$$

$$\nabla^2 \varphi_d - k_d^2 \varphi_d = 0 \text{ for } Z > L_c \quad (\text{B.3})$$

Expanding the Dirac delta function of equation (B.2) into cylindrical co-ordinates, allowing $\mathbf{R}_1 = 0$

$$\nabla^2 \varphi_c - k_c^2 \varphi_c = -\frac{Q}{2\pi \epsilon_{si} \epsilon_0} \frac{\delta(\mathbf{R})}{R} \delta(Z - Z_1) \text{ for } Z > 0 \quad (\text{B.4})$$

The solution of the channel potential will involve solving a general and a particular solution. In this model there will be two general solutions corresponding to the regions on either side of the point charge in the channel. Expressing the channel potential in this form as

$$\varphi_c = \varphi_c^{G1} + \varphi_c^P + \varphi_c^{G2} \quad (\text{B.5})$$

where the superscripts $G1$ denote the source end of the channel, $G2$ the drain end of the channel and P the particular solution of the point charge. The first step is to find the general solution which for the channel potential is found by allowing the right-hand side (RHS) of equation (B.4) to

B.1 Linearized Poisson's Equation

equal zero. As this form is identical to that of the source and drain regions a universal form can be written

$$\nabla^2 \varphi_x - k_x^2 \varphi_x = 0 \quad (\text{B.6})$$

where x denotes either the source (S), channel (C), or drain (D) region. This solution is found for the single interface case in appendix section A.3 and can be used here, again using the same radial boundary condition for the Bessel function.

$$\varphi_x = \int_0^\infty dk a(k) J_0(kR) \left(\exp\left(-Z\sqrt{k^2 + k_x^2}\right) + \exp\left(Z\sqrt{k^2 + k_x^2}\right) \right) \quad (\text{B.7})$$

Although this is a universal form for the solution each region has different behaviour as depicted in Figure 7.2. This figure represents the expected behaviour of the general (red curve) and particular (blue curve) Z dependent components of the potential in each of the regions.

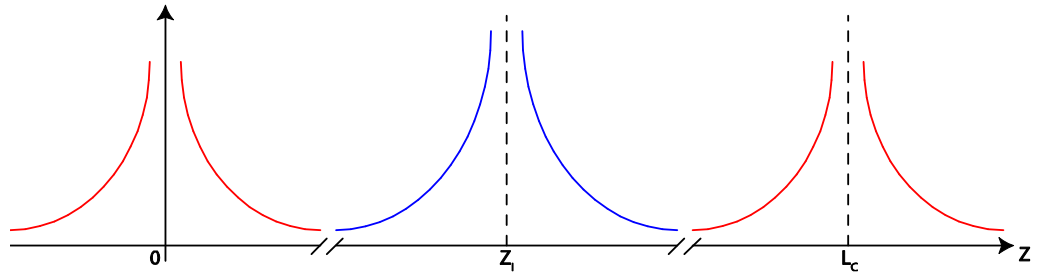


Figure 7.2: Expected behaviour of the Z component of the potential with the source region $Z < 0$, the drain region $Z > L_C$ and the impurity at $Z = Z_I$.

From Figure 7.2 the behaviour of the Z dependence of the potential in the source and drain is depicted by the red curve in the $Z < 0$ and $Z > L_C$ regions respectively. Applying the boundary condition such that the potential tends to zero at large Z distance, $\lim_{Z \rightarrow -\infty} \varphi_S = 0$ and $\lim_{Z \rightarrow \infty} \varphi_D = 0$, gives the following solutions for the source and drain.

$$\varphi_S = \int_0^\infty dk A_S(k) J_0(kR) \exp\left(Z\sqrt{k^2 + k_S^2}\right) \text{ for } Z < 0 \quad (\text{B.8})$$

$$\varphi_D = \int_0^\infty dk A_D(k) J_0(kR) \exp\left(-Z\sqrt{k^2 + k_D^2}\right) \text{ for } Z > 0 \quad (\text{B.9})$$

B.2 Solution of Coefficients

For the channel potential there are two general solutions describing the regions on either side of the point charge. Referring to the red curves in Figure 7.2 the Z behaviour is expected to decrease from the source interface and increase towards the drain interface. This corresponds with the limiting boundary condition that the potential must tend to zero at large distances, $\lim_{Z \gg 0} \phi_C^{G1} = 0$ and $\lim_{Z \ll L_C} \phi_C^{G2} = 0$. Applying these boundary conditions to equation (B.7) provides the general solutions for the channel potential.

$$\phi_C^{G1} = \int_0^\infty dk k A_C(k) J_0(kR) \exp\left(-Z\sqrt{k^2 + k_C^2}\right) \quad (B.10)$$

$$\phi_C^{G2} = \int_0^\infty dk k B_C(k) J_0(kR) \exp\left(Z\sqrt{k^2 + k_C^2}\right) \quad (B.11)$$

The particular solution for the double interface model is identical to that of the single interface model allowing the solution to be repeated here. Using equation (A.49)

$$\phi_C^P = \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} \int_0^\infty dk J_0(kR) \frac{k}{\sqrt{k^2 + k_C^2}} \exp\left(-|Z - Z_I|\sqrt{k^2 + k_C^2}\right) \quad (B.12)$$

Substituting the general and particular solutions for the channel potential into equation (B.5) and re-arranging gives the following form.

$$\begin{aligned} \phi_C = & \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} \int_0^\infty dk J_0(kR) \frac{k}{\sqrt{k^2 + k_C^2}} \exp\left(-|Z - Z_I|\sqrt{k^2 + k_C^2}\right) \\ & + \int_0^\infty dk J_0(kR) \left\{ A_C(k) \exp\left(-Z\sqrt{k^2 + k_C^2}\right) + B_C(k) \exp\left(Z\sqrt{k^2 + k_C^2}\right) \right\} \end{aligned} \quad (B.13)$$

B.2 Solution of Coefficients

To find the coefficients for the source, drain and channel potentials given by equations (B.8), (B.9) and (B.13) respectively, the electric field boundary conditions must be applied at both the $Z = 0$ and $Z = L_C$ interfaces. The boundary conditions for the source interface are

$$\frac{\partial \phi_s(Z=0)}{\partial R} = \frac{\partial \phi_C(Z=0)}{\partial R} \quad (B.14)$$

B.2 Solution of Coefficients

$$\epsilon_{si}\epsilon_0 \frac{\partial \varphi_s(Z=0)}{\partial Z} = \epsilon_{si}\epsilon_0 \frac{\partial \varphi_c(Z=0)}{\partial Z} \quad (\text{B.15})$$

and for the drain interface are

$$\frac{\partial \varphi_c(Z=L_c)}{\partial R} = \frac{\partial \varphi_d(Z=L_c)}{\partial R} \quad (\text{B.16})$$

$$\epsilon_{si}\epsilon_0 \frac{\partial \varphi_c(Z=L_c)}{\partial Z} = \epsilon_{si}\epsilon_0 \frac{\partial \varphi_d(Z=L_c)}{\partial Z} \quad (\text{B.17})$$

Using the following expressions allow the potentials to be simplified. These simplified terms will be used throughout the remainder of this appendix.

$$K_c = \sqrt{k^2 + k_c^2} \quad (\text{B.18})$$

$$K_s = \sqrt{k^2 + k_s^2} \quad (\text{B.19})$$

$$K_d = \sqrt{k^2 + k_d^2} \quad (\text{B.20})$$

Starting with the boundary condition at the source-channel interface and finding the derivatives of the potentials:

$$\frac{\partial \varphi_s(Z=0)}{\partial R} = \int_0^\infty dk A_s (-kJ_1(kR)) \quad (\text{B.21})$$

$$\frac{\partial \varphi_c(Z=0)}{\partial R} = \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \int_0^\infty dk (-kJ_1(kR)) \left\{ \frac{k}{K_c} \exp(-Z_l K_c) + A_c + B_c \right\} \quad (\text{B.22})$$

Setting these derivatives equal to one another and re-arranging gives

$$A_s - A_c - B_c = \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \frac{k}{K_c} \exp(-Z_l K_c) \quad (\text{B.23})$$

For the second source-channel interface electric field BC:

B.2 Solution of Coefficients

$$\frac{\partial \varphi_s(Z=0)}{\partial Z} = \int_0^\infty dk A_s J_0(kR) K_s \quad (\text{B.24})$$

$$\frac{\partial \varphi_c(Z=0)}{\partial Z} = \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \int_0^\infty dk J_0(kR) \{k \exp(-Z_I K_C) - A_C K_C + B_C K_C\} \quad (\text{B.25})$$

Substituting these into equation (B.15) and manipulating yields

$$A_s \frac{K_s}{K_C} + A_C - B_C = \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \frac{k}{K_C} \exp(-Z_I K_C) \quad (\text{B.26})$$

For the channel-drain interface electric flux BC:

$$\begin{aligned} \frac{\partial \varphi_c(Z=L_C)}{\partial R} &= \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \int_0^\infty dk (-kJ_1(kR)) \left\{ \frac{k}{K_C} \exp(-|L_C - Z_I| K_C) \right. \\ &\quad \left. + A_C \exp(-L_C K_C) + B_C \exp(L_C K_C) \right\} \end{aligned} \quad (\text{B.27})$$

$$\frac{\partial \varphi_D(Z=L_C)}{\partial R} = \int_0^\infty dk A_D (-kJ_1(kR)) \exp(-L_C K_D) \quad (\text{B.28})$$

Using these equation to find the electric field BC at the drain interface:

$$\begin{aligned} &A_D \exp(-L_C K_D) - A_C \exp(-L_C K_C) - B_C \exp(L_C K_C) \\ &= \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \frac{k}{K_C} \exp(-(L_C - Z_I) K_C) \end{aligned} \quad (\text{B.29})$$

For the channel-drain interface electric field BC:

$$\begin{aligned} \frac{\partial \varphi_c(Z=L_C)}{\partial Z} &= \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \int_0^\infty dk J_0(kR) \{(-k) \exp(-(L_C - Z_I) K_C) \\ &\quad + A_C (-K_C) \exp(-L_C K_C) \\ &\quad + B_C K_C \exp(L_C K_C)\} \end{aligned} \quad (\text{B.30})$$

$$\frac{\partial \varphi_D(Z=L_C)}{\partial Z} = \int_0^\infty dk A_D J_0(kR) (-K_D) \exp(-L_C K_D) \quad (\text{B.31})$$

The final BC is then

B.2 Solution of Coefficients

$$\begin{aligned}
 & A_D \frac{K_D}{K_C} \exp(-L_C K_D) - A_C \exp(-L_C K_C) + B_C \exp(L_C K_C) \\
 &= \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} \frac{k}{K_C} \exp(-(L_C - Z_I) K_C)
 \end{aligned} \tag{B.32}$$

Introducing the following expressions to simplify the RHS of the resulting simultaneous equations (B.23), (B.26), (B.29) and (B.32).

$$\gamma = \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} \frac{k}{K_C} \exp(-Z_I K_C) \tag{B.33}$$

$$\gamma' = \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} \frac{k}{K_C} \exp(-(L_C - Z_I) K_C) \tag{B.34}$$

Using these four simultaneous equations to find the coefficients is too complex for a basic elimination method. Instead an inverse matrix method is employed to solve the coefficients, e.g. arranging the simultaneous equations into the matrices $\mathbf{AX} = \mathbf{b}$ presented as equation (B.35), the solution for the coefficients can be found from $\mathbf{X} = \mathbf{A}^{-1}\mathbf{b}$.

$$\begin{bmatrix} 1 & -1 & -1 & 0 \\ 0 & -\exp(-L_C K_C) & -\exp(L_C K_C) & \exp(-L_C K_D) \\ K_S & K_C & -K_C & 0 \\ 0 & -K_C \exp(-L_C K_C) & K_C \exp(L_C K_C) & K_D \exp(-L_C K_D) \end{bmatrix} \begin{bmatrix} A_S \\ A_C \\ B_C \\ A_D \end{bmatrix} = \begin{bmatrix} \gamma \\ \gamma' \\ \gamma \\ \gamma' \end{bmatrix} \tag{B.35}$$

Computing the inverse of the first matrix on the LHS by hand is very tedious, instead Wolfram's Mathematica [131] application has been utilised to solve the coefficients. Following the computation in Mathematica to solve the matrix problem above and after some manipulation the coefficients can be written as follows.

$$A_S = \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} 2k \exp(-Z_I K_C) A_m \tag{B.36}$$

$$A_C = \frac{Q}{4\pi\epsilon_{Si}\epsilon_0} \frac{k}{K_C} (K_C - K_S) \exp(-Z_I K_C) A_m \tag{B.37}$$

$$A_m = \frac{K_C (\exp(2L_C K_C) + \exp(2Z_I K_C)) + K_D (\exp(2L_C K_C) - \exp(2Z_I K_C))}{(K_C^2 + K_S K_D) (\exp(2L_C K_C) - 1) + K_C (K_S + K_D) (\exp(2L_C K_C) + 1)} \tag{B.38}$$

B.1 Double Interface Solution

for the source interaction coefficients and

$$B_C = \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \frac{k}{K_C} (K_C - K_D) \exp(-Z_I K_C) A_n \quad (B.39)$$

$$A_D = \frac{Q}{4\pi\epsilon_{si}\epsilon_0} 2k \exp(-Z_I K_C) \exp(L_C (K_C + K_D)) A_n \quad (B.40)$$

$$A_n = \frac{K_C (\exp(2Z_I K_C) + 1) + K_S (\exp(2Z_I K_C) - 1)}{(K_C^2 + K_S K_D) (\exp(2L_C K_C) - 1) + K_C (K_S + K_D) (\exp(2L_C K_C) + 1)} \quad (B.41)$$

for the drain interaction coefficients.

B.1 Double Interface Solution

Substituting the coefficients found in the previous section into the potentials from section B.1 , gives the finalised forms.

$$\varphi_s = \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \int_0^\infty dk 2k J_0(kR) \exp(ZK_S) \exp(-Z_I K_C) A_m \quad (B.42)$$

$$\begin{aligned} \varphi_C = \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \int_0^\infty dk J_0(kR) \frac{k}{K_C} \{ & \exp(-|Z - Z_I| K_C) \\ & + (K_C - K_S) \exp(-(Z + Z_I) K_C) A_m \\ & + (K_C - K_D) \exp(-(Z - Z_I) K_C) A_n \} \end{aligned} \quad (B.43)$$

$$\varphi_D = \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \int_0^\infty dk 2k J_0(kR) \exp(-(Z - L_C) K_D) \exp(-(Z_I - L_C) K_C) A_n \quad (B.44)$$

Here the coefficients A_m and A_n are given by the equations (B.38) and (B.41) respectively, and the terms K_x are given by equations (B.18)-(B.20). Again, k is introduced as a separation variable and should not be confused with the carrier wave vector of the same symbol.

Appendix C Full Single Interface Scattering Model

This appendix will present the scattering model for the full single interface model which is used in section 4.2.5.2 to compare the mobility of the full and strongly screened models. This model is not used extensively in this research work but is included in the appendix for future reference.

The full or complete single interface model is based on the potential found in section 4.2.1 with the accompanying detailed calculation in Appendix A. Unlike the strongly screened model which assumes a metallic source and is used for scattering calculations in this PhD work, the model developed here will include the exact interaction of the doped source region of semiconductor.

Here an identical approach to that of Chapter 5 to calculate a scattering model will be used. A spherically-symmetric scattering potential using the Z-aligned simplification discussed in section 5.2.3 is assumed in the calculation which follows Fermi's Golden Rule approach assuming spherical, non-parabolic bands. Initially the scattering matrix element will be calculated from the scattering potential in section C.1 . The scattering probability and scattering rate are then obtained in section C.2 .

C.1 Matrix Element

The matrix element is found by completing the Fourier transform of the interaction potential over cylindrical co-ordinates, equation (5.6).

$$\mathbf{H}_{\mathbf{k}'\mathbf{k}} = \frac{1}{\Omega} \int_{-\infty}^{\infty} dZ \int_0^{2\pi} d\phi \int_0^{\infty} d\mathbf{R} U_s(\mathbf{R}, Z) \exp(-i\mathbf{q}_{\perp} \cdot \mathbf{R}) \exp(-iq_z Z) \quad (\text{C.1})$$

For the complete model the full interaction potential calculated in detail in Appendix A will be used and is repeated here as equations (C.2)-(C.3).

$$\varphi_s = \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \int_0^{\infty} dk J_0(kR) \frac{2k}{K_C + K_S} \exp(-Z_I K_C) \exp(Z K_S) \quad (\text{C.2})$$

$$\begin{aligned} \varphi_C = \frac{Q}{4\pi\epsilon_{si}\epsilon_0} \int_0^{\infty} dk J_0(kR) \frac{k}{K_C} \left\{ \exp(-|Z - Z_I| K_C) \right. \\ \left. + \frac{K_C - K_S}{K_C + K_S} \exp(-(Z + Z_I) K_C) \right\} \end{aligned} \quad (\text{C.3})$$

where

$$K_C = \sqrt{k^2 + k_C^2} \quad (C.4)$$

$$K_S = \sqrt{k^2 + k_S^2} \quad (C.5)$$

It should be noted that in equations (C.2)-(C.5) the variable k is not the carrier wave vector used in general notation but is in fact a separation variable introduced in the solution of the potential. Using the following form, the source and drain interaction potentials can be substituted into equation (5.6).

$$U_S(\mathbf{R}, Z) = eV(\mathbf{R}, Z) = e(\theta(-Z)\phi_S + \theta(Z)\phi_C) \quad (C.6)$$

Here e is the electronic charge and θ is the unit step function. Re-arranging the form of equation (5.6) taking care with the unit step functions of equation (C.6) gives

$$\mathbf{H}_{\mathbf{k}'\mathbf{k}} = \frac{1}{\Omega} \int_0^{2\pi} d\phi \int_0^\infty d\mathbf{R} \exp(-i\mathbf{q}_\perp \cdot \mathbf{R}) \left\{ \int_{-\infty}^0 dZ e\phi_S \exp(-iq_Z Z) + \int_0^\infty dZ e\phi_C \exp(-iq_Z Z) \right\} \quad (C.7)$$

where $\mathbf{q}_\perp$ is the momentum transfer in the plane perpendicular to the Z-axis and q_Z is the momentum transfer along the Z-axis. After some lengthy integration and algebraic manipulation, the Fourier transform of the potentials is found to be

$$\begin{aligned} \mathbf{H}_{\mathbf{k}'\mathbf{k}} = & \frac{eQ}{4\pi\epsilon_{Si}\epsilon_0} \frac{2\pi}{\Omega} \left[\frac{2}{K_C + K_S} \exp(-Z_I K_C) \frac{K_S + iq_Z}{\mathbf{q}_\perp^2 + q_Z^2 + k_S^2} \right. \\ & + \frac{1}{K_C} \left(\exp(-iq_Z Z_I) \frac{2K_C}{\mathbf{q}_\perp^2 + q_Z^2 + k_S^2} \right. \\ & \left. \left. - \exp(-Z_I K_C) \left(\frac{K_C + iq_Z}{\mathbf{q}_\perp^2 + q_Z^2 + k_S^2} - \left(\frac{K_C - K_S}{K_C + K_S} \right) \frac{K_C - iq_Z}{\mathbf{q}_\perp^2 + q_Z^2 + k_S^2} \right) \right) \right] \quad (C.8) \end{aligned}$$

where the terms K_x have now become

$$K_C = \sqrt{\mathbf{q}_\perp^2 + k_C^2} \quad (C.9)$$

$$K_S = \sqrt{\mathbf{q}_\perp^2 + k_S^2} \quad (C.10)$$

C.2 Scattering Rate

Before this scattering matrix element can be used in Fermi's Golden Rule, the magnitude-squared must be found. After some extensive manipulation, the solution is found as

$$|\mathbf{H}_{\mathbf{k},\mathbf{k}'}|^2 = \left(\frac{eQ}{4\pi\epsilon_{Si}\epsilon_0} \right)^2 \left(\frac{2\pi}{\Omega} \right)^2 \frac{1}{(\mathbf{q}_\perp^2 + q_z^2 + k_C^2)^2} f_{sgl}(k_C, Z_I) \quad (\text{C.11})$$

where the f_{sgl} function can be expressed as

$$f_{sgl}(k_C, Z_I) = 4 \left(\cos(q_z Z_I) A_{sgl} + \sin(q_z Z_I) B_{sgl} \right) + \exp(-2Z_I K_C) (C_{sgl} + D_{sgl}) \quad (\text{C.12})$$

$$A_{sgl} = \cos(q_z Z_I) - \exp(-Z_I K_C) \times \left(1 - \frac{1}{K_C + K_S} \left((K_C - K_S) + 2K_S \left(\frac{q_z^2 + K_C^2}{q_z^2 + K_S^2} \right) \right) \right) \quad (\text{C.13})$$

$$B_{sgl} = \sin(q_z Z_I) + \exp(-Z_I K_C) \frac{q_z}{K_C} \times \left(1 + \frac{1}{K_C + K_S} \left((K_C - K_S) - 2K_C \left(\frac{q_z^2 + K_C^2}{q_z^2 + K_S^2} \right) \right) \right) \quad (\text{C.14})$$

$$C_{sgl} = 1 - \frac{1}{K_C + K_S} \left(2(K_C - K_S) - \frac{(K_C - K_S)^2}{K_C + K_S} + 4K_S \left(\frac{q_z^2 + K_C^2}{q_z^2 + K_S^2} \right) \left(1 - \frac{K_S}{K_C + K_S} \left(\frac{q_z^2 + K_C^2}{q_z^2 + K_S^2} \right) - \left(\frac{K_C - K_S}{K_C + K_S} \right) \right) \right) \quad (\text{C.15})$$

$$D_{sgl} = \frac{q_z^2}{K_C^2} + \frac{q_z^2}{K_C(K_C + K_S)} \left(\frac{2(K_C - K_S)}{K_C} + \frac{(K_C - K_S)^2}{K_C(K_C + K_S)} - 4 \left(\frac{q_z^2 + K_C^2}{q_z^2 + K_S^2} \right) \left(1 - \frac{K_C}{K_C + K_S} \left(\frac{q_z^2 + K_C^2}{q_z^2 + K_S^2} \right) + (K_C - K_S) \right) \right) \quad (\text{C.16})$$

C.2 Scattering Rate

The scattering rate is found using Fermi's Golden Rule approach given by equation (5.9), which describes the probability of scattering from a state $\mathbf{k}$ to a state $\mathbf{k}'$ for an elastic interaction.

$$P(\mathbf{k}, \mathbf{k}') = \frac{2\pi}{\hbar} |\mathbf{H}_{\mathbf{k}'\mathbf{k}}|^2 \delta(E(\mathbf{k}') - E(\mathbf{k})) \quad (\text{C.17})$$

Substitution of the scattering matrix element into the Golden Rule gives

$$P(\mathbf{k}, \mathbf{k}') = \frac{2\pi}{\hbar} \left(\frac{eQ}{4\pi\epsilon_{si}\epsilon_0} \right)^2 \left(\frac{2\pi}{\Omega} \right)^2 \frac{\delta(E(\mathbf{k}') - E(\mathbf{k}))}{(\mathbf{q}_\perp^2 + q_z^2 + k_C^2)^2} f_{sgl}(k_C, Z_I) \quad (\text{C.18})$$

where f_{sgl} is given by equations (C.12)-(C.16). The scattering and momentum relaxation rates (for an elastic interaction) can be evaluated from the scattering probability using equations (5.14) and (5.15) respectively.

$$\Gamma(\mathbf{k}) = \sum_{\mathbf{k}'} P(\mathbf{k}, \mathbf{k}') = N_k \int_{\mathbf{k}'} P(\mathbf{k}, \mathbf{k}') d\mathbf{k}' \quad (\text{C.19})$$

$$\frac{1}{\tau_m(\mathbf{k})} = \sum_{\mathbf{k}'} P(\mathbf{k}, \mathbf{k}') (1 - \cos \theta) = N_k \int_{\mathbf{k}'} P(\mathbf{k}, \mathbf{k}') (1 - \cos \theta) d\mathbf{k}' \quad (\text{C.20})$$

$$N_k = \frac{\Omega}{(2\pi)^3} \quad (\text{C.21})$$

The scattering can be calculated to give

$$\Gamma(\mathbf{k}) = \left(\frac{Ze^2}{4\pi\epsilon_{si}\epsilon_0} \right)^2 N_I \frac{2\pi m^* k}{\hbar^3} (1 + 2\alpha E) \int_0^\pi d\theta \frac{\sin \theta}{(\mathbf{q}^2 + k_C^2)^2} f_{sgl}(k_C, Z_I) \quad (\text{C.22})$$

where the final integral is left to numerical integration. The momentum relaxation rate can be found by substituting the scattering weighting term into the integral.

$$\frac{1}{\tau_m(\mathbf{k})} = \left(\frac{Ze^2}{4\pi\epsilon_{si}\epsilon_0} \right)^2 N_I \frac{2\pi m^* k}{\hbar^3} (1 + 2\alpha E) \int_0^\pi d\theta \frac{\sin \theta (1 - \cos \theta)}{(\mathbf{q}^2 + k_C^2)^2} f_{sgl}(k_C, Z_I) \quad (\text{C.23})$$

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