Dopants and Roughness induced Resonances in thin Si Nanowire transistors: A self-consistent NEGF-Poisson study

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Abstract. Non-Equilibrium Green Function simulations of the effect of discrete ionised dopants and surface roughness in Silicon nanowire transistors show the strong presence of resonances in the transmission coefficients. These resonances or quasi-bound states are the main component in the screening of dopants and play an important role in the current flow. Resonances appear through a self-consistent calculation of the electron density and potential. In this work we study several examples that exhibit different types of resonances. We start with a single impurity case and gradually evolved to a complex case with several random impurities. Interface roughness in a very narrow nanowire could induce resonant cavities as is proven in this paper. The effect of these resonances in the current-voltage characteristic of the transistors is considered in detail.
1. Introduction

Present day bulk Si MOSFET technology is very close to exhausting its possibilities for further device miniaturisation. Silicon nanowire transistors are considered as one of the potential candidates in future Integrated Circuit technologies. The Gate-All-Around (GAA) silicon nanowire transistor architecture exhibits higher mobility and better electrostatic control than the corresponding bulk MOSFET architecture. Two of the most important factors that affect small transistor behaviour, or the electron propagation, are the intrinsic discreteness of the dopant atoms and the roughness of the Si/SiO₂ interface.

Device simulation consists of the self-consistent solution of two equations: firstly, the Poisson equation, which is used to compute the electrostatic potential from the fixed and mobile charge, and through the use of adequate boundary conditions; the other equation, which can be called a transport model, allows for the calculation of the electron and current density. There are different types of transport model, which differ in their degree of sophistication. The drift-diffusion model is the simplest and most widely used in the electronics community. It treats the electron as a charged fluid, which drifts and diffuses. The drift is caused by the local electric field and the diffusion is due to the fact that the electrons have a random kinetic energy of the order of $k_B T$. This model successfully catches the field-charge interaction and the effect of the temperature. Parameters such as electron mobility and density of states are necessary in this model. The MOSFET transistor is an electrostatic beast, which means that the electric field controls most of the transistor behaviour and induces the current flow. The interplay between the charge and the field, through trying to minimize the electrostatic energy and concentration gradients, determines the device characteristics. Fully functional transistors with body thickness as small as 0.7 nm have been fabricated [1]. Despite the strong confinement induced by the narrow channel, electrons are pushed through the channel by the powerful electric field.

Refined transport models, which treat electrons as Newtonian balls with renormalized masses due to the electron interaction with the perfect crystal, are also deployed. The collision with imperfections and vibrations of the crystal are included through the abrupt change of momentum and energy of the electron after a certain drift time. The drift time is calculated by quantum transition probabilities using the first Born approximation. This model allows for a spectral representation of the density, which at highly inhomogeneous electric fields, deviates from the Maxwellian or Fermi-Dirac distribution. The physical parameters of this model are effective electron masses or energy dispersions, electron-phonon coupling constants, sound velocity, elastic constant, etc., which are more fundamental than the parameters used in drift-diffusion. Average physical parameters such as electric field dependent mobility can be calculated from this model, if low field mobility is known.

Both models have been corrected to accommodate the quantum effects associated with the reduction of the transistor dimensions. The most successful of these corrections is the density gradient. This accounts for a repulsion energy (not associated to electric repulsion) associated with large concentration gradients or a strong localization of electrons, which pushes electrons away from the interfaces and mimics a ground state distribution of electrons in the wells. The origin of this force or potential comes from a striking similarity between the Hamilton-Jacobi equation and the Schrödinger equation for the phase of the wave function. The equation for the phase contains an additional potential, which varies as $\nabla^2 \left( \sqrt{n} \right) / \sqrt{n}$, where $n$ is the electron density. This potential is considered as a quantum potential that corrects the classical potential in the transport equation. Using the drift-diffusion model and the density gradient correction, it is possible to simulate the volume inversion i.e. when the electron density becomes larger in the middle of the channel as compared with that at the interface, which is really a property of the ground state. This effect occurs at body thicknesses below 20 nm [2]. Gate capacitances become smaller due to volume inversion and quantum confinement in
the triangular well, induced by the band bending at the Si/SiO₂ interface creating the need for a larger gate voltage in order to achieve the same inversion charge.

The intrinsic discreteness of the impurities in the device needs to be considered as the size of the device reduces. Technologically identical devices, which differ in the microscopic spatial configuration of dopants and the number of dopants, present different behaviours due to the non-self-averaging inherent in small structures and the small number of dopants. Capturing of these effects is essential for an accurate description of the current flows in devices.

In this work we present a study of the influences of different types of spatial inhomogeneities such as discrete dopants/surface roughness on the electron transport through a thin Si nanowire transistor [3, 4]. The shape of the self-consistent electrostatic potential around an ionised donor impurity induces resonant states. These states shape the transmission function and are an important element in the propagation of the electron through the nanostructure. Surface roughness can, under certain conditions, also induce resonant levels. Studies of the effect of dopants on the device characteristics in a statistical ensemble of devices, which differ in the particular realisations of disorder, will be presented. In this work we have deployed a full 3D Non-Equilibrium Green Function (NEGF) formalism coupled with the Poisson equation. The NEGF equations are written in the effective mass approximation and use Hartree’s approximation for the interacting electron system. The rest of the paper is divided into three parts. Section 2 provides an introduction to the use of NEGF describing the coupling of the NEGF transport equation and the Poisson equation; a brief description of the NEGF-Poisson algorithm is presented. Section 3 describes models of different sources of inhomogeneous potential, such as those created by the roughness of the SiO₂/Si interface and the discreteness of the dopant atoms. We discuss the role of these inhomogeneities in the creation of resonance states that control electron flow. Furthermore, we computed the impact of these resonances on transistor performance. The final section presents the conclusions.

2. Non-Equilibrium Green’s Function Approach to Device Simulation

The quantum carrier transport is described using the NEGF approach, which is a generalisation of Landauer’s formalism [5, 6, 7, 8] to treat many body systems at room temperature in the context of the one particle Green’s function. The Hamiltonian used in the discretisation of the NEGF equations is an effective-mass Hamiltonian that folds the full crystal interaction into the electron effective masses:

$$ H = -\frac{\hbar^2}{2} \nabla \left( \frac{1}{m_{ij}} \right) \nabla_j + V(\vec{r}) $$

(1)

Where \((1/m)_{ij}\) is the inverse of the mass tensor which contains the effective masses and \(V(r)\) is the self-consistent electrostatic potential coming from the solutions of Poisson’s equations.

The effective masses of the transport valleys are extracted from Tight Binding calculations that capture the dependence of the electron band structure on the nanowire diameter [9]. Due to the small dimensions of the wire cross-section we only include four of the six lowest valleys of the silicon conduction band. The two valleys that have been neglected have transversal masses 0.3\(m_0\) in the directions perpendicular to the transport direction, resulting in large ground-state energy shifts associated with the transversal confinement. As a result the electron population of these valleys is negligible compared to the other four valleys for the simulated nanowire diameter, temperature and bias conditions. Sources of incoherent scattering such as phonon interaction, and the corresponding self-energies, are not included in our NEGF simulations. We calculate the correlation matrix, \(G^c\), using the recursive algorithm described in [10, 11, 12]. From the correlation matrix, the electron and current densities are calculated by the following equations:

$$ n(E,x) = iG^c(E,x,x) $$

(2)
The boundary conditions of the Green’s function equations at the contacts, which are given through the contact self-energies, are defined using the algorithm described in [13].

\[ J(E, x) = -i \frac{eh}{2m} (\nabla - \nabla')G^<(E, x, x') \Big|_{x'=x} \]  

(3)

Fig. 1 shows the flow chart of our simulator illustrating the computational procedure used to solve the coupled Poisson-NEGF equations. The electrostatic potential and the electron density obtained from a density gradient (DG) solution of the Drift-Diffusion (DD) equations [14] serve as an initial condition for the Poisson-NEGF cycle. The DD solver has Neumann boundary conditions for Poisson’s equation in the source and drain instead of the Dirichlet boundary conditions usually used in the DD formalism [15, 16], which matches well with the Green’s function boundary conditions. A close initialisation of the potential distribution at the beginning of the Poisson-NEGF loop reduces drastically the number of NEGF iterations.

After the first Poisson-NEGF iteration the change in electron concentration from the initial DG solution to the new NEGF solution is moderated by damping. A gradual change in the electron density prevents oscillatory behaviour of the solution around the impurities leading to divergence. The
solution instabilities are associated with the extreme sensitivity of the quantum density to the shape of the attractive potential. This is related to the discrete nature of the quasi-bound states and their energy sensitivity to the shape of the potential.

We have found that solving the non-linear Poisson equation results in a much more stable convergence of the Poisson-NEGF system than if the linear version is used. Once a new electron density is obtained from the NEGF solver, a quasi-Fermi level, $f_n$, is calculated using the new density and the old potential [17]. This quasi-Fermi level is used to update the electron concentration and the Jacobian when solving the non-linear Poisson equation iteratively (see Fig. 1). Adaptive damping is used after the solution of the Poisson equation to limit the change in potential and to improve convergence. The alternate solutions of Poisson and NEGF are iterated until density and current converge.

3. Modelling of Surface Roughness and Discrete Dopants

The random discrete dopants have been introduced in a 4 nm region of the source/drain (S/D) leads between the channel and the continuously doped S/D regions next to the contacts. Each Si lattice site in these regions is considered and whether this site has a dopant or not is determined using a rejection technique based on the ratio between the nominal doping concentration and the silicon atom density at that point [18]. The resulting total number of dopants in the discrete dopant regions closely follows a Poisson distribution. The charge of each dopant is distributed to the surrounding nodes of the discretisation mesh using the cloud-in-cell technique. The region with continuous doping between the discretely doped regions and the contacts guarantees a homogeneous injection into the source/drain from the reservoirs. The random rough interface between Si and SiO$_2$ is introduced using the approach described in [19]. The interface is modelled by a randomly generated surface with exponential autocorrelation function and specified rms amplitude and correlation length selected based on results reported in [20]. The correlation length of the order of 2 nm is similar to the one typically used in Monte Carlo simulations used to reproduce the universal mobility curve [21]. The generated ‘analogue’ random surface is quantised to two levels on the scale of one inter-atomic layer.

The simulated Si NWTs have a 6 nm undoped channel with 2.2x2.2 nm$^2$ cross-section, 0.8 nm SiO$_2$ oxide and 10 nm S/D regions doped at $10^{20}$ cm$^{-3}$. The transport in the nanowire occurs in the <100> direction. The diameter-dependent effective masses are extracted from $sp^3d^5$ second-neighbour-basis tight-binding calculations [9]. All the simulations in this work have been done at room temperature.

3.1. Discrete Dopants

In the following subsections we present and discuss the simulation of discrete dopants. Firstly we analyzed the case of a donor in the middle of a doped silicon wire. This example illustrates the relationship between the shape of the potential and the type of resonance/anti-resonance. These resonances will be present in all the cases studied. The second example concentrates on simulations of the effect on the Si gate-all-around nanowire transistor of random discrete donors in the source and drain. This example has practical applications, as random dopant variability is an important issue in the reliability of digital circuits.
3.1.1. *A donor in the middle of the Si wire.*

We introduced a donor-like impurity in the middle of a doped nanowire. The impurity is modeled as a charge distributed in the cubic volume of $0.2\text{nm} \times 0.2\text{nm} \times 0.2\text{nm}$, which is the range of the dielectric screening length [22]. A tuning of the gate potential can partially control the shape of the impurity potential. This allows us to study the effects of the shape of the impurity potential on the electron transmission. The gate potential introduces a barrier around the impurity that partially repels the electrons from the channel. As the gate potential increases, the electrons are attracted to the channel and their presence screens the potential of the impurity. The density of electrons and its shape around the impurity depends on the self-consistent potential and the nature of the quantum states around it.

That has to account also for the polarization including the image charge induced at the dielectric/semiconductor interface as well as at the dielectric/metal interface. An impurity placed in the middle of the channel will create a deep potential surrounded by potential barriers, the so-called...
inverted sombrero type potential (also a double Gaussian type potential [23] since it can be constructed from two Gaussians). Fig. 2 shows that this potential initially exhibits wide barriers around the dip at an applied gate bias of 0.3 V. As the potential applied to the metal gate increases, the barriers are lowering and become nearly flat at a gate bias of 0.65 V. Fig. 3 shows the corresponding electron density along the channel of the nanowire at the same gate biases. The corresponding transmission coefficients as a function of the electron energy for this potential are presented in Fig. 4. At Vg=0.3 V, there is a pronounced resonance at an energy of 0.2805 eV.

The transmission at this resonance energy falls to almost zero before the first energy mode of the nanowire starts to appear. The wave function of this resonance mode is strongly localised around the impurity. This can be seen in the upper panels of Fig. 5, which shows the single-electron density at the resonant energy (0.2805eV). The electron wave function is strongly localised at the impurity position with no wave reflection and is fully transmitted. The two middle panels of Fig. 5 show the probability density of electrons with energies 0.35 eV and 0.65 eV corresponding to low and high transmission probability. In contrast to the resonant electron, these electrons have a de-localised wave function.
This de-localised electron wave is partially reflected while the transmission probability increases with the electron energy approaching the next energy mode. The following resonance is less pronounced compared to the first occurrence at the single energy mode leading to much smaller decline in transmission probability.

The situation changes at large gate biases when the shape of the self-consistent potential becomes Coulomb-like (a single Gaussian-type potential) which has no barriers as illustrated in Fig. 6. The electron density will now exhibit a typical asymmetry, as demonstrated in Fig. 7, for indicated energy modes. Fig. 8 shows corresponding transmission with an asymmetric Fano resonance [24]. This resonance appears due to the existence of a localised level in the continuum. Fig. 9 shows the probability density for three different energies. The energy of the electron in the upper panel is close to the Fano resonance and its wave function is strongly localised around the impurity. The Fano resonance state has the largest contribution to the screening of the impurity charge. The electron wave function at Fano resonance will be fully reflected and makes no contribution to the electron transport through the nanowire.

![Figure 10. Transmision coefficients for the uncoupled mode case. Full line: the total transmission. Dashed line: transmission of a single mode](image1)

![Figure 11. Transmision coefficients for the coupled mode case. Full line: the total transmission. Dashed line: transmission of a single mode](image2)

The middle and lower panels of Fig. 9 show non-resonant electron states, which are de-localised thus exhibiting several nodes along the wire. The Fano resonances will always appear at the same amount of energy below the next transversal mode. This observation was already pointed out in [23], which presents indications that the resonances are due to the interaction between the modes. In order to confirm the relation of the Fano resonance with the coupling between the modes with have carried out the simulation in a coupled mode-space approach, which allows the coupling and decoupling of the modes in an undoped wire. The results are presented in Figs. 10 and 11 for the transmission coefficients for the case of the coupled and uncoupled cases respectively. The non-resonant electron states have very small contributions to the screening of the impurity charge but will contribute significantly into the electron transport. Fig. 10 does not exhibit anti-resonances because the modes are not coupled, but in Fig. 11 the anti-resonances are present confirming the hypothesis.
3.1.2. Dopants in the Source and Drain of GAA Si Nanowire Transistor.

Due to the significant computational burden associated with the 3D NEGF approach, and its slow convergence in the presence of attractive impurity potentials, the statistical simulation study has been restricted to a small statistical sample of 30 randomly generated device configurations. All simulations were carried out at $V_D=1$ mV in the linear mode of device operation. Fig. 12 shows, on a linear and logarithmic scale, the current-voltage characteristics of the 30 microscopically different NWTs with different random dopant (RD) configurations. The nanowire with continuous doping (labelled as ‘smooth’ in the figure), and one with no dopants at all in the random dopant regions, are shown for comparison. At $V_G<0.3$ V, which marks the transition between the sub-threshold and the linear region of the transistor operations, the device configurations with a high concentration of discrete dopants located close to the channel lower the gate barrier potential, leading to a higher current than in the smooth case. At $V_G>0.3$ V the smooth device always delivers a higher current than in the RD devices. This is mainly associated with the coherent impurity scattering in RD devices, which reduces the current due to partial reflection from the impurity potentials. The degree of backscattering, for a particular RD configuration, depends strongly on the gate voltage. As a consequence, the on-current in ‘unlucky’ RD devices is reduced to as low as 20% of the current for the smooth device. A particular configuration may have low scattering at low $V_G$ and high scattering at high $V_G$, or vice versa, relative to other configurations. This sensitivity to the gate voltage is a result of the relative proximity of the discrete dopants to the tail of the channel potential barrier and lead to a crossing of the $I_D-V_G$ curves as can be seen in Fig.12.

There is a variation in the sub-threshold slope of the $I_D-V_G$ curves produced by the different atomistic configurations. Devices with configurations of dopants close to the central axis of the wire, far from the SiO$_2$ interfaces, will have relatively poor electrostatic control compared with devices with dopants distributed closer to the interfaces and to the channel/source and channel/drain junctions. In addition to the sub-threshold slope variation due purely to electrostatics, which have been observed in drift-diffusion simulations, there is an additional contribution from the varying degrees of source-to-drain tunnelling.
At \( V_G = 0.4 \) V, we have investigated the behaviour of the device configurations with: the lowest current (L), the median current (M) and the highest current (H). The corresponding 3D self-consistent electrostatic potential distributions are shown in Fig. 13 (although not all the impurities are evident in the figure). The device with the shortest effective channel length exhibits the largest current. This is clear from Fig. 14, which shows the electron concentration and self-consistent electrostatic potential along the middle of the channel. The device with the largest current has six dopants in the source, producing a region of average dopant concentration much larger than the dopant concentration of the continuously doped smooth device.

The physical effects shaping the impact of the discreteness of the donors on the current-voltage characteristics can be explained qualitatively using the transmission coefficients, which are directly related to the current through the well-known Landauer formula [25],

\[
J = \frac{e^2}{h} \int T(\varepsilon)(f_S(\varepsilon) - f_D(\varepsilon)) \, d\varepsilon
\]  

(3)

where \( T \) is the transmission coefficient and \( f_S(\varepsilon)/f_D(\varepsilon) \) are the Fermi distributions in the source/drain.

Fig. 15 shows the transmission coefficients for the three RD devices and for the smooth device presented as a reference. For the highest current device the shape of the self-consistent potential around some impurities produces Fano-type resonances as seen in Fig. 14. These result in zero transmission at the resonance energies and can be interpreted as back scattering for the corresponding electrons. The electrons at these resonant energies (or quasi-bound states) are the main source of the screening of the impurity potential. For the other two devices we have transmission resonance peaks due to the inverted sombrero shape of the self-consistent potential of the impurities (see Fig.14). The relative value of the on-current between the L, M and H devices can be understood using the Landauer formula (Eq.3) with the transmission coefficients (Fig. 14) of the L, M and H devices at around 0.3 eV (the Fermi Level in Source is 0.2). Note that the transmission for the smooth device has a stair-type characteristic as expected. Therefore, the irregular shape and dips in the transmission for the devices with discrete impurities can be interpreted as a fraction of carriers being reflected back or back scattered. This feature is not visible at lower gate bias because of the dominant reflection of the carriers by the channel barrier potential.
3.2. Surface Roughness
In this section the effect of the interface roughness will be considered. We have assumed rough interface only in the channel and have ignored any roughness between the oxide and the gate material. In order to study the statistical effect associated with the interface roughness the $I_d-V_G$ characteristics of thirty nanowire transistors with different randomly generated interface roughness patterns were simulated and analysed. The collection of individual $I_d-V_G$ characteristics of the devices with different surface roughness configurations is shown in Fig. 16. The devices with a smooth interface, and with the smallest possible cross-section (all the interface roughness steps are in the direction that decreases the body thickness of the channel) are also presented in Fig. 16 for comparison.

The three surface roughness cases selected for analysis produce the lowest, median and the second highest current at all gate biases. The device that produces the highest off-current has a distinct surface roughness pattern and will be analyzed later. At 2.2 nm body thickness even a small intrusion of the interface into the channel is sufficient to raise the ground state of the transverse wave function resulting in the step increases in transmission occurring at higher energies. This effect, together with the roughness-induced scattering, means that the current of the rough devices are generally lower compared to that of the smooth device. It is possible to have a rough device with a higher current than that of the smooth device if there is no overall narrowing of the channel, but the probability for this is very low. The body thickness confinement variation causes a large spread in threshold voltage which (for the 30 devices simulated here) spans 124 mV. In the extreme random roughness case there is a decrease in the on-current by more than 25% compared to that of the smooth device if the threshold voltages are aligned.

![Figure 16](image1.png)

**Figure 16.** $I_d-V_G$ characteristics of the nanowire transistor with surface roughness in the channel. The solid line represents the device with the smallest possible cross-section (2.0×2.0 nm$^2$) where all the interface roughness steps are in the direction that decreases the body thickness of the channel. The smooth device is also shown for comparison.

![Figure 17](image2.png)

**Figure 17.** Potential for the low, median and high current (from top to bottom) of the surface roughness devices at $V_G$=0.4 V.

The 3D distribution of the self-consistent electrostatic potential for the three selected devices at high gate ($V_G$=0.4V) are shown in Fig. 17 with the lowest current device at the top and the highest current device at the bottom. The impact of the reductions in channel body thickness on the potential distribution can be seen in the figure. This together with the corresponding up-shift in the ground-state sub-band resulting from the increased confinement leads to a decrease in the electron current.
The transmission coefficients at high gate bias are compared in Fig. 18. It is possible for the surface roughness to result in specific arrangements of body-thickness variations that resemble a resonant structure. The impact of such resonance is evident in the second sub-band of the lowest current device in Fig. 18. As mentioned previously, surface roughness can also induce quasi-bound states. To illustrate the point we have selected a device in which the particular surface roughness pattern produces a cavity in the channel. This device has a current slightly larger than the smooth device at low gate bias. Fig. 19 shows the surface roughness in two perpendicular planes along the channel length. There is a well-defined cavity between 10 and 15 nm. Fig. 20 shows the transmission of this device and the smooth device. The transmission coefficient of the rough device shows resonances that are clearly Breit-Wigner-type for the first two sub-bands. The first resonance appears before the onset of the smooth device transmission, implying a large current in this device compared to the smooth one. Another manifestation of the resonances is the two maxima in the middle of the channel in the Local Density of States plotted in Fig. 21. The first sub-band energy is also plotted with a dashed line in the same figure in order to clarify the position of the longitudinal resonant cavity.
4. Conclusions
A statistical study of variability due to random discrete dopants at the source/drain and interface roughness in a Si nanowire transistor has been carried out using a full 3D NEGF formalism. The role of resonances in electron transport and transistor performance has been widely studied. The relationship between the shape of the potential and the type of resonances has also been investigated in simple and more complex cases. The transmission coefficients have been used to correlate the spatial inhomogeneities of electrostatic potential with device behaviour. In this small transistor we have proven that the self-average of microscopic roughness in the interface and the discreteness of dopants does not occur and a continuum model will fail to describe the relevant physics involved.

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