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Chapter

Analysis of Quantum Confinement and Carrier Transport of Nano-Transistor in Quantum Mechanics

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Abstract

Quantum mechanics is the branch of physics that consists of laws explaining the physical properties of the nature of nano-particles and their characteristics on an atomic scale. The study of nano-particles significantly challenges our current perception of the universe and the fabric of reality itself. Quantum particles have both wave-like and particle-like characteristics. The fundamental equation that predicts the physical behaviour of a quantum system is the Schrödinger equation and the Poisson equation using Monte Carlo simulations. This gives rise to the *wavefunction, electron and hole densities, energy levels and band structure* of the system which contains all the measurable information about the particle such as time and position, where position is represented using probabilities. This is because particles do not have one definite position during the time before measurement. In fact, they exist as a fuzzy distribution of all possible states where the likelihood of finding the particle in some states is more probable than others. This is known as being in a *superposition* of all states. When the quantum system is observed, however, its wavefunction *collapses* so it consequently falls into one specific position. Moreover, in this chapter we present the simulation results of conduction band profile, electron density (classical and quantum mechanical), eigenstate and eigenfunctions for Si, SOI and III-V MOSFET structures at bias voltage 1.0 V using 1D Poisson-Schrödinger solver.

Keywords: nano-devices, nano-particles, MOS, SOI and III-V structures, 1D Poisson-Schrödinger solver, conduction and valence band profile, carrier density and wavefunctions in the potential well, wave-particle duality

1. Introduction

In this chapter, a connection between the band structure and quantum confinement effects with device characteristics in nano-scale devices is established. Three different devices are presented: a 25 nm gate length Si MOSFET, a 32 nm SOI MOSFET and a 15 nm $In_{0.3}$ $Ga_{0.7}As$ channel MOSFET. We use a 1D Poisson-Schrödinger solver across the middle of the gate along the channel of the devices. The goal is to obtain the calculations of an energy of bound states and associated carrier wavefunctions which are carried out self consistently with electrostatic potential.

The obtained wavefunctions are then used to calculate a carrier density which allows to obtain a sheet density across the structure at given bias.

One of the architectures seriously considered the Silicon-On-Insulator (SOI) transistor as a replacement for bulk MOSFETs. SOI transistors have many advantages compared with the conventional bulk MOSFET architecture. One of the most important is a better electrostatic integrity. SOI devices tolerate thicker gate oxides and low channel doping, allowing scaling to sub-10 nm channel lengths without substantial loss of performance.

However, the transition to this new device architecture and the eventual introduction of new materials in order to further boost device performance is a challenging task for the industry. However, the simulation of UTB transistors has to consider the impact of quantum confinement effects on the device electrostatics. The confinement effects can be induced into classical device simulation approaches using various approximations which include the density gradient approach [1, 2], the effective potential approach [3] and 1D Poisson-Schrödinger solver acting across the channel [4].

This idea leads onto another fundamental quantum superpower called quantum tunnelling. Quantum tunnelling causes particles to simply pass through physical barriers. If a particle was trapped in a well where it has not got enough kinetic energy to escape the well, it would stay in the well as one would expect, however, there is a slight difference. There will also be an exponentially decaying probability that the particle is found outside the well (under specific conditions, that is)! This has to do with the fact that the particles have a 'wave' of probable locations it can be in which extends beyond the well.

2. Quantum mechanics in a semiconductor

The purpose of this chapter is to understand the behaviour and properties of the particles of semiconductor material and devices. In order to get a conception of conduction band and valence band profile, drift velocity, energy, characteristics of the electrical field, wavefunction, carriers density and the mobility of carriers, we need to have an idea on the behaviour of carriers and then proper analysis about semiconductor materials which is related to the different potential. For more understanding about the particles in the theory of semiconductor physics we need to increase our knowledge extensively on the area of quantum mechanical wave theory. Furthermore, we will get idea about the physical behaviour of the materials in semiconductor physics whose electrical properties are related to the behaviour of the carriers in the crystal lattice structure. We will do an analysis of these carriers with the formulation of quantum mechanics, so called 'wave mechanics'. One of the most important parts to describing wave mechanics is 'Schrödinger wave equation'. The gradient of Poisson equation describes about the carriers density of the materials in the semiconductor devices. More details about the characteristics and behaviour of carriers of the semiconductor materials related with the quantum mechanical behaviour are described in this chapter.

2.1 Action of quantum mechanics

Generally, in quantum mechanics, we need to know the basic idea about the principle of tiny energy behaviour (photon), the wave-particle duality, wavefunction behaviour in the potential well, Heisenberg uncertainty principle, and the Schrödinger and Poisson equation.

2.1.1 Wave and photon energy

In general, a wave is a 'perturbation' from the surrounding or 'collision' between particles that travel from one position to another position over time. As we know a wave like classically or electromagnetic wave, which carries momentum and energy during changing the position, while in quantum mechanically a wavefunction can be applied to find out probabilities. We can say the equation for such wavefunction, so called Schrödinger wave equation, which will be described and developed mathematically with more details in the next section [1, 2].

We will now explore the physics behind the photoelectric effect. If light (monochromatic) falls on a smooth and clean surface of any material, then at some specific conditions, electrons are emitted from the surface. According to classical physics, the high intensity of light where the work function of the material will be overcome and an electron will be emitted from the surface, does not depend on the incident frequency, which is not observable. The observed effect is that, at a constant intensity of the incident light, the kinetic energy of the photoelectron increases linearly with frequency, start at specific frequency ν_0, below this frequency we did not observe any emission of photoelectron, as shown in **Figure 1(a)** and **(b)**.

After heating the surface, from that surface, thermal radiation will be emitted continuously (Planck), which form in discrete packets of energy called 'quanta'. The energy of these quanta is generally described by $E = h\nu$, where ν is the frequency of radiation and h is a Planck's constant. However, Einstein explained that the energy in a light wave also contains photon or quanta, whose energy is also given by $E = h\nu$. A photon with high energy can emit an electron from the surface of the material. The required energy to emit an electron is equal to the work function of the material, and rest of the incident photon energy can be converted into the kinetic energy of the photoelectron [1–3]. The maximum kinetic energy of the photoelectron can be written below as in the equation form:

$$T_{max} = \frac{1}{2} mv^2 = h\nu - h\nu_0 \tag{1}$$

2.1.2 Wave-particle duality

As we know the light waves in the photoelectric effect behave like particles. In the Compton effect experiment, an X-ray beam was incident on a solid - individual photons collide with single electrons that are free or quite loosely bound in the atoms of matter, as a result colliding photons transfer some of their energy and momentum of electrons.

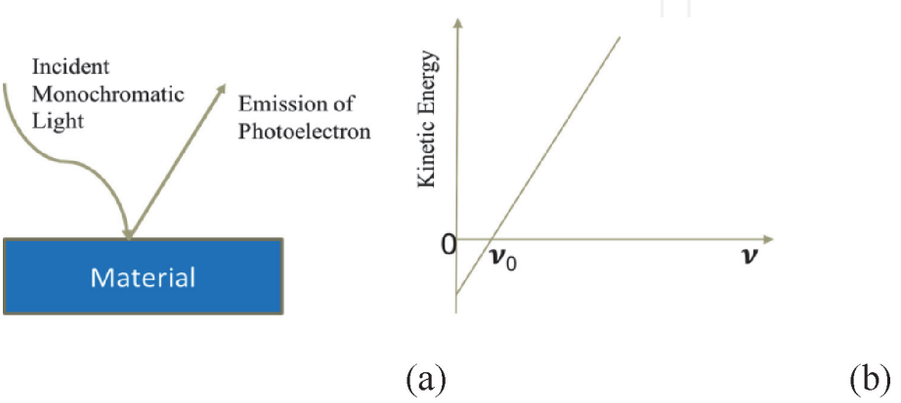

Figure 1.
(a) The photoelectric effect and (b) the kinetic energy of the photoelectron as a function of the incident frequency.

A portion of the X-ray beam was deflected and the frequency of the deflected wave had shifted compared to the incident wave as shown in **Figure 2**. The observed change in frequency and the deflected angle corresponded exactly to the collision between an X-ray (photon) and an electron in which both energy and momentum are conserved [1, 2].

In 1924, de Broglie observed that just as the waves exhibit particle-like behaviour, the particles also show wave-like characteristics. So, the assumption of the de Broglie was the existence of a wave-particle duality principle. The momentum of a photon is given by:

$$\boldsymbol{p} = \frac{\boldsymbol{h}}{\boldsymbol{\lambda}}; = \frac{\boldsymbol{h}}{\boldsymbol{p}}, \tag{2}$$

where $\boldsymbol{p}$ is the momentum of the particle and $\boldsymbol{\lambda}$ is known as the de Broglie wavelength of the matter wave. In general, electromagnetic waves behave like particles (photons), and sometimes particles behave like waves. This wave-particle duality principle quantum mechanics applies to small particles such as electrons, protons and neutrons. The wave-particle duality is the basis on which we will apply wave theory to explain the motion and behaviour of electrons in a crystal.

2.1.3 Uncertainty principle

The uncertainty principle describes with absolute accuracy the behaviour of subatomic particles, which makes two different relationships between conjugate variables, including position and momentum and also energy and time [1, 2].

For the case 1, it is impossible to simultaneously explain with accuracy the position and momentum of a particle. If the uncertainty in the momentum is $\Delta\boldsymbol{p}$, and the uncertainty in the position is $\Delta\boldsymbol{x}$, then the uncertainty principle is stated as

$$\Delta\boldsymbol{p}\Delta\boldsymbol{x} \geq \frac{\hbar}{2} \; \boldsymbol{or} \; \hbar, \tag{3}$$

where $\hbar$ is defined as $\hbar = \frac{\boldsymbol{h}}{2\pi} = 1.054 \text{ x} 10^{-34}$ J-s and is called international Planck's constant.

For the case 2, it is impossible to simultaneously describe with accuracy the energy of a particle and the instant of time the particle has this energy. So, if the uncertainty in the energy is given by $\Delta\boldsymbol{E}$ and the uncertainty in the time is given by $\Delta\boldsymbol{t}$, then the uncertainty principle is stated as

$$\Delta\boldsymbol{E}\Delta\boldsymbol{t} \geq \hbar \tag{4}$$

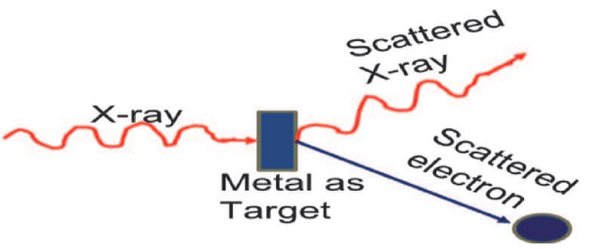

Figure 2.
Compton scattering diagram showing the relationship of the incident photon and electron initially at rest to the scattered photon and electron given kinetic energy.

One consequence of the uncertainty principle is that we cannot, for example, determine the exact position of an electron. We, instead, will determine the probability of finding an electron at a particular position [5, 6].

2.2 Basic principle of Schrödinger and Poisson equation

Generally, the Schrödinger equation description depends on the physical situation. The most common form is the time-dependent Schrödinger equation which gives an explanation of a system related with time and also predicts that wave functions can form standing waves or stationary states. The stationary states can also be explained by a simpler form of the Schrödinger equation, the time-independent Schrödinger Equation [7–9]. We will explain here the motion of electrons in a crystal by theory, which is described by Schrödinger wave equation.

2.2.1 Time dependent and time independent Schrödinger wave equation and the density probability function

The Schrödinger equation is one of the fundamental tools for the understanding and prediction of nano-scaled semiconductor devices. For the case of one dimension the wave vector and momentum of a particle can be considered as scalars, so relating the de Broglie equation, we can write as

$$\boldsymbol{E} = \hbar\boldsymbol{\omega}\ \boldsymbol{p} = \hbar\boldsymbol{k} \tag{5}$$

We use these equation and properties of classical waves to set up a wave equation, known as the Schrödinger wave equation. We solve this equation for the particles which are confined to a potential well, and also to find the solution for particular discrete values of the total energy. However, we develop a theory by considering a particle, moving under the influence of a potential, V (x, t). For this case, the total energy E is equal to the sum of the kinetic and potential energies which can be written as,

$$\boldsymbol{E\psi} = \boldsymbol{H\psi} = \left(\frac{\boldsymbol{p}^2}{2\boldsymbol{m}} + \boldsymbol{V}\right)\boldsymbol{\psi} \tag{6}$$

As we know the momentum operator, and energy are given by

$$\boldsymbol{p} = -\boldsymbol{i}\hbar\frac{\partial}{\partial\boldsymbol{x}}, \boldsymbol{E} = \boldsymbol{i}\hbar\frac{\partial\boldsymbol{\Psi}\ (\mathbf{x},\mathbf{t})}{\partial\boldsymbol{t}} \tag{7}$$

After solving Eqs. (6) and (7), we can develop the one-dimensional time-dependent Schrödinger equation, which can be written as

$$\boldsymbol{i}\hbar\frac{\partial\boldsymbol{\psi}\ (\boldsymbol{x},\boldsymbol{t})}{\partial\boldsymbol{t}} = -\frac{\hbar^2}{2\boldsymbol{m}}\frac{\partial^2\boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{t})}{\partial\boldsymbol{x}^2} + \boldsymbol{V}(\boldsymbol{x})\boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{t}), \tag{8}$$

where $\boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{t})$ is the wave function, which describes the behavior of an electron in the device and V(x) is the potential function assumed to be independent of time, and $\boldsymbol{m}$ is the mass of the particle. Assume that the wave function can be written in the form

$$\boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{t}) = \boldsymbol{\psi}(\boldsymbol{x})\boldsymbol{\phi}(\boldsymbol{t}), \tag{9}$$

where $\boldsymbol{\psi}(\boldsymbol{x})$ is a function of the position $\boldsymbol{x}$ only and $\boldsymbol{\phi}(\boldsymbol{t})$ is a function of time $\boldsymbol{t}$ only. Substituting this form in the Schrödinger wave Eq. (8), we get

$$i\hbar\,\psi(x)\frac{\partial\phi(t)}{\partial t} = -\frac{\hbar^2}{2m}\phi(t)\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\,\psi(x)\,\phi(t) \tag{10}$$

Now, if we divide both sides of the Eq. (10) by the wave function, $\psi(x)\,\phi(t)$, we get

$$i\hbar\,\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V(x) \tag{11}$$

After solving the Eq. (11) (using differential equation), the solution of the above equation can be written as

$$\phi(t) = e^{-i\left(\frac{E}{\hbar}\right)t} \tag{12}$$

We notice the solution of Eq. (12) is the classical exponential form of a sinusoidal wave. As we see from Eq. (11) on the left hand side with function of time, which is equal to the constant of total energy of the particle, and the right hand side is a function of the position x only. After simplification of the above equation the time-independent portion of the Schrödinger wave equation can now be written as

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V(x) = E$$

$$\frac{\partial^2\psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\,\psi(x) = 0 \tag{13}$$

Now, the total wave function can be written as in the form of product of the position or time independent function and the time dependent function,

$$\psi(x,t) = \psi(x)\,\phi(t) = \psi(x)e^{-i\left(\frac{E}{\hbar}\right)t} \tag{14}$$

According to the Max Born, the function $|\psi(x,t)|^2 dx$ is the probability of finding the particle between x and $x + dx$ at a given time, we can express also $|\psi(x,t)|^2\,dx$ as a probability density function.

$$|\psi(x,t)|^2\,dx = \psi(x,t)\cdot\psi^*(x,t), \tag{15}$$

where $\psi^*(x,t)$ is the complex conjugate function. Following Eq. (14), we can rewrite:

$$\psi^*(x,t) = \psi^*(x)e^{i\left(\frac{E}{\hbar}\right)t} \tag{16}$$

Finally, we can develop the density of the probability function using Eq. (14), and Eq. (16), which is independent of time.

$$|\psi(x,t)|^2\,dx = \psi(x)\cdot\psi^*(x) = |\psi(x)|^2 \tag{17}$$

The main difference between classical and quantum mechanics is that in classical mechanics, the position of a particle can be determined precisely, whereas in quantum mechanics the position of a particle is related in terms of probability [1, 2].

2.2.2 Wave function behaviour: finite square well, infinite square well, and tunnelling behaviour

In quantum mechanics, finite square well is an important invention to explain the particle wave function behaviour in the crystal. It is a further development of the infinite potential well, in which particle is confined in the square well. The finite potential well, there is a probability to find the particle outside the box. The idea in quantum mechanics is not like the classical idea, where if the total energy of the particle is less than the potential energy barrier of the walls it is not possible to find the particle outside the box. Alternatively, in quantum mechanics, there is a probability of the particle existing outside the box even if the particle energy is not enough by comparing the potential energy barrier of the walls [1, 8, 9].

We apply here the time independent Schrödinger equation for the case of an electron in free space. Consider the potential function $V(x)$ will be constant and energy must have the condition $E > V(x)$. For analysis, we assume that the potential function $V(x) = 0$ for the region II inside the box, as shown in **Figure 3**, and then the time-independent wave equation can be written as from Eq. (13) as

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\psi(x) = 0 \tag{18}$$

Letting $k = \sqrt{2mE}/\hbar$ or $E = \hbar^2 k^2/2m$, then Eq. (18) leads to

$$\frac{\partial^2 \psi(x)}{\partial x^2} = -k^2 \psi(x) \tag{19}$$

After solving the Eq. (19) using differential equation, the general solution becomes

$$\psi(x) = A \sin(kx) + B \cos(kx),$$

where A and B are complex numbers, and k is any real number.

Now, for the region I and region III, outside the box, where the potential assumed to be constant, $V(x) = V_0$, and Eq. (13) becomes

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\psi(x) = 0$$

$$-\frac{\hbar^2}{2m}\frac{\delta^2 \psi(x)}{\delta x^2} = (E - V_0)\psi(x) \tag{20}$$

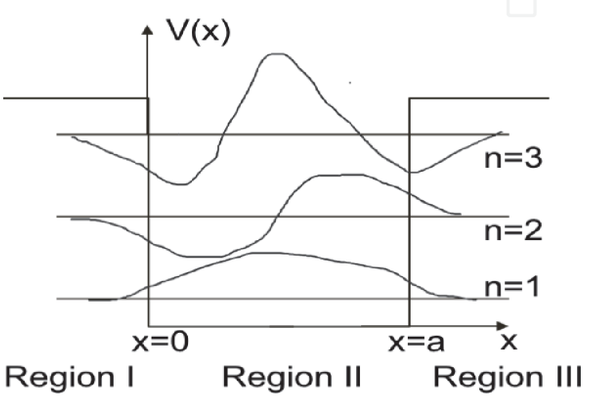

Figure 3.
Potential function of the finite potential well for different regions along the x-direction, with three discrete energy levels and corresponding wave function.

We will get here two possible solutions, depending on energies, where $\boldsymbol{E}$ is smaller than $\boldsymbol{V_0}$, that means the particle is bound the potential and $\boldsymbol{E}$ is greater than $\boldsymbol{V_0}$, that means the particle is moving in free space, which is represented by travelling wave (shown in **Figure 3**).

The potential $V(x)$ as a function of the position is shown in **Figure 4**. The particle is assumed to exist in region II so the particle is contained within a finite region of space. The time-independent Schrödinger wave equation can be written as

$$\frac{\partial^2\psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\,\psi(x) = 0, \tag{21}$$

where E is the total energy of the particle. If E is finite, the wave function must be zero, or $\psi(x) = 0,$ in both regions I and III. A particle cannot penetrate these infinite potential barriers, so the probability of finding the particle in regions I and III is zero.

In the quantum mechanics, the particle in a box (also known as the infinite potential well) describes a particle free to move in a small space surrounded by impenetrable barriers (shown in **Figure 4**). In classical systems, for example, a particle trapped inside a large box can move at any speed within the box and it is no more likely to be found at one position than another. However, when the well becomes very narrow (on the scale of a few nanometers), quantum effects become important. The particle may only occupy certain positive energy levels [1, 9, 10].

The energy of the incident particle ($\boldsymbol{E > V}$) in region I and transmitted particle ($\boldsymbol{E > V}$) in region III through the potential barrier ($\boldsymbol{E < V}$) in region II, where the tunnelled particle is the same but the probability amplitude is decreased. There is a finite probability that a particle impinging a potential barrier will penetrate the barrier and will appear in region III (shown in **Figure 5**). This quantum mechanical tunnelling phenomenon can be applied to semiconductor devices.

Quantum tunnelling is the quantum mechanical phenomenon where a subatomic particle's probability disappears from one side of a potential barrier and appears on the other side without any probability appearing inside the well. Quantum tunnelling is not predicted by the laws of classical mechanics where surmounting a potential barrier requires enough potential energy [9, 10].

2.2.3 Maxwell's equations: Poisson equation

To develop the Poisson equation we need to describe the famous Maxwell's equations in their differential form. In mathematics, Poisson's equation is a partial differential equation, which describe the potential field caused by a given charge distribution [2, 8]. Our goal is to find the density of the electron in the crystal of the

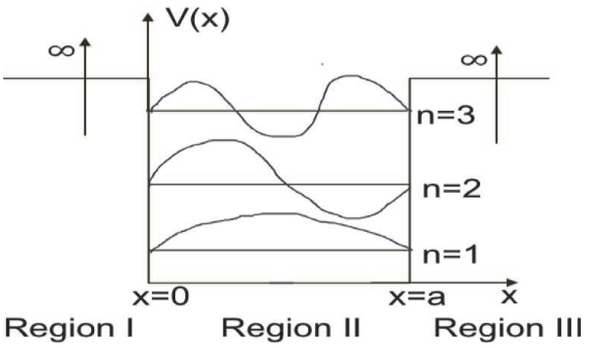

Figure 4.
Potential function of the infinite potential well for different regions along the x-direction, with three discrete energy levels and corresponding wave function in the box or potential well.

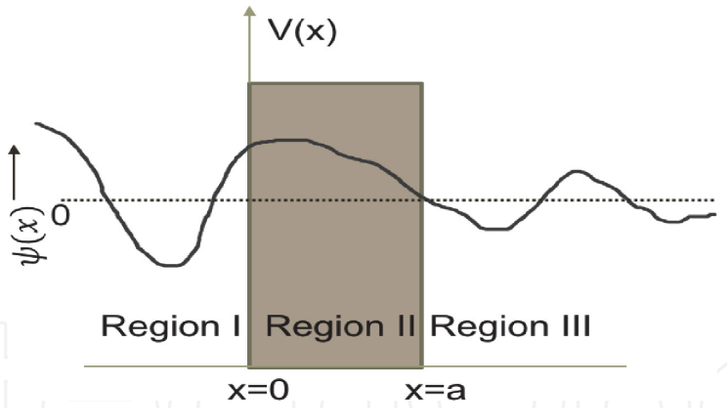

Figure 5.
Quantum tunnelling: The wavefunctions through the potential barrier, a significant tunnelling effect can be seen in three different regions.

semiconductor device classically. As we know the Gauss's law is $\nabla \cdot \boldsymbol{D} = \boldsymbol{\rho}$, where ∇ is the divergence operator, **D** is the electric displacement law ($\boldsymbol{D} = \boldsymbol{\varepsilon E}$), $\boldsymbol{\rho}$ is the free charge density, $\boldsymbol{\varepsilon}$ is the permittivity of the medium, and **E** is the electric field ($\boldsymbol{E} = -\nabla \mathbf{V}$). Maxwell's four equations describe the electric and magnetic fields arising from distributions of electric charge and currents, and how those fields change in time. Maxwell's equations described as follows [2]:

$$\nabla \cdot \boldsymbol{E} = \frac{\boldsymbol{\rho}}{\boldsymbol{\epsilon_0}}, \tag{22}$$

$$\nabla \cdot \boldsymbol{B} = \mathbf{0} \tag{23}$$

$$\nabla \times \boldsymbol{E} = -\frac{\boldsymbol{\delta B}}{\boldsymbol{\delta t}}, \tag{24}$$

$$\nabla \times \boldsymbol{B} = \boldsymbol{\mu_0 j} + \boldsymbol{\mu_0 \epsilon_0} \frac{\boldsymbol{\delta E}}{\boldsymbol{\delta t}} \tag{25}$$

We can substitute the value of electric displacement in the basic equation of Gauss's law, which can be rewritten as $\nabla \cdot \boldsymbol{E} = \frac{\rho}{\epsilon_0}$, so called Eq. (22). In electrostatic, we suppose that there is no magnetic field, then Eq. (24) can be rewritten as $\nabla \times \boldsymbol{E} = 0$, The electric field as the gradient of a scalar function **V**, is called electrostatic potential. Thus we can write $\boldsymbol{E} = -\nabla \mathbf{V}$, and the minus sign is chosen so that **V** is introduced as the potential energy per unit charge. Finally, we can develop the derivation of Poisson's equation using Eq. (22), and Eq. (24), which leads to

$$\nabla \cdot \boldsymbol{E} = \nabla \cdot (-\nabla \mathbf{V}) = \frac{\boldsymbol{\rho}}{\boldsymbol{\epsilon_0}}$$

$$\nabla^2 \mathbf{V} = -\frac{\boldsymbol{\rho}}{\boldsymbol{\epsilon_0}} \tag{26}$$

2.3 Contribution of Schrödinger and Poisson equation in nano-particles

In this section, a connection between the bandstructure and quantum confinement effects with device characteristics in nano-scale devices is established. Three different devices are presented: a 25 nm gate length Si (Silicon) MOSFET (Metal Oxide Semiconductor Field Effect Transistor), a 32 nm Silicon-on-insulator (SOI) MOSFET and a 15 nm implant free (IF) $In_{0.3}Ga_{0.7}As$ (Indium Gallium Arsenide) channel MOSFET. We use a 1D Poisson-Schrödinger solver across the middle of the

gate along the channel of the devices. The goal is to obtain the calculations of an energy of bound states and associated carrier wavefunctions which are carried out self consistently with electrostatic potential. The obtained wavefunctions are then used to calculate a carrier density which allows to obtain a sheet density across the structure at given bias. We have chosen the SOI MOSFET for comparison because it is considered for low power applications. The SOI technology is developing now into the commercial area and is included in the ITRS. The SOI based MOSFETs have a silicon channel made of a narrow layer of less than 10 nm grown on a relatively thick SiO_2 layer. Such strongly confined device channel creates an ultra-thin body (UTB) which provides enhanced carrier transport and, therefore, this transistor architecture is better to be referred as UTB SOI. The FD (fully depleted) SOI MOSFET has superior electrical characteristics and a threshold control from a bottom gate compared to the bulk CMOS device, which are described as follows [11, 12]:

1. decrease in a power dissipation and faster speed due to reduced junction area,

2. steep subthreshold slope,

3. negligible floating body effects,

4. increased channel mobility,

5. reduced short-channel effects and an excellent latchup immunity.

From a point of simplicity, we will first consider the UTB SOI transistor architecture because it is quite illustrative for quantum-mechanical calculations of a confined structure. We will consider a semiconductor material with a small energy gap sandwiched between energy barriers from a material with a larger energy gap. In this way, a quantum well is formed between the barriers which introduce a potential well with discrete energy levels, where particles are confined in one dimension and move free in other two directions as shown in **Figure 6** [13].

We will now focus exclusively on the calculation of quantum states related to electrons. The calculation of quantum states related to holes or any other particles or quasi-particles are equivalent. In the calculations, we will determine the conduction band profile, electron density, energy levels (eigenstates), wavefunctions (eigenfunctions) and electron sheet density in the semiconductor device structure under external potential. In this case, both Schrödinger and Poisson equations have to be solved self-consistently. The one-dimensional, time independent Schrödinger's wave equation for a particle in a potential distribution is a second order ordinary differential equation, which is given by [14].

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\,\psi(x) = 0$$

$$\left(-\frac{\hbar^2}{2}\frac{\delta}{\delta x}\frac{1}{m(x)} + V(x)\right)\psi(x) = E\psi(x) \tag{27}$$

$$\boldsymbol{H}\psi(x) = E\psi(x),$$

where

$$\boldsymbol{H} = -\frac{\hbar^2}{2}\frac{\delta}{\delta x}\frac{1}{m(x)} + V(x), \tag{28}$$

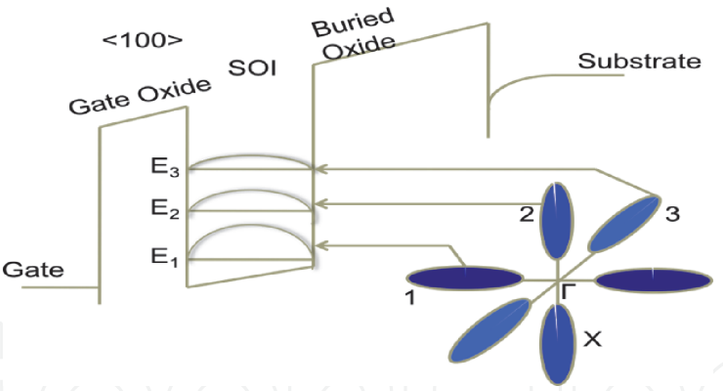

Figure 6.
Schematics of conduction band structure of silicon in <100> oriented narrow channels [assumed (100) plane for the Si-SiO$_2$ interface]. The energy levels are also shown in the silicon quantum well.

where ψ is the wave function, E is the energy eigenvalue, $V(x)$ is the potential energy assumed to be independent of time, $\hbar$ is Planck's constant divided by 2π, $m \equiv m(x)$ is the effective mass of an electron which is a position dependent, $\boldsymbol{H}$ represents the Hamiltonian operator associated with the sum of the kinetic and potential energies of the system.

The potential distribution $\phi(x)$ in the semiconductor can be determined from a solution of the 1 D Poisson Eq. (26), which is given by

$$\frac{d}{d(x)}\left(\varepsilon_S(x)\frac{d}{d(x)}\right)\phi(x) = \frac{-\rho(x)}{\varepsilon_0} \tag{29}$$

The charge density ρ is given by

$$\rho = N_D(x) - N_A(x) + p(x) - n(x). \tag{30}$$

Eq. (25) can be written as

$$\frac{d}{d(x)}\left(\varepsilon_S(x)\frac{d}{d(x)}\right)\phi(x) = \frac{-q[N_D(x) - N_A(x) + p(x) - n(x)]}{\varepsilon_0}, \tag{31}$$

where ϕ is the electrostatic potential, ε_S is the semiconductor dielectric constant, ε_0 is the permittivity of free space. In the static behaviour, N_D and N_A are called the ionised donor and acceptor concentrations and, in the case of dynamic behaviour, n and p are known as electron and hole density distributions. When dealing with n-type majority carriers semiconductor devices, we can ignore the holes contribution due to their slow movement compared to the electron dynamics. Then only the electrons and donors are considered. As a result the above Eq. (31) can be written as

$$\frac{d}{d(x)}\left(\varepsilon_S(x)\frac{d}{d(x)}\right)\phi(x) = \frac{-q[N_D(x) - n(x)]}{\varepsilon_0} \tag{32}$$

The potential energy V in the Hamiltonian is related to the electrostatic potential ϕ as follows [15]:

$$V(x) = q\phi(x) + \Delta E_C(x), \tag{33}$$

where ΔE_C is the pseudopotential energy due to the band offset at the heterointerface. The wavefunction $\psi(x)$ in Eq. (27) and the electron density $n(x)$ in Eq. (32) are related by

$$n(x) = \sum_{k=1}^{M} \psi_k^*(x)\psi_k(x)n_k, \tag{34}$$

where the summation runs over all the subbands, M is the number of bound states, and n_k is the electron occupation for each state. The electron occupation of a state k is given by the Fermi-Dirac distribution:

$$n_k = \frac{m}{\pi\hbar^2}\int_{E_k}^{\infty} \frac{1}{1 + exp\,(E - E_F/k_BT)}dE, \tag{35}$$

where E_k is the eigenenergy, is the E_F Fermi energy, and k_BT is the thermal energy. An iteration procedure is employed to obtain self-consistent solutions for Eqs. (27) and (32). Starting with a trial potential (x), the wave functions, and their corresponding eigenenergies, E_k are used to calculate the electron density distribution n_x using Eqs. (34) and (35).

2.4 Simulation results: wavefunctions behaviour of particles in the semiconductor devices: 1D Poisson-Schrödinger solver

The previous method of solving the Schrödinger-Poisson equations (see Section 2.3) has been applied to calculate the conduction band profile, electron concentration, energy levels (eigenstates) and wavefunctions (eigenfunctions) in a cross-section placed in middle of the gate of Metal-Oxide-Semiconductor (MOS) structure.

2.4.1 Si MOS structure

The MOS structure consists of a Metal-Oxide-Semiconductor capacitor, which is in the heart of the MOSFET. **Figure 7** shows the ideal MOS structure for p-type silicon in the flat band condition. The MOS structure is called the flat-band condition if the two following conditions are met [16]:

1. The work function of metal and silicon are equal, which implies that in all the materials, all energy levels in both the silicon and oxide are flat. When there is no applied voltage between the metal and silicon, their Fermi levels line up.

2. There exists no charge, the electric field is zero everywhere in the oxide and at the Si-SiO_2 interface.

The energy bands in the semiconductor near the oxide-semiconductor interface bend as a voltage is applied across the MOS capacitor [13]. We will assume three different bias voltages. One is below the threshold voltage, V_T, the second is just above the threshold voltage, and third one is at an on-current condition. The threshold voltage is defined as the applied gate voltage required to create the inversion layer charge and is one of the important parameters of MOSFETs. For enhancement mode, n-type MOS structure, the accumulation is for $V_G < 0$, the depletion for $V_T > V_G > 0$, the inversion for $V_G \sim V_T$ and the strong inversion for $V_G >> 0$ [14].

An accumulation layer of holes occurs in the oxide-semiconductor junction typically for negative voltages when the negative charge on the gate attracts holes from the substrate to the oxide-semiconductor interface. The induced space charge region is created for positive voltages. The positive charge on the gate pushes the

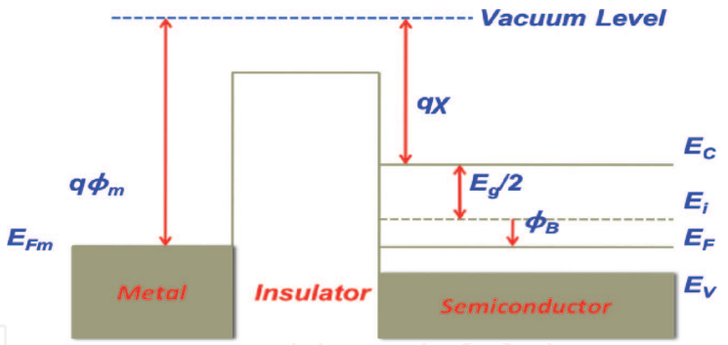

Figure 7.
Ideal metal-oxide-semiconductor (MOS) structure with p-type silicon substrate in a flat band condition.

mobile holes into the substrate. Therefore, the semiconductor is depleted of mobile carriers and a negative charge occurs at the interface because the fixed ionised acceptor atoms are in fixed positions [16].

We will investigate a Si MOS structure at a cross-section in the middle of a gate of the 25 nm gate length Si MOSFET. The structure shown in **Figure 8(a)** has a p-type silicon substrate, oxynitride (ON) gate oxide with a thickness of 1.6 nm, a dielectric constant of ε_{ON} = 7 and a metal gate.

The conduction band profile in a MOS structure of bulk silicon, biased at gate voltage of VG = 1.0 V is shown in **Figure 8(b)**. The ground state energy rises from the conduction band edge as shown in **Figure 8(b)**. This phenomenon is called surface quantization by applied higher gate voltage. The surface quantization is often expressed by a triangular well approximation and the potential near the interface has almost a triangular shape because the potential barrier of SiO_2 is relatively high in silicon MOS structure [13]. **Figure 8(b)** shows also the classically calculated electron density which will peak at the interface and predicts a much larger electron density and higher energy level when compared to the lower gate voltage [14, 16]. The quantum-mechanically calculated electron density is smaller and a displacement of the charge from the interface occurs when compared to the classical calculation.

2.4.2 Silicon-on-insulator (SOI) MOS structure

The investigated 32 nm gate length silicon-on-insulator (SOI) MOSFET is grown on a silicon (Si) substrate. The SOI structure has a layer of silicon dioxide (SiO_2)

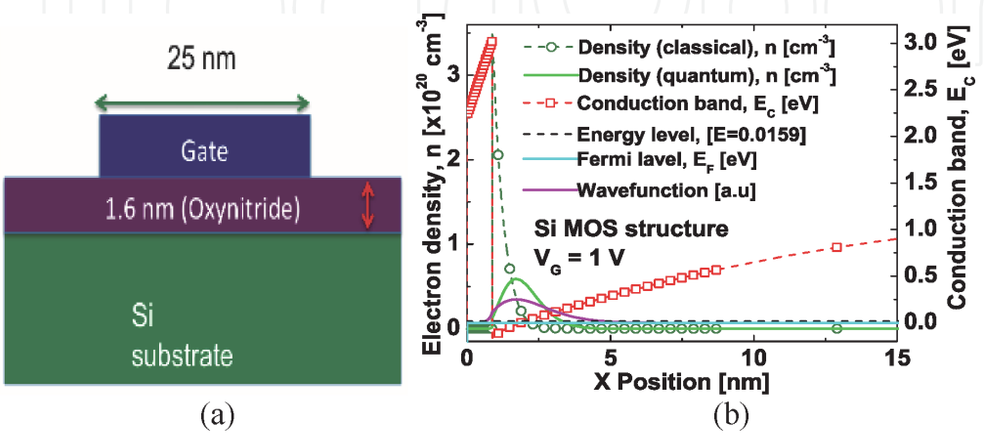

Figure 8.
(a) A schematic metal-oxide-semiconductor (MOS) structure for the 25 nm gate length MOSFET with p-type silicon substrate, (b) conduction band, electron density (classical and quantum-mechanical), energy level, Fermi energy level and wavefunction under an applied bias of V_G = 1.0 V across the channel for the MOS structure of the 25 nm gate length Si MOSFET, where T = 300 K.

with a thickness of 20 nm, which is called buried oxide (BOX) and is fabricated on a Si substrate, and a silicon body (which creates a device channel) with a thickness of 8 nm. A Hafnium Oxide (HfO_2) layer is deposited above the silicon body as a gate oxide with a thickness of 1.19 nm and a dielectric constant of $\varepsilon_{HfO_2} = 20$ and a top metal contact referred to as a gate as shown in **Figure 9(a)**. The metal gate will be able to bend the semiconductor bands with the application of a gate potential [13].

We have investigated the specified 32 nm gate length SOI MOSFET using, again, a self-consistent solution of 1D Schrödinger and Poisson equations. **Figure 9(b)** shows the electron conduction band and density profiles, which are obtained along a slice taken through the middle of a SOI MOS structure, from the surface to the substrate biased at V_G = 1.0 V at room temperature. In this structure, the potential energy creates a square quantum well, because the potential difference between the front interface and the back interface is small and the potential barriers are very high. Electrons are therefore confined in the ultra-thin Si body, which is sandwiched between the gate oxide and the BOX. The electron energy in the perpendicular direction is quantized and the energy of the ground state rises [14, 16] when compared to the conduction band. We can find two discrete energy levels in the quantum well. The classically calculated electron density will again peak at the interface of oxide and semiconductor. The quantum-mechanically calculated electron density will peak away from the oxide-semiconductor interface due to displacement of the charge from the interface [13].

2.4.3 MOS structure for an InGaAs channel transistor

We have selected an $In_{0.3}Ga_{0.7}As$ channel because of its optimal electron mobility and low effective mass. We investigate the effect of a confined channel in the implant free (IF) $In_{0.3}Ga_{0.7}As$ channel MOSFET with a gate length of 15 nm aimed for the future sub-22 nm Si technology. The IF MOSFET is derived from a HEMT structure which has

1. an oxide layer to prevent gate tunnelling,

2. a δ-doping layer placed below the channel. This placement allows the metal gate to maintain a good control of carrier transport in the channel, and

3. an ultra-thin body channel to the heterostructure used in a transistor design.

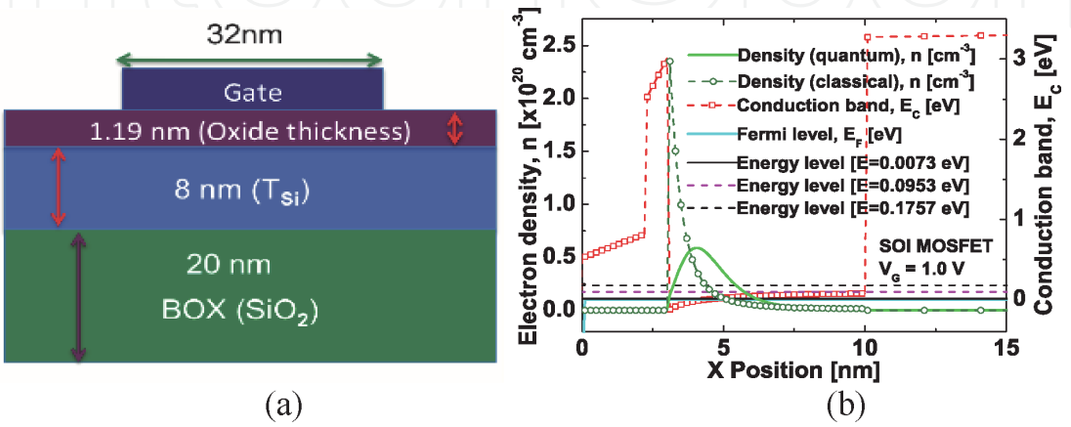

Figure 9.
(a) A schematic for silicon on insulator (SOI) structure with the 32 nm gate length. (b) Electron density (classical and quantum-mechanical) distribution, conduction band and energy levels under an applied bias of V_G = 1.0 V.

We have used, again, the 1D self-consistent solution of the Poisson-Schrödinger equation to obtain the conduction band profile, energy levels, wavefunctions and electron density in a confined body of this heterostructure MOSFET.

The III-V MOSFET consists of $In_{0.3}Ga_{0.7}As$ channel with thickness of 5 nm, high-ε dielectric layer of Gadolinium Gallium Oxide (GdGaO) as a gate dielectric with a thickness of 1.5 nm and whose dielectric constant is $\varepsilon_{GGO} = 20$. The $In_{0.3}Ga_{0.7}As$ channel is located between an $Al_{0.3}Ga_{0.7}As$ layer with a thickness of 1.5 nm and an $Al_{0.3}Ga_{0.7}As$ layer of a thickness of 3 nm. The δ-doping layer is placed below the channel with a concentration of 7×10^{12} cm^{-2}. The $Al_{0.3}Ga_{0.7}As$ layer at the bottom of the structure is grown as a thick buffer layer of 50 nm as shown in **Figure 10(a)**. The whole device is grown on a GaAs substrate [13, 14].

Figure 10(b) shows the conduction band, five discrete energy levels and electron concentration (classical and quantum mechanical) across the channel for the 15 nm gate length $In_{0.3}Ga_{0.7}As$ MOSFET biased at V_G = 1.0 V.

At V_G = 1.0 V, we obtain three discrete energy levels in the quantum well with corresponding wavefunction for these energy levels shown in **Figures 11(a)** in SOI MOSFET. We summarise that in future technology the bulk MOSFET will be replaced by an ultra-thin-body (UTB) silicon-on-insulator (SOI) on the basis of better electrostatistic integrity, low channel doping to get high mobility, high dielectric material to prevent gate leakage and metal gate [17–19].

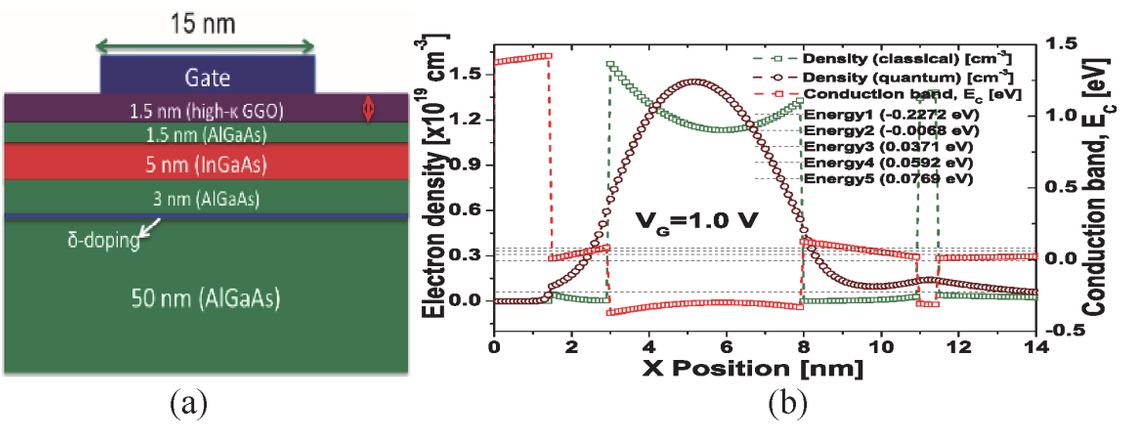

Figure 10.
(a) Cross-section of the 15 nm gate length $In_{0.3}Ga_{0.7}As$ channel MOS structure with a high- ε dielectric layer which is located below the metal gate, and (b) conduction band, electron density and discrete energy levels under an applied bias of VG = 1.0 V, across the channel for a MOS structure of the 15 nm gate length $In_{0.3}Ga_{0.7}As$ MOSFET.

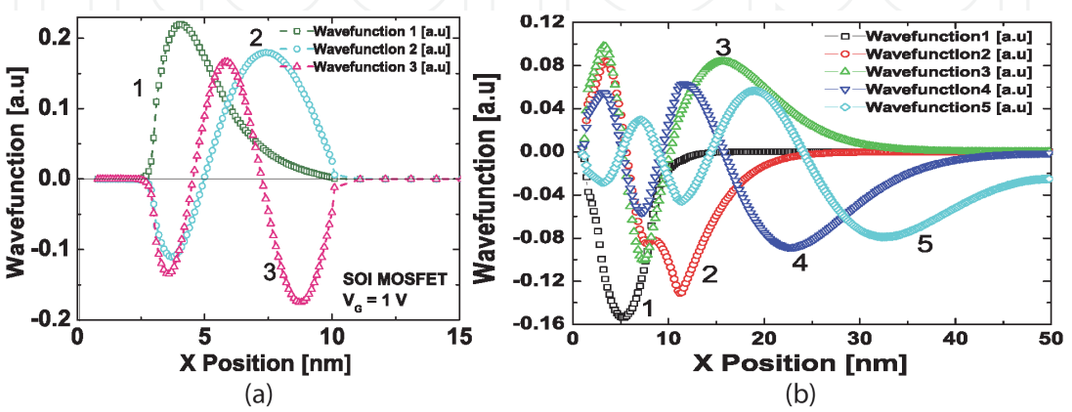

Figure 11.
(a) Electron wave functions under an applied bias of V_G = 1.0 V across the channel for a MOS structure of the 32 nm gate length SOI MOSFET. (b) The wavefunctions under an applied bias of V_G = 1.0 V, across the channel for a MOS structure of the 15 nm gate length $In_{0.3}Ga_{0.7}As$ MOSFET.

Figure 10(b) shows the conduction band and electron concentration for the 15 nm gate length In0.3Ga0.7As MOSFET biased at V_G = 1.0 V. Five discrete energy levels can be observed at this high bias with the corresponding wave functions in the quantum well shown in **Figure 11(b)** [20].

3. Conclusions

We have been carried out using a self-consistent solution of 1D Poisson-Schrödinger equation to determine conduction band profiles, electron density, energy levels (eigenstates) and wavefunctions (eigenfunctions) in the Si, SOI and InGaAs MOS structures under external potential. We have afterwards simulated the electron sheet density as a function of the applied gate bias and made a comparison among the three device structures, the 25 nm gate length bulk Si, 32 nm UTB SOI, and 15 nm gate length InGaAs MOSFETs.

We have investigated the effect of electron confinement in nanoscaled transistor channels using 1D simulation through cross-sections of the devices. These investigations have been carried out using a self-consistent solution of 1D Poisson-Schrödinger equation to determine conduction band profiles, electron density, energy levels (eigenstates) and wavefunctions (eigenfunctions) in the Si, SOI and $In_{0.3}Ga_{0.7}As$ MOS structures under external potential. We have afterwards simulated the electron sheet density as a function of the applied gate bias and made a comparison among the three device structures, the 25 nm gate length bulk Si MOSFET, the 32 nm UTB SOI Si MOSFET, and the 15 nm gate length IF $In_{0.3}Ga_{0.7}As$ MOSFET [20].

I can envisage that my future work could be related to the investigations of the new physical phenomena present in the UTB MOSFET architectures. As explained previously, the planar and non-planar UTB device architectures are preferred solutions for future technology nodes because the conventional bulk MOSFETs suffer from a poor electrostatic behaviour when scaled to sub-22 nm gate lengths exhibiting unsatisfactory short channel effects. These short channel effects can be summarised as follows:

1. reduced carrier mobility at high channel doping, hampering the device performance,
2. band-to-band drain leakage current [19],
3. and high gate tunnelling current and poor electrostatic control despite employment of metal/high-ϙ gate stacks, etc. [1, 3].

The UTB MOSFET architectures do not show such severe short channel effects because they have superior electrostatic integrity thanks to the electron confinement of their channel region.

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