A two-dimensional Self-Consistent Solution to Schrödinger -Poisson Equation Using Finite Element Method

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A thesis submitted in conformity with the requirements
for the degree of Masters of Science
Department of Physics
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Abstract

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Masters of Science

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2014

In this paper, we show a method of solving the Schrödinger equation and Poisson equation self-consistently using the Finite Element Method. We ran a simulation for a wafer of GaAs/AlGaA heterojunction with GaAs doping of $2 \times 10^{18}/cm^3$ quantum wafer. We achieve convergence for Fermi level range between $E_f = (1000.0, 2000.0)$ MeV.

Contents

Chapter 1

Introduction

Modern day electronics have reached scales of extremely small magnitudes, typically, a few hundred nanometers. When we enter this regime, it is important to take into account quantum mechanical phenomenons as they have a larger impact on smaller scale electronics. These quantum effects will impose substantial amount of change on device performance. One way to understand the behavior of materials at such scales is to incorporate quantum mechanics along with semi-classical electrostatics. A complete picture requires a self-consistent solution of both Schrödinger and Poisson equation. These types of systems are extremely complex to be solved analytically. Therefore, we resort to numerical approximations. Ideally, one would device a numerical simulation flexible enough to capture wide range of applicability, while at the same time accurate to experimental data. A lot of literature have utilized a conventional approach to the solution of Schrödinger and Poisson equation called finite-difference method (FDM). In this paper, we use another method in finding a self-consistent solution called finite-element method (FEM). The reason why we decided to use FEM is that it is easy to have complex geome-

tries, such as combinations of cylinders, spheres, and cubes. In chapter 1 we will discuss the formulation of Schrödinger and Poisson equations in the FEM regime. In chapter 2, we will discuss the theory behind our numerical simulation. Lastly, in chapter 3, we will discuss the results for a simple two-dimensional heterojunction.

Chapter 2

Formulation

2.1 Finite Element Method

More often than not, we need to numerically solve partial differential equations. In this paper, we will use the finite Element method to study the Schrödinger and Poisson equations. This method is powerful because allows us to solve PDEs for obscure geometries. For generic formulation for a PDE of the form

$$[D]u(x) = f(x) \in \Omega \tag{2.1}$$

Where D is an arbitrary operator, and Ω defines our geometry. We have to rewrite this equation in weak variational form so that we can solve it using FEM. Let us consider the boundary conditions

$$\begin{cases} u(x) = u_0(x) & \text{on } \Gamma_D \quad (2.2) \\ \dfrac{\partial u}{\partial n} = g_0(x) & \text{on } \Gamma_N \quad (2.3) \end{cases}$$

Where Γ_D and Γ_N signifies Dirichlet and Neumann boundary condition. The general idea of finite element method is to rewrite a PDE into a variational problem. The way to do that is to introduce an arbitrary function v and multiply the PDE with v. Then we integrate over the domain Ω and separate every second-order derivative using integration by parts. The original PDE then can be written in the weak form as

$$\int_\Omega [D'](u \cdot v)\, d\Omega + \int_{\Gamma_N} gv\, \partial\Omega = \int_\Omega fv\, d\Omega \quad \forall v \in \hat{V} \tag{2.4}$$

Where D' is the reduced operator after performing integration by part to the second-order derivatives, and $\hat{V}$ is the function space where our arbitrary function v lives. The function u lies in V, which could be different than $\hat{V}$. Now, to perform the calculation numerically, we need to reformulate the continuous variational problem to a discrete problem. We just need to define a discrete space $\hat{V}_d \subset \hat{V}$ and $V_d \subset V$ so that we can write our boundary problem as

$$\int_\Omega [D'](u_d \cdot v)\, d\Omega + \int_{\Gamma_N} gv\, \partial\Omega = \int_\Omega fv\, d\Omega \quad \forall v \in \hat{V}_d \subset \hat{V} \tag{2.5}$$

It convenient to use unified notation for linear weak forms

$$a(u, v) = L(v) \tag{2.6}$$

with

$$a(u,v) = \int_{\Omega} [D'](u_d \cdot v)\ d\Omega \tag{2.7}$$

$$L(v) = \int_{\Omega} fv\ d\Omega - \int_{\Gamma_N} gv\ \partial\Omega \tag{2.8}$$

2.2 Poisson in weak variational form

Here, we want to solve Poisson equation that arises in electrostatics. The general Poisson equation for electrostatics is giving by

$$\frac{d}{dx}\big(\epsilon_s(x)\frac{d}{dx}\big)\phi(x) = \frac{-q[N_D(x) - n(x)]}{\epsilon_0} \tag{2.9}$$

Where ϵ_s is the dielectric constant of the material, N_D is the ionized donor concentration, ϕ is our electrostatic potential, and n is the electron density. Here, we will only consider a piecewise dielectric constant, therefore, we only need to divide the domain into subdomain with different dielectric constants. The Poisson equation can be rewritten as

$$\epsilon_s \nabla^2 \phi(x) = \frac{-q[N_D(x) - n(x)]}{\epsilon_0} \tag{2.10}$$

Notice that our operator $[D]$ is replace with ∇^2, and our source term $f(x)$ is replaced with the scaled difference of the ionized donor concentration and the electron density. It is pretty straight forward to reformulate the Poisson equation to the weak variational

form, all we need to do is to follow the procedure explained in the previous section. We get our final weak variational as

$$\int_{\Omega} \epsilon_s \epsilon_0 \nabla\phi \cdot \nabla v \;\; d\Omega = \int_{\Omega} q[N_D(x) - n(x)]v(x) \;\; d\Omega \tag{2.11}$$

Now can use finite element method to solve for $\phi(x)$.

2.3 Schrödinger in weak variational form

To rewrite Schrdinger's equation in the variational form, we start with Schrödinger 's equation in differential form

$$-\frac{\hbar^2}{2}\frac{d}{dx}\big(\frac{1}{m^*(x)}\frac{d}{dx}\big)\psi(x) + V(x)\psi(x) = E\psi(x) \tag{2.12}$$

Where $m*(x)$ is the effective mass. Since we are going to have a constant mass within the region we are exploring, we can take that out of the derivative. With a little algebra we can rewrite the equation as

$$\frac{\hbar^2}{2m^*}\nabla^2\psi(x) + [E - V(x)]\psi(x) = 0 \tag{2.13}$$

Multiply both sides by a test function v. This function is arbitrary with the condition that it vanishes on the boundaries of our system.

$$\frac{\hbar^2}{2m^*}\nabla^2\psi(x)v(x) + [E - V(x)]\psi(x)v(x) = 0 \tag{2.14}$$

Integrate both terms over the domain and using integration by parts yields

$$\int_{\Omega} \frac{\hbar^2}{2m^*} \frac{\partial \psi}{\partial x} \frac{\partial v}{\partial x} d\Omega + \int_{\Omega} V(x)\psi(x)v(x)d\Omega = \int_{\Omega} E\psi(x)v(x)d\Omega \tag{2.15}$$

Notice that we drop the surface term because we require that our test function v vanishes where ψ is known.

Chapter 3

Numerical Simulation

3.1 Relevant Equations

In this section, we will cover the basic equations that we need to satisfy in our numerical simulation. The basic equations combines quantum mechanics with semi-classical physics. We need to solve Schrödinger and Poisson using

$$-\frac{\hbar^2}{2}\frac{d}{dx}\big(\frac{1}{m^*(x)}\frac{d}{dx}\big)\psi(x) + V(x)\psi(x) = E\psi(x) \tag{3.1}$$

$$\frac{d}{dx}\big(\epsilon_s(x)\frac{d}{dx}\big)\phi(x) = \frac{-q[N_D(x) - n(x)]}{\epsilon_0} \tag{3.2}$$

$$V(x) = -q\phi(x) + \Delta E_c(x) \tag{3.3}$$

$$n(x) = \sum_{k=1}^{m} \psi_k^*(x)\psi_k(x)n_k \tag{3.4}$$

$$n_k = \frac{m^*}{\pi\hbar^2} \int_{E_k}^{\infty} \frac{1}{1 + e^{(E-E_F)/KT}} dE \tag{3.5}$$

Where $\Delta E_c(x)$ is the pseudopotential energy due to the band offset at the heterointerface, n_k is the electron occupation number which can calculated by Fermi-Dirac distribution function with E_F being the Fermi level, ψ_k is the wavefunction in the k^{th} state, and E_k is the eigen energy in state k. These five equations have to be solved and produce a self-consistent solution in order for us to have a good approximation of the behavior of our system.

3.2 Approximations

In this section, we will cover the basic approximations that we employ in our numerical simulation. We first start with approximating the occupation number n_k. since the complete Fermi-Dirac integral is an exponential function

$$\mathcal{F}_j(x) = \frac{1}{\Gamma(j+1)} \int_0^{\infty} \frac{t^j}{exp(t-x)+1} dt \tag{3.6}$$

Where $x = E - E_F$. In this paper, we will only consider the two dimensional case, in which $j = -1/2$. Since we are taking the integral of $\mathcal{F}_j(x)$ from E_k to ∞, we need the

argument E to be $E \leq 0$. Therefore the distribution function falls of exponentially as

$$\mathcal{F}_{-1/2}(E) \sim exp(-E), \quad E \gg 0 \tag{3.7}$$

Therefore, we only need to calculates relatively few quantum states the are lower than Fermi level. The second approximation involves treating $m^*(x)$ as a step function. Where it is (for two subdomains)

$$m^*(x) = \begin{cases} a_1 m_e & \in \ \Omega_1 \quad (3.8) \\ a_2 m_e & \text{otherwise} \quad (3.9) \end{cases}$$

Where m_e is the mass of electron (≈ 0.511 MeV), and a_1 and a_2 are coefficients that depends on the materials.

3.3 Algorithm

In this section, we will describe the process of producing a self-consistent solution. We first start with an arbitrary potential $V(x)$ and plug it in equation 3.1 to solve for the wavefunctions. After we get the wavefunctions, we compute the electron density function and the occupation number using equations 3.4 and 3.5. Then we can solve Poisson equation because we have $n(x)$. Finally, we use the solution of 3.2, $\phi(x)$, to find the new corrected potential, $V(x)$, using 3.3. After finding the new potential and the new electron density, we compute the difference between them and their old values to test for convergence. We repeat this process until we achieve convergence, we choose our criteria

for convergence to be on the order of 10^{-5} error.

3.4 Geometry

We will consider a GaAs/AlGaAs structure for our simulation. We chose GaAs/AlGaAs because it preforms better than most of semiconductors at high frequency. Also, GaAs/AlGaAs is pretty much insensitive to temperature. Lastly, GaAs/AlGaAs has a high electron mobility. Ideally, our simulation would work for all sorts of materials but we will only show GaAs/AlGaAs in this paper. Our wafer is depicted in Figure **??**. Our wafer's boundary conditions at $\phi(0, y) = 0$ and $\phi(1, y) = 0$ at both ends on the x-axis, and is periodic, $\phi(x, 0) = \phi(x, 1)$ on the y-axis. Notice that we use normalized coordinate system in which our domain is $\Omega \in [0, 1] \times [0, 1]$. The last two boundary conditions take care of the fact that we dope the GaAs layer with 2×10^{18} electrons/cm^3.

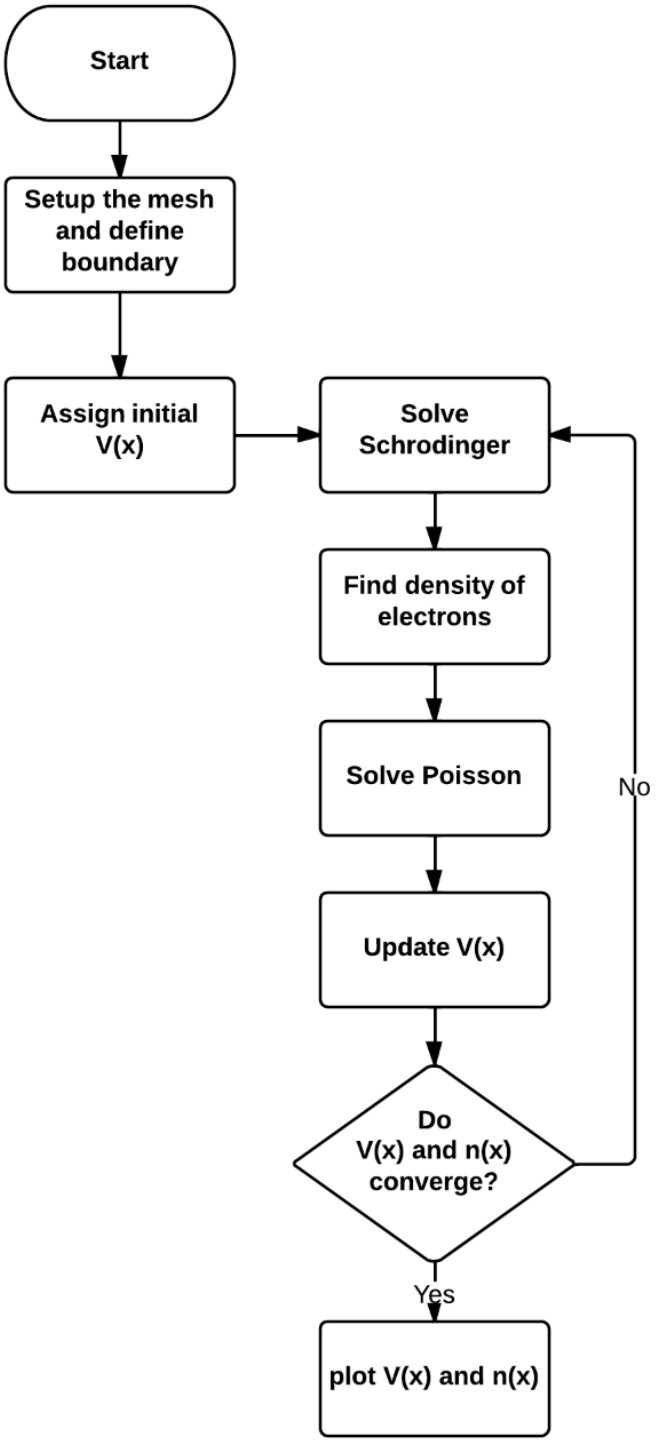


Figure 3.1: A flowchart of the self-consistent simulation

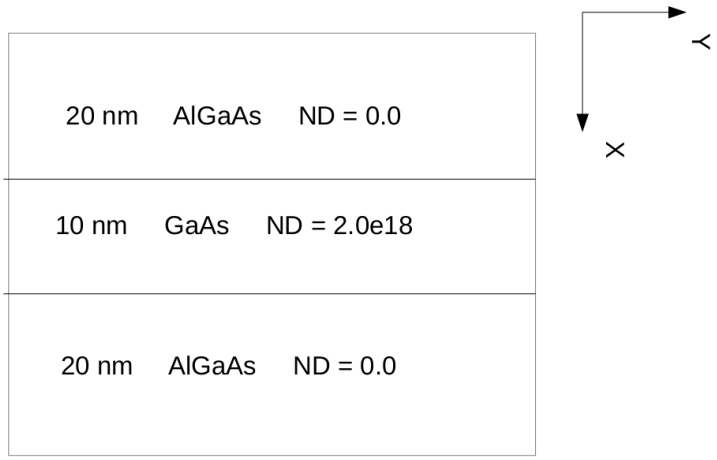


Figure 3.2: Structure of the wafer that we used for our simulation. Here, we use alloy fraction of GaAs/$Al_{0.3}Ga_{0.7}As$

Chapter 4

Results

In this section, we will device our efforts to find the right Fermi level that will have a convergent solution while preserving the properties of the system. We start with Fermi Level of the order $\sim O(10^5)$. From figure **??**, we can see that Fermi levels of the order $\sim O(10^5)$ are not good candidates for our wafer because they do not reach our 10^{-5} error requirement. We next try Fermi levels of the order $\sim O(10^4)$

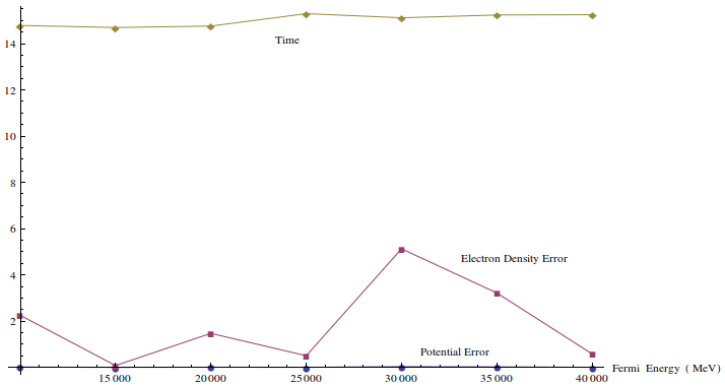


Figure 4.1: shown above is the time it took the simulation to run (in minutes), the error in electron density, and the error in potential plotted against different values of Fermi level on the order of 10^5

For Fermi levels of the order $\sim O(10^4)$, we get some convergent solutions. Namely,

for the Fermi levels $Ef = 1000.0$, 1500.0, and 2000.0 all in 4 iterations.

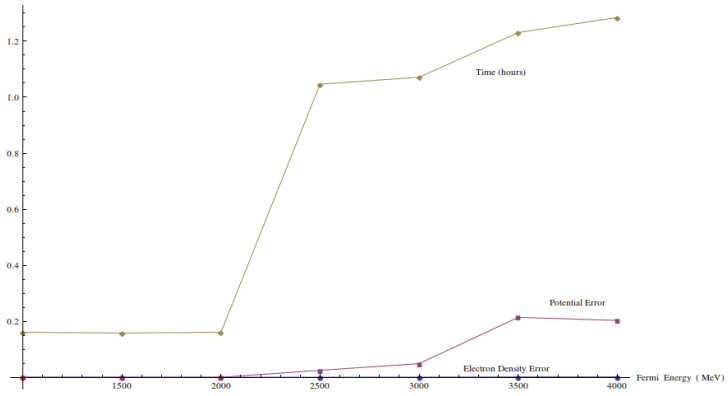
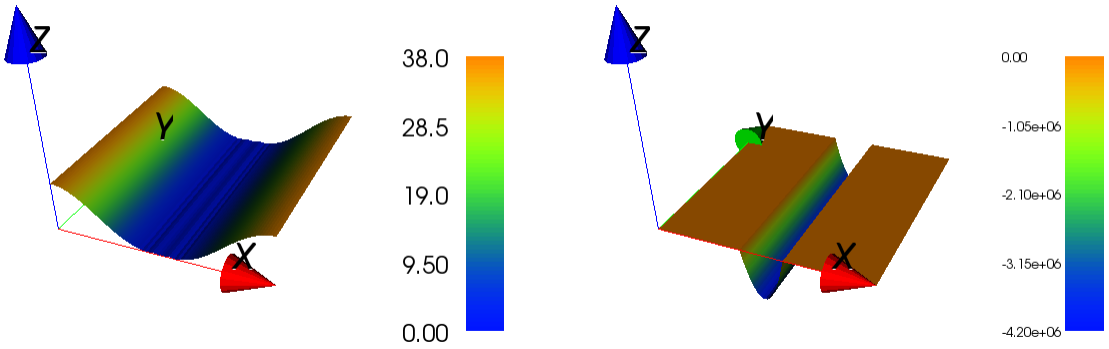


Figure 4.2: shown above is the time it took the simulation to run (in hours), the error in electron density, and the error in potential plotted against different values of Fermi level on the order of 10^4. The values E_f≧2000.0 did not converge

Next, we Plot the electron density and potential for a Fermi energy in the convergent range.

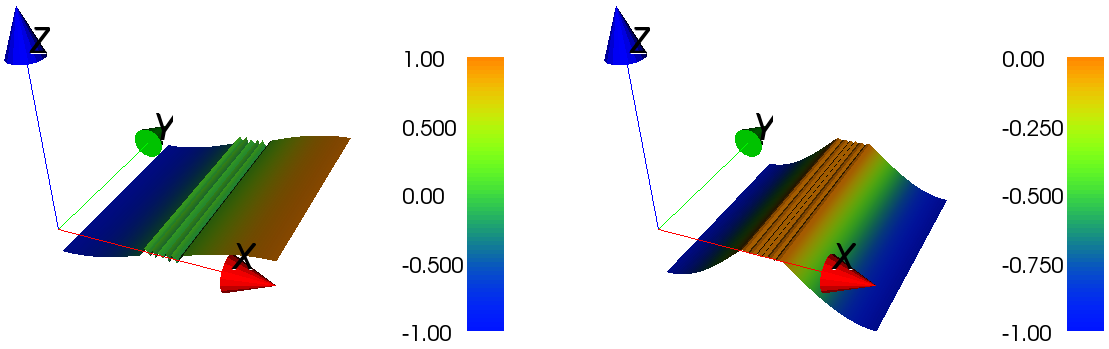


(a) Electron Density ($10^{11}/cm^3$ (b) Potential (MeV)

Figure 4.3: Convergent solution for electron density n(x,y) and potential V(x,y)

Conclusion

As electronic chips becomes smaller, more work required to determine their electronic properties. When devices reaches the nanometer range, quantum effects become



(a) wavefunction k = 1 (b) wavefunction k=2

Figure 4.4: First two eigenfuctions of $\psi(x, y)$

non-negligible. A self-consistent solution to the Schrödinger and Poisson equation is necessary to get accurate predictions of the system properties. Due to the complexity of the system, only numerical simulation are possible. We use FEM to simulate a self-consistent solution for a GaAs/AlGaAs quantum wafer. We achieve convergence for values of Fermi level ranging from $1000.0MeV$ to $2000.0MeV$

Acknowledgements

I would like to thank Prof. Woowon Kang for his immense patience and allocating some of his precious time to sponsor and review this thesis. I would also like to thank the Saudi Arabian Cultural Mission (SACM) for sponsoring this research.

Bibliography

[1] Tan, IH., G. L. Snider, L. D. Chang, and E. L. Hu. "A self-consistent solution of Schrödinger-Poisson equations using a nonuniform mesh." Journal of applied physics 68, no. 8 (1990): 4071-4076.

[2] Trellakis, Alex, Till Andlauer, and Peter Vogl. "Efficient solution of the schrödinger-poisson equations in semiconductor device simulations." In Large-Scale Scientific Computing, pp. 602-609. Springer Berlin Heidelberg, 2006.

[3] Serra, AM Cruz, and H. Abreu Santos. "A onedimensional, self-consistent numerical solution of Schrödinger and Poisson equations." Journal of applied physics 70, no. 5 (1991): 2734-2738.

[4] Huang, Chung-Kuang, and Neil Goldsman. "2-D self-consistent solution of Schrödinger equation, Boltzmann transport equation, Poisson and current-continuity equation for MOSFET." SISPAD 2001 (2001): 148-51.

[5] Ruic, Dino, and Christoph Jungemann. "A self-consistent solution of the Poisson, Schrodinger and Boltzmann equations by a full Newton-Raphson

approach for nanoscale semiconductor devices."

[6] Kittel, Charles, and Paul McEuen. Introduction to solid state physics. Vol. 8. New York: Wiley, 1986.

[7] Simon, Steven H.. The Oxford solid state basics. Oxford: Oxford University Press, 2013.