ECE 539 Course Project
Study of two-dimensional Shrödinger-Poisson Solver.

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Abstract

We solve the 2-Dimensional Shrödinger-Poisson system of equations using a self consistent scheme (like Gummel Iteration). We study a double gate Silicon Mosfet oriented in the 100 direction using the above setup. We assume a simple 6-valley bandstructure for Silicon.

1 Introduction

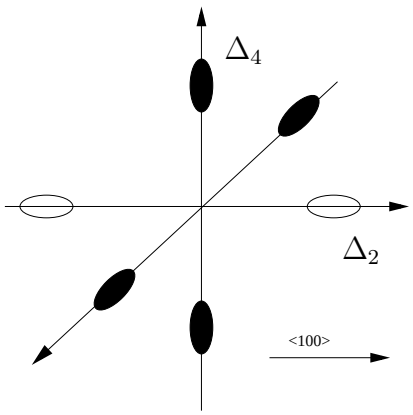

Figure 1: Conduction band model for Silicon

The bandstructure model used in the Shrödinger equation is the multivalley six band conduction valley model as shown in Fig. 1, where each valley corresponds to a constant energy surface, and can be captured by a parabolic effective mass equation. This model allows us to capture the mass anisotropy in Silicon. The Valley pair pointing in the (100) direction have a mass m_l = 0.91m_0 and the transverse mass is m_t = 0.19m_0. The two valleys in this direction are degenerate. The other valley pairs also have the same longitudinal and transverse mass along their respective axes.

The Shrödinger equation is given by:

$$i\hbar\dot{\psi} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi \tag{1.1}$$

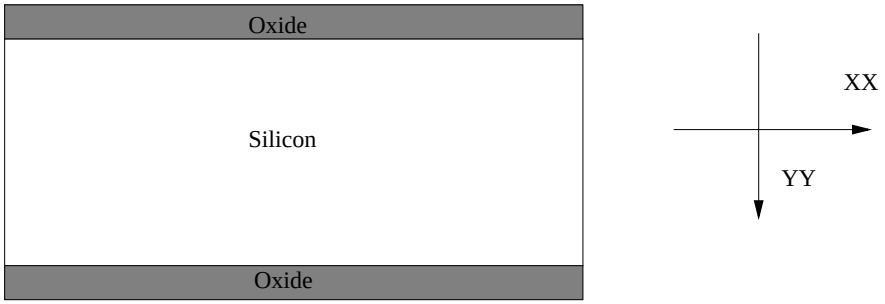

Figure 2: Two Dimensional Double Gate MOSFET

which has a time-independent version given by:

$$\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \tag{1.2}$$

or

$$\hat{H}\psi = E\psi \tag{1.3}$$

where $\hat{H}$ is the Hamiltonian operator given by:

$$\hat{H} = \frac{\hbar^2}{2m}\nabla^2 + V \tag{1.4}$$

We consider a 2-D version of the above equation for a Double-gate structure shown in Fig. 2

$$\Big[-\frac{\hbar^2}{2m_x^v}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m_y^v}\frac{\partial^2}{\partial y^2} + V(x,y)\Big]\psi_j^v(x,y) = E_j^v\psi_j^v(x,z) \tag{1.5}$$

At each iteration step of the scheme, we solve the above equation three times, for each equivalent valley pair v.

and the linear Poisson equation is given by:

$$\nabla(\epsilon_r\nabla V) = -\frac{\rho}{\epsilon_0} \tag{1.6}$$

The ψ calculated from 1.5 in the previous iteration is used in the following formula to calculate the new charge density ρ:

$$\frac{\rho}{q} = n_q = \sum_v \frac{1}{\pi}\left(\frac{2m_z^v k_B T}{\hbar^2}\right)^{\frac{1}{2}} \sum_n \psi_n^v \psi_n^{v*} \mathcal{F}_{-\frac{1}{2}}\left(\frac{E_F - E_n}{k_B T}\right) \tag{1.7}$$

The value of ρ is then used in 1.6 to get the potential V and this procedure is repeated until convergence is achieved.

Our test device is a Double gate Si MOSFET as shown in Fig. 2. Hence our 2-D space would be a rectangle. The top and bottom of that rectangle are the gate contacts where we apply a fixed potential. The rectangle itself is composed of three layers from top gate to bottom gate, consisting of Silicon dioxide, Silicon, and then Silicon dioxide again. The width of these layers is varied for different configurations of the device that are analyzed in this project.

We use finite difference approximation to discretize the physical space as mentioned in the last paragraph. Assuming we use same value for Δx and Δy (let's call it a), which can be selected based on the level of resolution we want to work with. Appropriate proportions of grid points along the vertical direction (top to bottom) are assigned to their respective layers. We used the five-point stencil formula for the 2-D double derivative as follows:

$$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \equiv \frac{-u_{i-1,j} - u_{i,j-1} + 4u_{i,j} - u_{i,j+1} - u_{i+1,j}}{a^2} \tag{1.8}$$

Once the discretization is done, our physical problem is transformed into a numerical problem as follows: The Poisson equation is converted into a linear system of equations:

$$\mathbf{Ax} = \mathbf{b} \tag{1.9}$$

where $\mathbf{A}$ is the finite-difference discretization of the double-derivative, $\mathbf{x}$ is the 2-D potential grid, and $\mathbf{b}$ is the charge density. The Shrödinger equation turns into an eigenvalue problem:

$$\mathbf{Ax} + \mathbf{Bx} = \lambda\mathbf{x} \tag{1.10}$$

where $\mathbf{A}$ is the finite-difference discretization of the double-derivative, $\mathbf{x}$ is the 2-D wave-function grid, $\mathbf{B}$ is a diagonal matrix that represents the potential at each grid point, and λ is the energy level corresponding to each wave-function.

Using 1.8 and the fact that our $\mathbf{x}$ is 2-D in space, the form of $\mathbf{A}$ is as follows:

$$\mathbf{A} = \begin{bmatrix}
-4 & 1 & 0 & \cdots & 0 & 1 & 0 & & \cdots & 0 \\
1 & -4 & 1 & & & & 1 & & & \\
0 & 1 & -4 & 1 & & & & \ddots & & \\
\vdots & & 1 & -4 & \ddots & & & & & \\
0 & & & \ddots & \ddots & & & & & \vdots \\
1 & & & & & & & & & \\
0 & 1 & & & & & & & & \\
 & & \ddots & & & & & & & \\
\vdots & & & & & & & & & \\
 & & & & & & & & & \\
0 & & & & \cdots & & & & &
\end{bmatrix} \tag{1.11}$$

As we can see, this is a five-band matrix with three adjacent diagonals in center (like a tridiagonal) and upper and lower diagonal at a spacing which is the number of grid points in one dimenstion. So for a 10-by-10 grid, each of the upper and lower diagonals would be 10 diagonals apart from the main diagonal. This means that for an m-by-n grid, the size of the vectors in 1.9 and 1.10 would be m-by-n and the size of the matrices would be m-by-n squared (e.g., for a 10x10 grid, $\mathbf{x}$ would have 100 elements and $\mathbf{A}$ would be a 100-by-100 matrix). This apparent $\mathcal{O}(n^4)$ complexity of the problem can be mitigated by the fact that only sparse matrices are involved and also only a

small number of eigenvalues from 1.10 are required to proceed with calculations. Hence efficient algorithms can be utilized which exploit these facts and speed up the process.

The application of Dirichlet boundary conditions as long as they are zero, don't require any change in the matrix or the numerical equation. But for Neumann bounary conditions, absolute value of the appropriate elements on the diagonal needs to be decremented by 1, e.g., -3 instead of -4, or 3 instead of 4. Those appropriate elements depend on where we are applying the Neumann BCs. For example, if they are applied to right and left edges of the 2-D physical space, the elements would be 1st, n'th, $(n+1)$'th, $2n$'th, $(2n+1)$'th, and so on.

In order to find the carrier concentration from ψ_n and E_n using 1.7 we need to calculate the Fermi integral of order half, for which an integration algorithm is used.

2 Results

We have used MATLAB as the programming environment. The electron density for the structure in Fig 2 is plotted below.

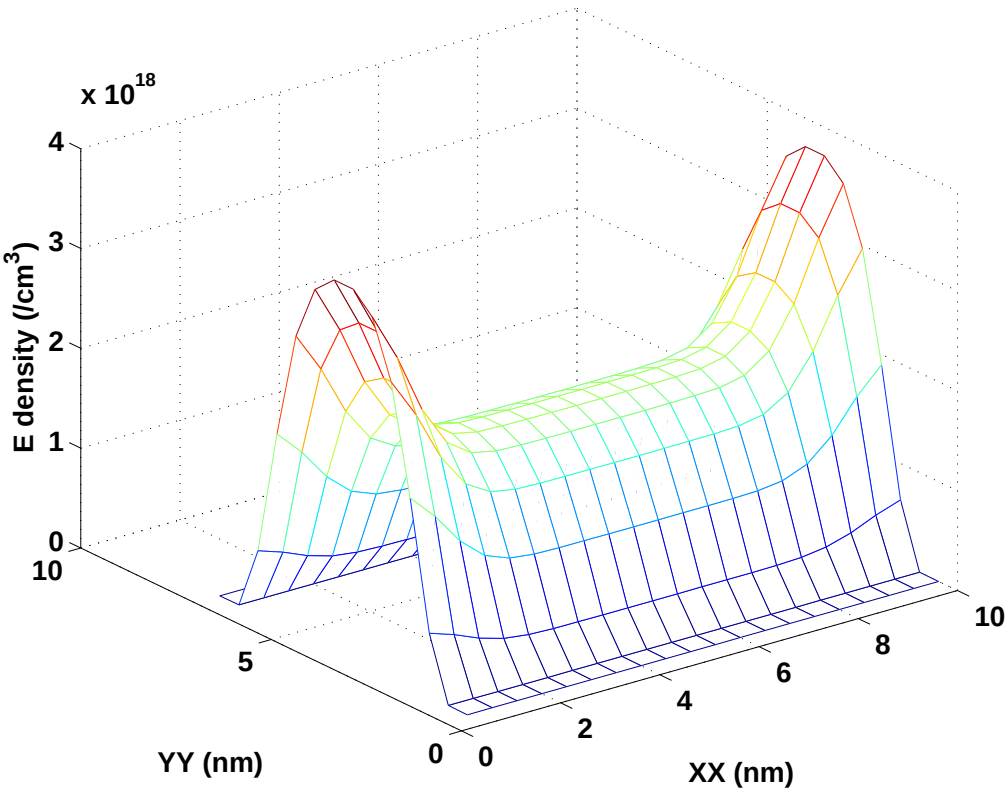

Figure 3: Electron density

We have also studied the effect of variation of the thickness of the body on the electron density, from Fig 4 one can observe the effect of confinement of carriers along thickness of the body. A

representative plot of the electron density with varying gate voltage is also plotted.

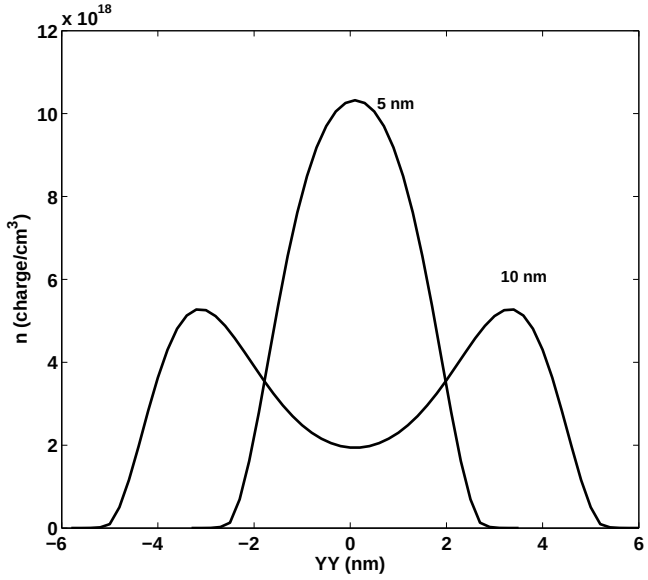

Figure 4: Effect of body thickness on the electron density

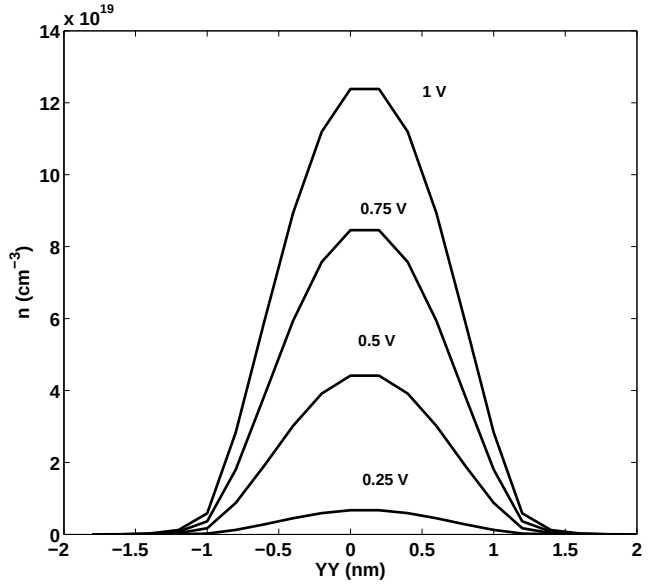

Figure 5: Effect of Gate voltage on electron density

3 Conclusion and Possibilities of Improvement

In conclusion we have developed a program to solve 2-D Poisson Shrödinger equation including band anisotropy using a simple six valley model. The program was tested on a Double gate

structure.

We intend to extend the program to 3-D and also try to include the full bandstructure using Tight Binding in the future.

References

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