Assignment 02

# Self-consistent Poisson-Schrodinger Solver for MOS Structure

Submitted by

Syed Nakib Hossain

1017062229

## 1. Theory

In the self-consistent method the Schrodinger equation is solved iteratively using the potential obtained from solving Poisson's equation until the system converged.
The solution starts with a guess, ideally from semi-classical or classical approximation. We start by guessing the potential distribution giving the doping level and assuming no mobile charge from Poisson equation-

$$\epsilon \nabla^2 \varphi = -\rho$$

$$\rho = q(p(x) - n(x) + Na - Nd)$$

With the potential derived we can solve the Schrodinger equation to obtain wave function and energy for bound state-

$$\left(-\frac{\hbar^2}{2m^*}\nabla^2 + V\right)\psi = \varepsilon\psi$$

$$n(x) = \sum N_i |\psi|^2$$

$$N_i = \frac{m_{DOS} kT}{\pi\hbar^2} \ln(1 + \exp(\frac{E_f - E_i}{kT}))$$

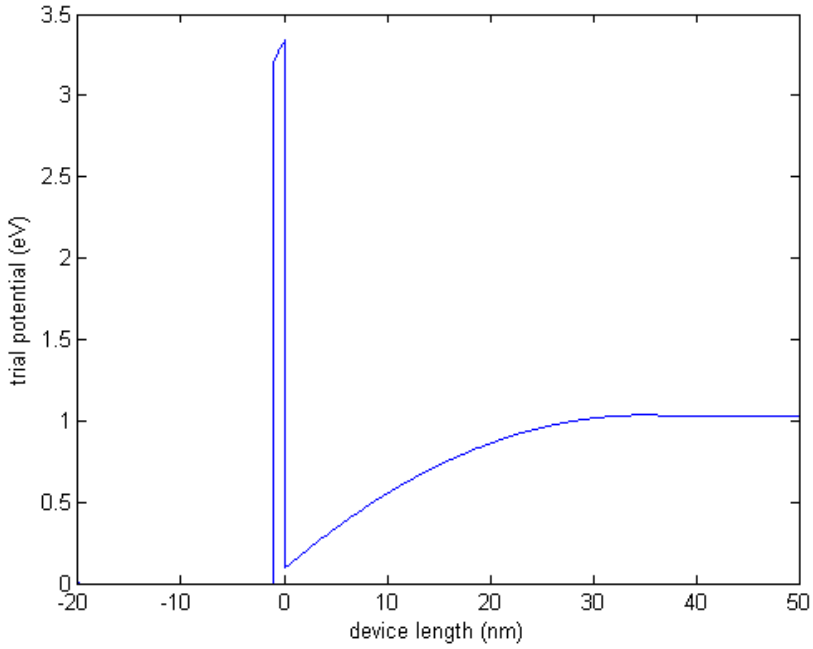
With this new charge distribution the Poisson's equations can be solved again to make a more accurate guess. The two equation is solved iteratively to reach a consistent solution

## 2. Device Geometry

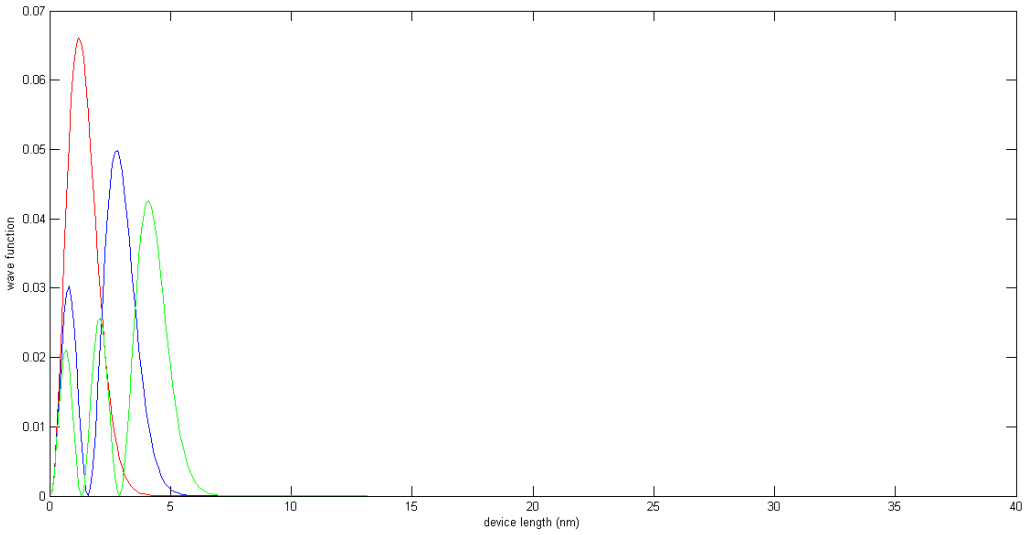
We have considered a MOS structure with Aluminum as gate, $SiO_2$ as gate oxide and p-type silicon substrate. The thickness of oxide layer is considered to be 1 nm. Although in this thickness penetration effect should be observable as open boundary condition is not considered the penetration effect is not seen in the oxide region in simulation result. The total device length is 70 nm where the substrate occupy 50 nm. The self-consistent simulation is done only on the quantum region formed near the oxide-substrate junction.

## 3. Simulation Result

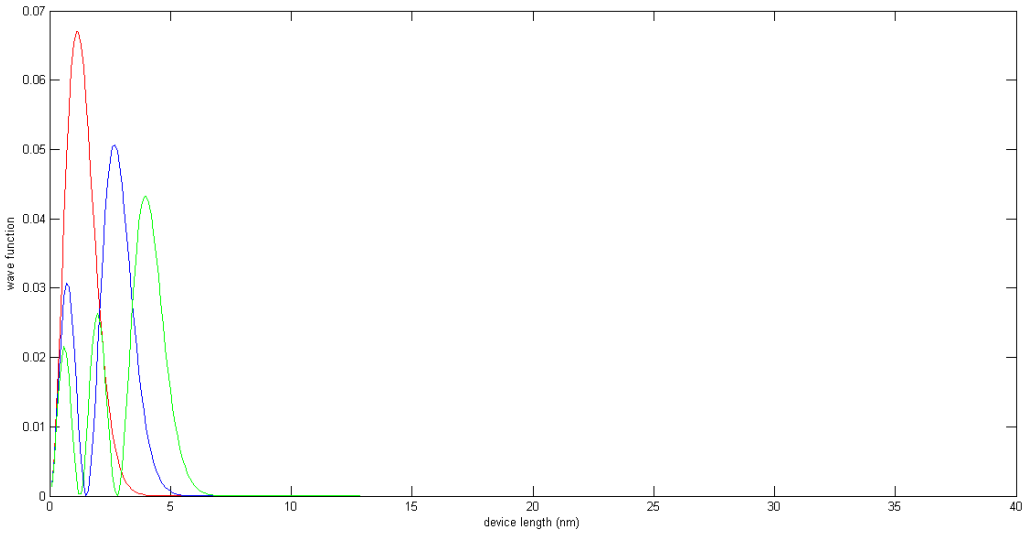
First the Poisson equation is solved to get the trial potential. The following figure shows the potential –




In all the iteration we have considered zero gate potential. The first three eigen function for iteration 1, 50 is shown below -

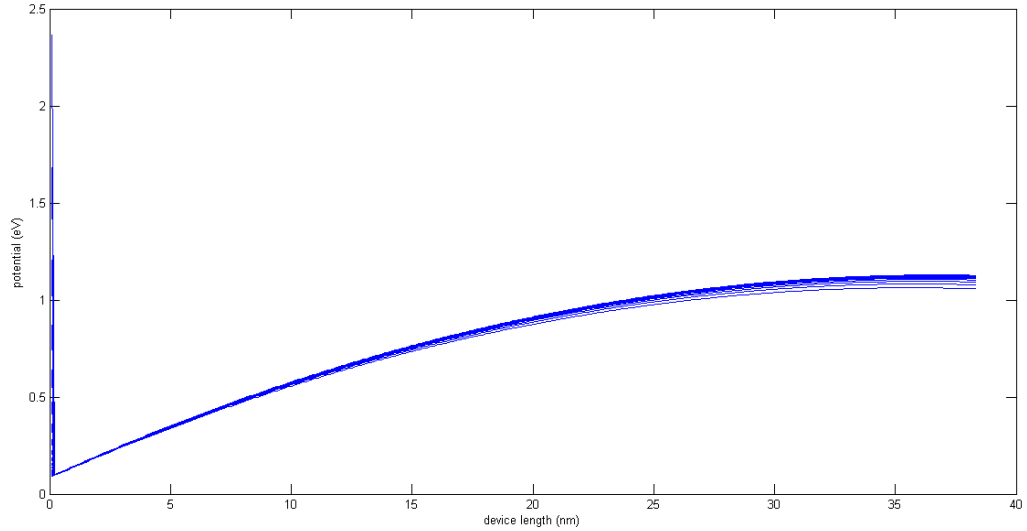



Iteration = 1

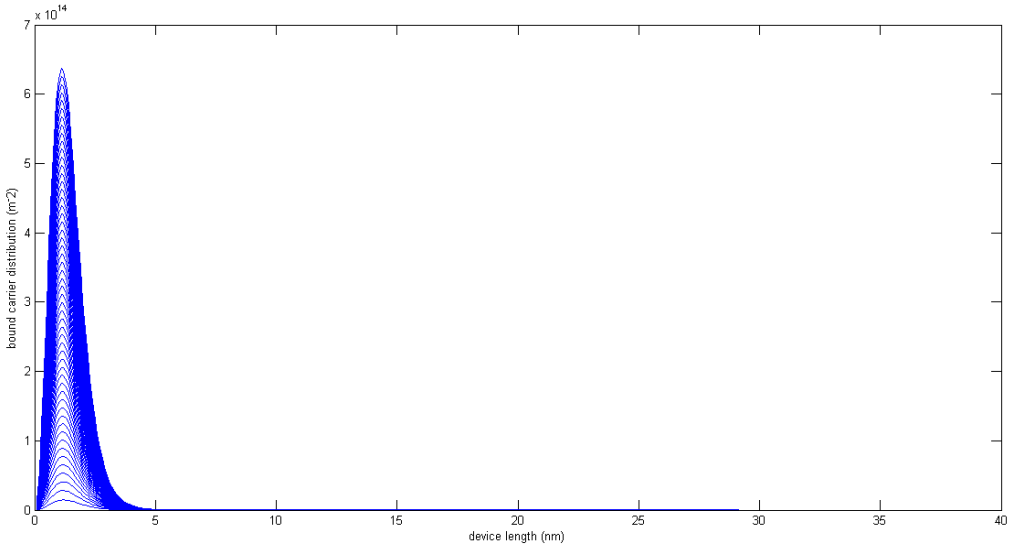



Iteration = 50

Below we show the evolution of the potential and bound charge carrier density inside the depletion region throughout the iteration –




Evolution of potential inside the depletion region

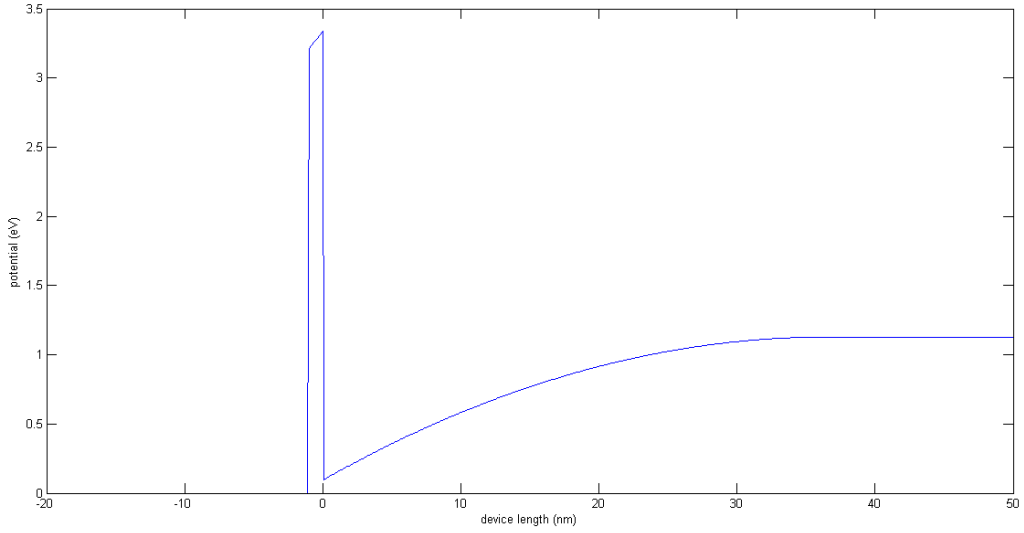



Evolution of density of bound charge carrier

The error rate for the last couple iterations are –

| iteration | error |
|---|---|
| 50 | 4.52374081766830e-09 |
| 51 | 3.16661463087995e-09 |
| 52 | 2.21662630728417e-09 |
| 53 | 1.55163447800418e-09 |
| 54 | 1.08614019693367e-09 |
| 55 | 7.60294204018633e-10 |

The final potential distribution –




Final potential distribution