Homework #8
Computational Microelectronics

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Due on November 1, 2018

1 Results

We have calculated the electron density and integrated electron density by using both the non-linear Poisson solver (Homework 6) and Schrödinger-Poisson solver. In the Schrödinger-Poisson solver, we first solve the non-linear Poisson equation to provide the initial guess on the potential ϕ. And we iteratively solve the Schrödinger equation and Poisson equation to satisfy the self-consistent condition. In our code, the iteration continues until the difference between the total energy and the updated total energy provided from the Schrödinger equation is less than 10^{-5} meV.

Fig. 1 shows the integrated electron density n_{2D} as a function of the gate voltage V_G. It shows very similar results compared to the figure provided in the Lecture note 11. The semi-classical density is larger than the density from the Schrödinger-Poisson solver, though the two show the same tendency; first, the density increases as V_G increases; secondly, the density increases exponentially at $V_G < 0.5$; lastly, the density increases linearly at $V_G > 0.5$.

Fig. 2 shows the electron density n, changing the gate voltage. For the both solvers, the density increases as V_G increases. However, n is high near the interfaces between SiO_2 and Si from the non-linear Poisson solver while n is mostly distributed near the midpoint of Si.

We had some troubles in the calculation with the Schrödinger-Poisson solver. After solving the Schrödinger equation, we had solved again the Poisson equation. When we solve the Poisson equation iteratively in this phase, the solution does not converge at $V_G > 0.24$. To avoid this, we solved the Poisson once and move to the Schrödinger equation again.

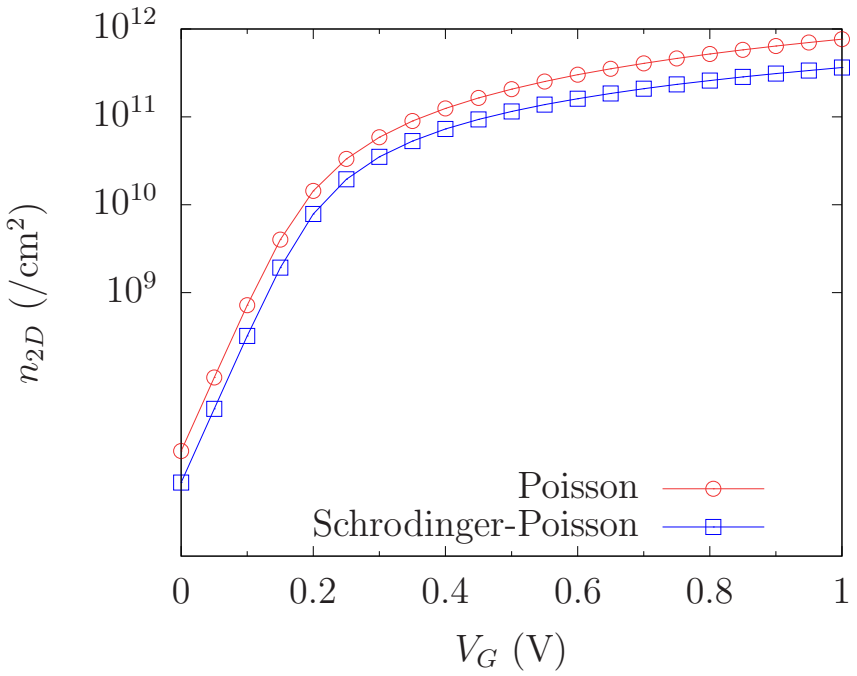

Figure 1: The integrated electron density n_{2D} as a function of the gate voltage V_G.

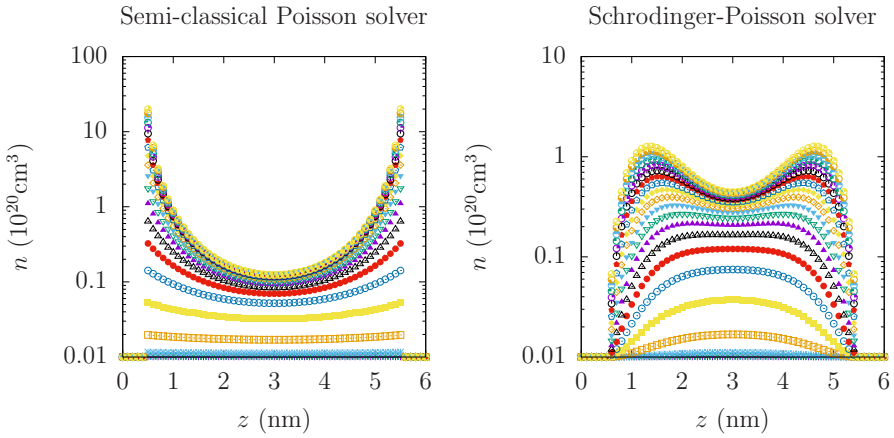

Figure 2: Snapshot of the electron density n in the z-direction. LEFT: the density obtained from the Poisson solver. RIGHT: the density obtained from the Schrödinger-Poisson solver.