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Self consistent with Poisson's equation and Boltzmann statistics

1. Setting the structure.

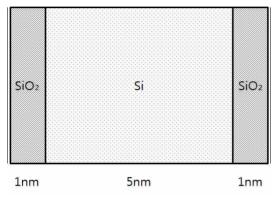


Fig 1. Simulation structure.

We set up the structure to simulate as above. The constants and setting values used in this structure are as follows.

Thickness of SiO_2 layers: 1nm Thickness of Si layer: 5nm Number of mesh points: 71 Initial acc electron density

 $1.0 \times 10^{18} \text{ cm}^3$

Electron charge : 1.602192×10^{-19} C

Vacuum permittivity

 $: 8.854187817 \times 10^{-12} \text{ F/m}$

Relative permittivity

: SiO₂ - 3.9, Si - 11.7

2. Poisson's equation With no self consistent.

Calculation of the Poisson's equation in this structure with no self consistent is next.

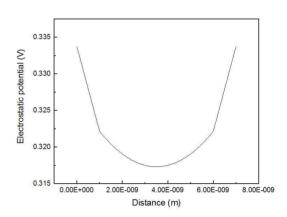


Fig 2. Electrostatic potential with no self consistent and zero gate voltage (about 0.33V of electrostatic potential).

Then we change the gate voltage,

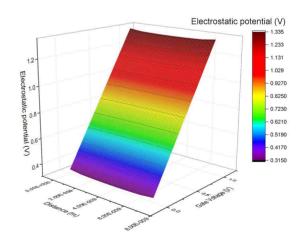


Fig 3. Electrostatic potential with no self consistent and gate voltage from 0V to 1V (additional about 0.33V of electrostatic potential).

Also using the Boltzmann statistics,

$$n(\mathbf{r}) = n_i \exp\left(\frac{q\phi}{k_B T}\right)$$
 (1)

We can calculate the electron density.

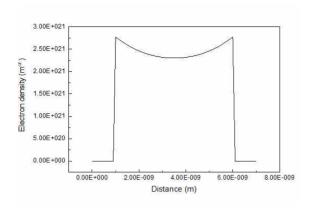


Fig 4. Electron density with no self consistent and zero gate voltage (about 0.33V of electrostatic potential).

Comparison between non-repeated solution and repeated solution.

We can calculate the difference between non-repeated electrostatic potential and 1 repeated electrostatic potential. The difference is displayed below.

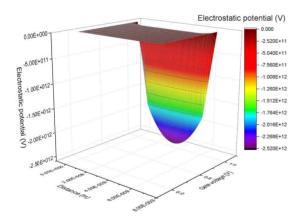


Fig 5. The difference between non-repeated electrostatic potential and 1 repeated electrostatic potential.

This result indicates that when the gate voltage exceeds a certain level, it exhibits an electrostatic potential which is impossible.

To see more detail, compare the maximum difference in each gate voltage.

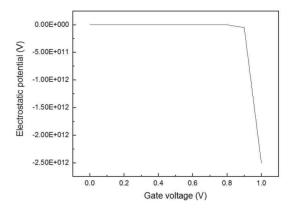


Fig 6. The maximum difference in each gate voltage.

When gate voltage is 0.1V, the difference is -0.001911V. However when the gate voltage is 0.2V, the difference is -0.09144V. It may be not acceptable to make self consistent convergence. Therefore the maximum gate voltage for convergence may be about 0.1V.

To confirm this assumption, we tried to calculate self consistent solution when the gate voltage is 0.2V. However there is no solution in that case.

In case of 0.1V, We can find the convergence solution.

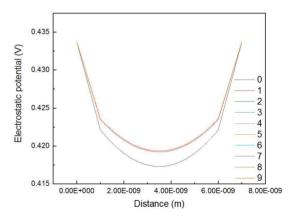


Fig 7. Self consistent solution of the structure for each repeat when the gate voltage is 0.1V (about 0.43V electrostatic potential)

Therefore, the maximum positive gate voltage is about 0.1V.