Computational Microelectronics HW.13

EECS, 20204003

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1. Double Gate FET with Self-Consistent nonlinear Poisson-Schrodinger

1) Numerical Expression

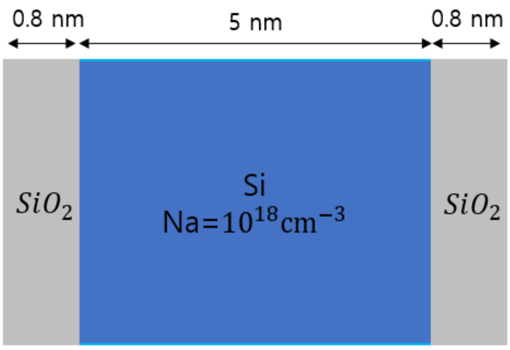

Fig. 1 Double Gate FET

이전 과제 12에서 사용했던 수식들이고, 과제12와의 차이는 단순히 Schrodinger-Poisson을 loop를 통해 self-consistent한 결과를 얻어내는 것이다.

$$-\frac{\hbar^2}{2m_{zz}}\frac{\partial^2}{\partial^2 z}\psi(z) + V(z)\psi(z) = E_{z,n}\psi(z) \quad \text{(n=1,2,3...)}$$

$$V(z) = -q\phi(z) + (E_c - E_i)$$

$$\sum_{i=interface1+1}^{interface2-1} \left|\psi_{z,n,i}\right|^2 \Delta z = 1$$

$$n(z)\ (cm^{-3}) = \frac{1}{L_x L_y}\sum_{n=1}^{\infty}\left|\psi_{z,n,i}\right|^2 \frac{L_x L_y}{(2\pi)^2}(2\pi)\frac{m_d}{\hbar^2}k_B T \ln(1+\exp\left(\frac{-E_{z,n}+E_F}{k_B T}\right))$$

$$n_{total}(z) = 2 \times 2 \times \sum_{valley=1}^{3} n(z)$$

위와 같은 Schrodinger solver를 구성하고, 풀게 되면 전자 농도가 나오게 되는데, 이 때 나오는 전자 농도를 Poisson solver에 다시 넣게 된다. Poisson solver를 풀게 되면 Schrodinger solver의 결과에 따라서 potential이 update가 되고, 이를 다시 Schrodinger solver를 푸는데, 사용하는 loop를 형성하게 된다. 이 결과가 어느 정도의 수렴도를 가질 때까지 반복을 한다.

하지만, 전자 농도를 넣을 때, 다음과 같은 2가지의 방식을 시도한다.

$$1. n_{new} = n_{Sch}(z)$$

$$2.\quad n_{new,0} = n_{Sch} \times e^{\frac{\delta\phi}{V_T}},$$

$$n_{new,n} = n_{new,n-1} \times e^{\frac{\delta\phi}{V_T}} \text{ (When repeated for n times)}$$

1번 방식은 Schrodinger solver를 풀어서 나온 전자 농도를 상수로서 Poisson solver에 넣는 것이다. 2번 방식은 Schrodinger solver를 풀어서 나온 전자 농도를 Poisson solver를 풀 때 계속 변하는 값으로 넣게 된다. 이 때 변하는 정도는 위와 같은 수식으로 나타나게 된다.

2) Results

A) Electron Density. Constant electron density is used. $(\mathbf{V_{gs}} = \mathbf{0V, 0.5V, 1V})$

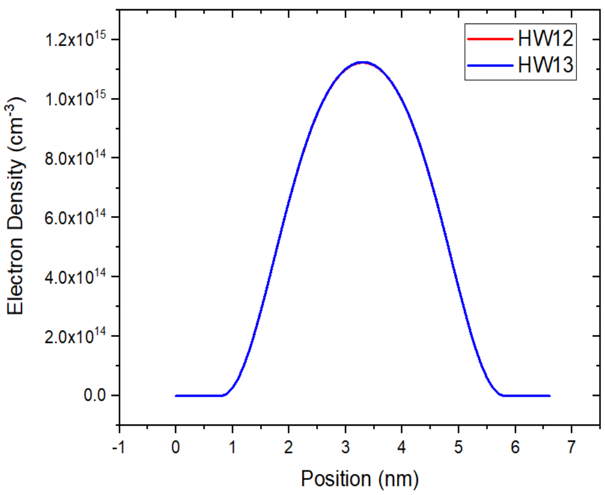

Fig 2. Position vs. Electron density graph. Red line represents the electron density which is non self- consistent result while blue line is self-consistent result when $\mathbf{V_{gs}} =$ 0V.

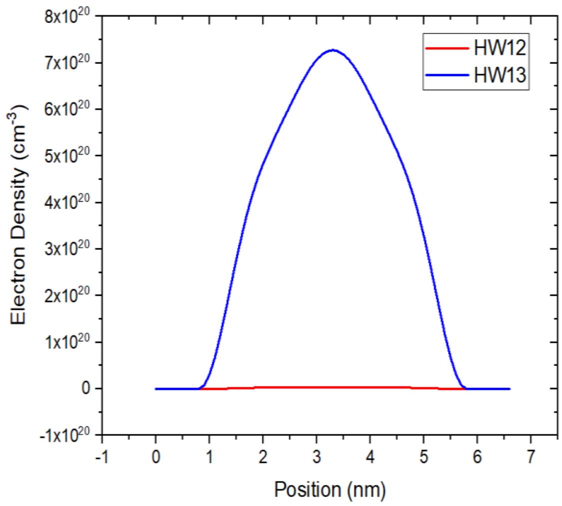

Fig 3. Position vs. Electron density graph. Red line represents the electron density which is non self-consistent result while blue line is self-consistent result when$\mathbf{V_{gs}} =$ 0.5V.

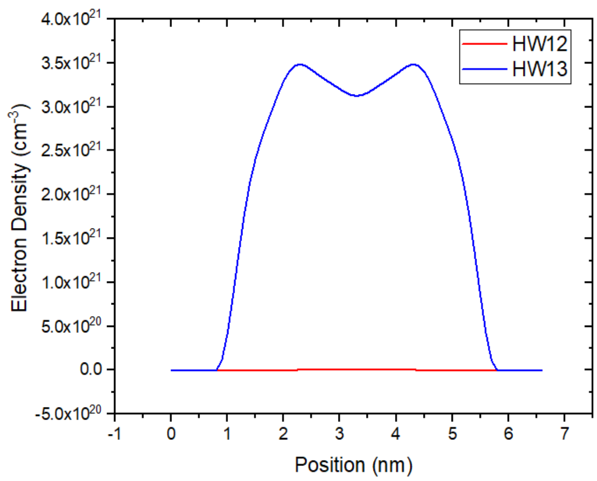

Fig 4. Position vs. Electron density graph. Red line represents the electron density which is non self- consistent result while blue line is self-consistent result when $\mathbf{V_{gs}} =$ 1V.

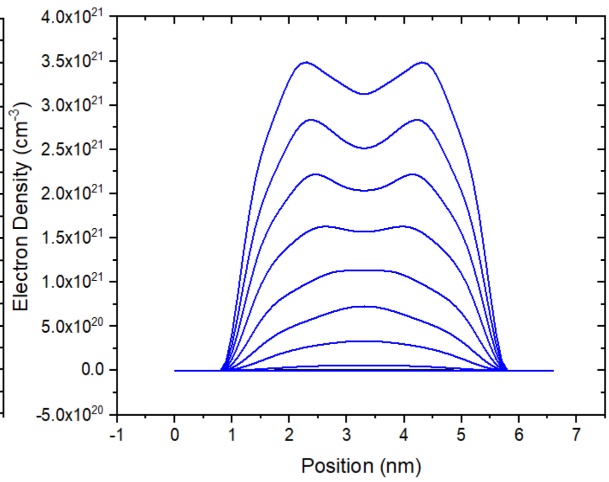

Fig 5. Position vs. Electron density graph. Black line represents the non self-consistent results which is solved by Poisson equation while blue line is solved by Schrodinger solver when $\mathbf{V_{gs}} =$ 0~1V with 0.1 step size.

위의 결과는 전자 밀도를 나타낸 결과로, 약 0.3V부터 급격하게 결과가 커지는 것을 확인하였다. 이 결과가 옳은 지 확인을 위해 Convergence graph를 확인한다.

B) Convergence Graph with constant electron density.

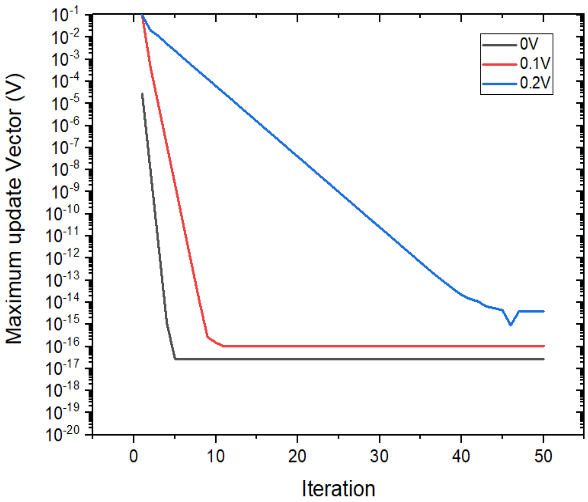

Fig 6. Iteration vs. Maximum update vector when gate voltage is 0~0.2V with voltage step 0.1V

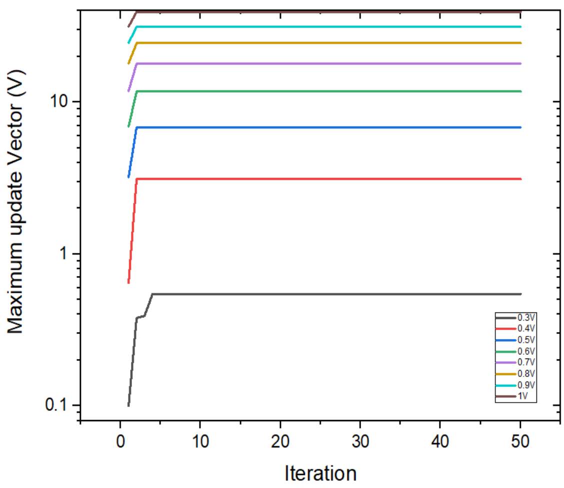

Fig 7. Iteration vs. Maximum update vector when gate voltage is 0.2V~1V with voltage step 0.1V

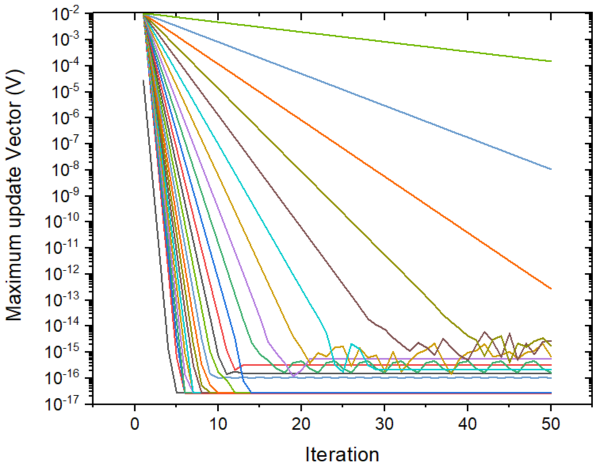

Fig 8. Iteration vs. Maximum update vector when gate voltage is 0~0.23V with voltage step 0.01V

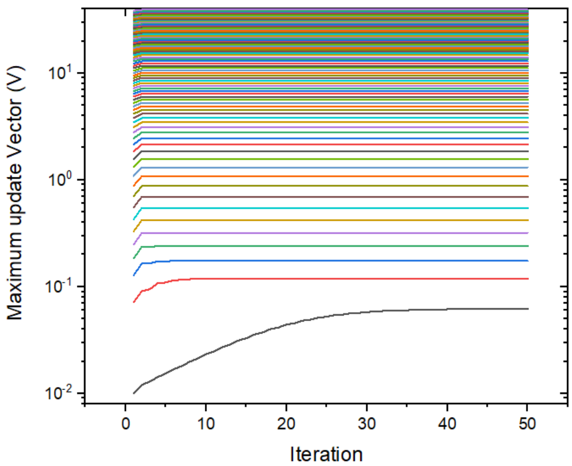

Fig 9. Iteration vs. Maximum update vector when gate voltage is 0.24~0.1V with voltage step 0.01V

Convergence graph를 확인한 결과 gate voltage 상승 step을 0.1V로 하였을 때, 약 0.3V부터 발산하는 것을 확인하였다. 수렴도를 올리기 위해 step size를 1/10를 했음에도 0.2V~0.3V 사이의 gate voltage에서 발산하는 것을 확인할 수 있다. 물론 Newton iteration을 늘리고 voltage increasement를 줄이면, 수렴성이 좋아지겠지만, 시간이 매우 오래 걸리게 되는 심각한 trade-off가 발생한다. 따라서 다른 방법을 사용하였다.

C) Electron Density. Updated electron density is used. ($V_{gs} = 0V \sim 0.5V, 1V$)

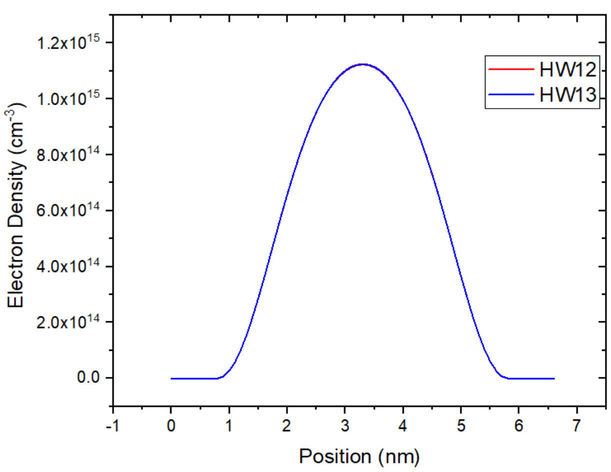

Fig 10. Red line represents the electron density which is non self- consistent result while blue line is self-consistent result when $\mathbf{V_{gs}} =$ 0V.

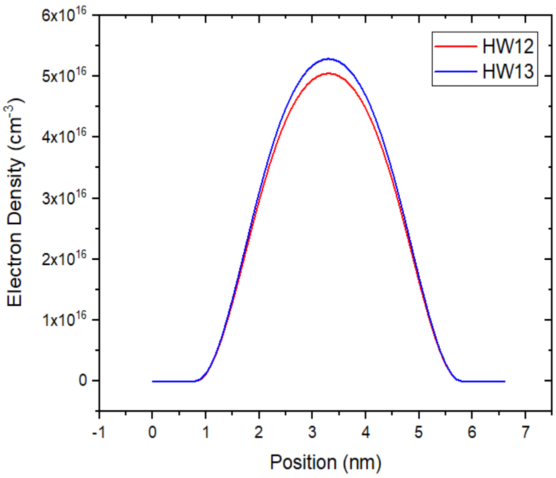

Fig 11. Red line represents the electron density which is non self- consistent result while blue line is self-consistent result when $\mathbf{V_{gs}} =$ 0.1V.

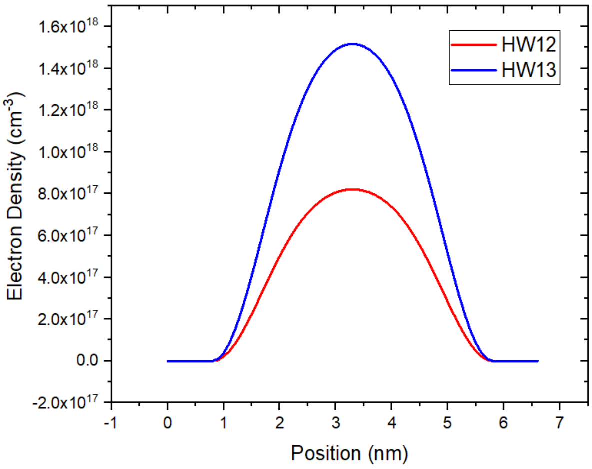

Fig 12. Red line represents the electron density which is non self-consistent result while blue line is self-consistent result when $\mathbf{V_{gs}} =$ 0.2V.

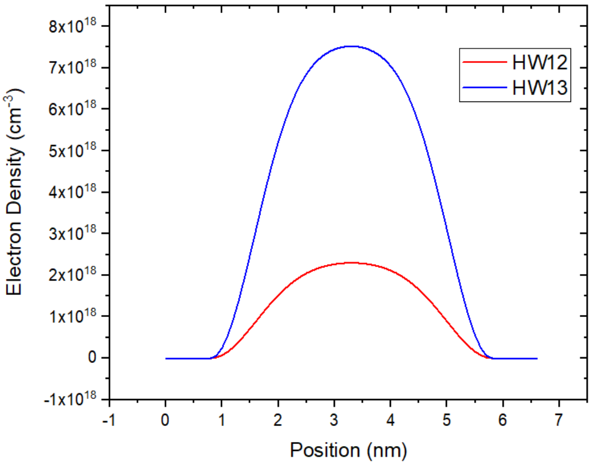

Fig 13. Red line represents the electron density which is non self-consistent result while blue line is self-consistent result when $\mathbf{V_{gs}} =$ 0.3V.

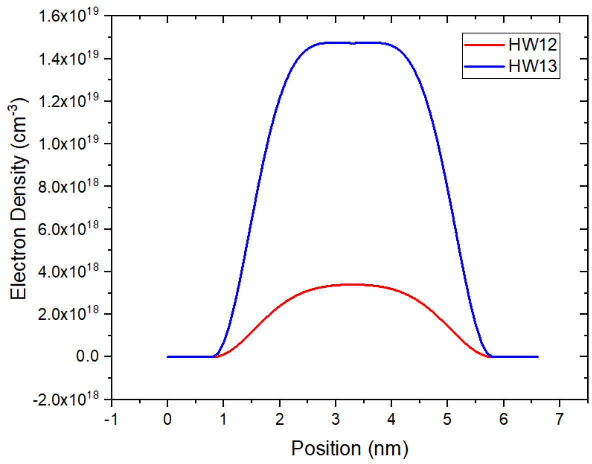

Fig 14. Red line represents the electron density which is non self-consistent result while blue line is self-consistent result when $\mathbf{V_{gs}} =$ 0.4V.

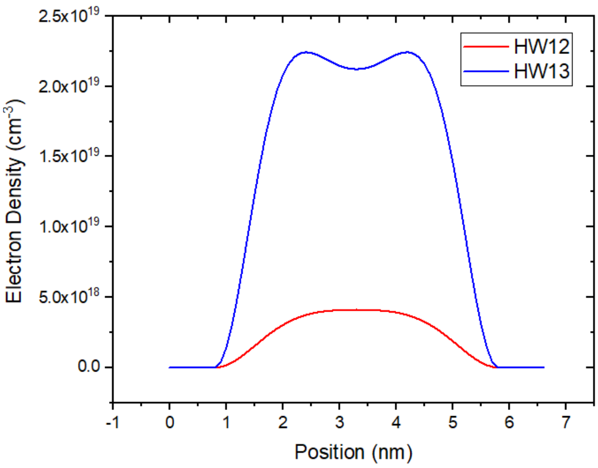

Fig 15. Red line represents the electron density which is non self-consistent result while blue line is self-consistent result when $\mathbf{V_{gs}} =$ 0.5V.

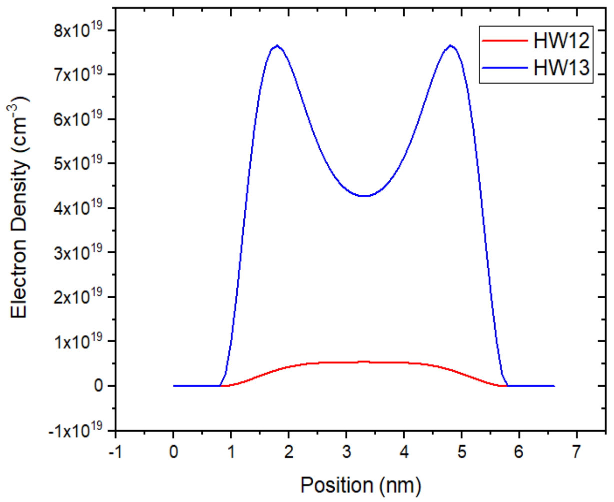

Fig 16. Red line represents the electron density which is non self-consistent result while blue line is self-consistent result when $\mathbf{V_{gs}}$ = 1V.

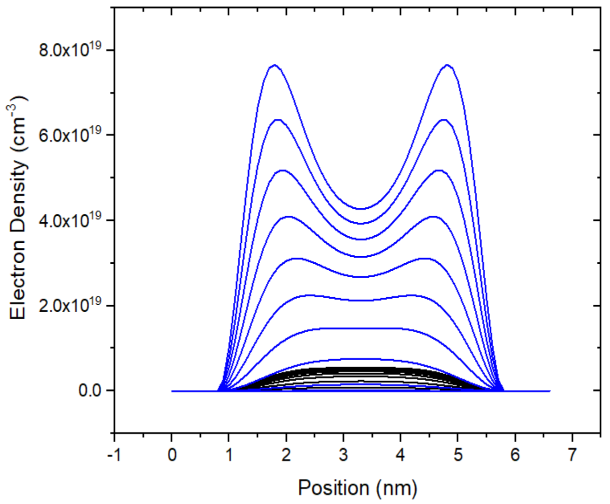

Fig 17. Position vs. Electron density graph. Black line represents the non self-consistent results while blue line is the self-consistent results when $\mathbf{V_{gs}}$ = 0~1V with 0.1 step size.

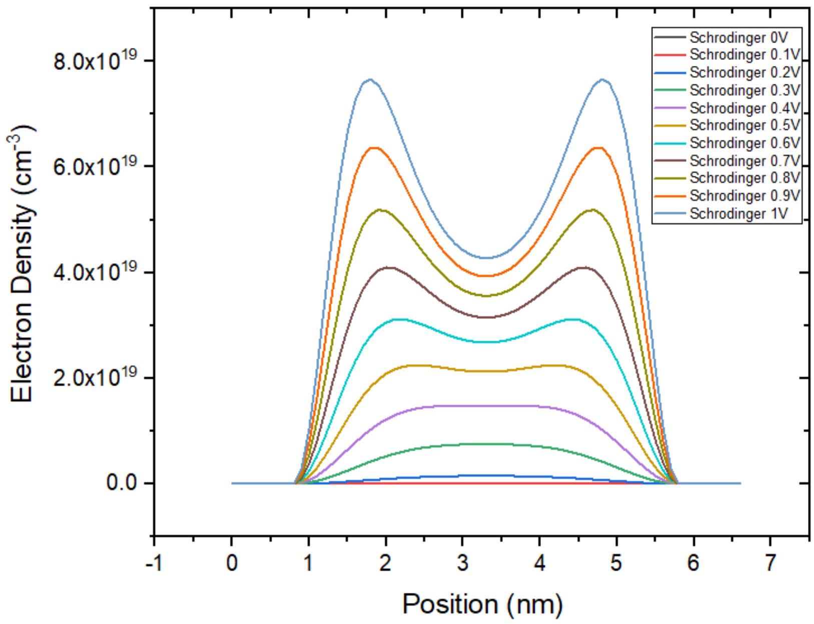

Fig 18. Position vs. Electron density graph which is solved by Poisson-Schrodinger solver.

위의 결과는 전자 밀도를 나타낸 결과로, 이전의 A), B) 파트와 달리 전자 농도가 Poisson solver의 internal loop에서 상수였던 것과 달리 계속 변하게 된다. 또한 Poisson의 결과와 맞춰지도록, 단순한 non self-consistent의 결과보다 커지며, 전자 농도의 최고점이 interface와 가까워지는 것을 확인할 수 있다. 결과가 옳은 지 확인을 위해 Convergence graph를 확인한다.

D) Convergence Graph with updated electron density is used.

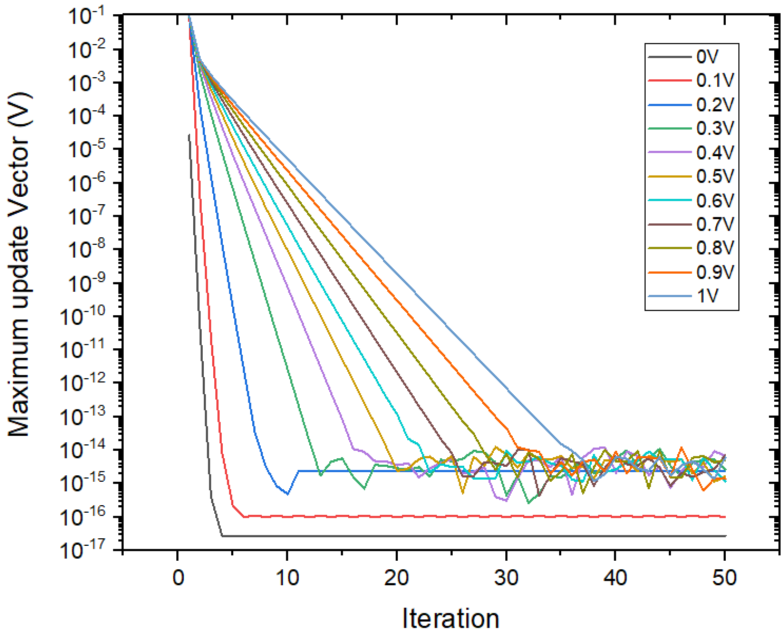

Fig 19. Iteration vs. Maximum update vector when gate voltage is 0~0.1V with voltage step 0.1V

이전의 결과와 달리, 수렴이 올바르게 이뤄지는 것을 확인할 수 있다. 특징은 Poisson에서의 Convergence 그래프와 달리, 로그 스케일로 그리면 직선으로 떨어지는 것을 확인할 수 있다. 매번 첫번째 Maximum Update vector 값이 0.1V인 이유는 gate voltage increasement가 0.1V이기 때문이다.