Numerical Solution of Poisson and Landau-Khalatnikov Equations for Negative Capacitance Devices with PZT and HZO Ferroelectric Films

Yu-Chin Tsai[1-2,5-6] and Yiming Li[1-8,*]

[1] *Parallel and Scientific Computing Laboratory;* [2] *Institute of Biomedical Engineering;* [3] *Institute of Communications Engineering;* [4] *Department of Electrical and Computer Engineering, National Yang Ming Chiao Tung University, 1001 Ta-Hsueh Rd., Hsinchu 300, Taiwan.*

[5] *Parallel and Scientific Computing Laboratory;* [6] *Institute of Biomedical Engineering;* [7] *Institute of Communications Engineering;* [8] *Department of Electrical and Computer Engineering, National Chiao Tung University, 1001 Ta-Hsueh Rd., Hsinchu 300, Taiwan.*

[*] *ymli@faculty.nctu.edu.tw*

In order to promise the high performance of devices, many researches have been proposed various methods in recent years [1-2]. Negative capacitance (NC) field-effect transistor (FET) is one of solutions which can boost the devices performance effectively based on the concept of the ferroelectric (FE) polarization [3-5]. Many groups have proposed the NC effect can improve the devices characteristic adequately [6-7], where the detail of numerical method used to solve NC devices plays a key role to explore their physics. To explore the physical insight of NC devices, such as the polarization phenomenon, we investigate and compare the NC device with different FE films by solving one-dimensional (1D) Poisson equation coupled with Landau-Khalatnikov (LK) equation.

Fig. 1 (a) shows the program flow chart of the numerical solution. In this flow, we discretize the Poisson equation by using the finite difference method (FDM) and solve it by using the monotone iterative (MI) method. The MI method replaces the Newton's method for the numerical solutions of the nonlinear algebraic equations due to its effective execution and global convergence [8]. The devices structure and parameters are listed in Fig. 1 (b). Fig 1(c) reveals the discretized equations of the Poisson equation by using FDM over the uniform rectangular mesh in the different region. The schematic of 1D MFIS discretization also demonstrate the boundary condition between the interface of different regions. Figs. 2 show the electrostatic potential of (a) metal-SiO_2-Si and (b) metal-HfO_2-SiO_2-Si under V_G is 1V. Because of the different dielectric constant, the larger voltage across the SiO_2 layer than that of the HfO_2 layer. The band diagram of HfO_2 and HZO are demonstrated in Figs. 2 (c) and (d). Notably, the dipoles in the FE layer will be rearranged due to occurring the polarization by applying the gate voltage, the potential in the FE and the insulator layer will drop in the opposite direction and increase the surface potential simultaneously. Therefore, the potential will be raised in the FE region. Figs. 3 illustrate the (a) PZT and (b) HZO's potential profile, respectively. We can observe that the slope is steeper in the HZO than that in PZT, which indicate the polarization in the HZO is strong. Fig. 3(c) shows the polarization of HZO and PZT along the FE layer. The FE layer will obtain the polarization term due to solving the LK equation. The result indicates that the HZO has higher polarization than the PZT. However, the variation of polarization at each grid points along the FE layer is much small. It means the FE polarization distribution is uniform in the 1D NC MOS simulation. Fig. 3 (d) shows the total capacitance which correspond to PZT and HZO. As the applied voltage increase, the charges which in the bulk region will reduce so that the effect of the FE series capacitance will not prominent. The NC MOS capacitance can be denoted by a series connection of FE, insulator and bulk capacitance. When the stronger polarized occur in the FE layer, the FE capacitance will influence the total capacitance of NC MOS. Thus, the higher capacitance can be observed in HZO due to the stronger NC effect which lead the HZO capacitance larger than that of PZT. Not shown here, we do also check the absolute error variation versus the number of iterations. The MI method converges globally for different voltage conditions. Thus, it provides a robust way to solve the Poisson equation coupled with LK equation.

In summary, we have explored the numerical method to solve Poisson equation coupled with LK equation and compare with different FE materials of NC devices. The results indicate that the voltage across the FE layer will increase the electrical potential due to the polarization occur in the FE layer. Compared with PZT, the material of HZO has strong NC effect which has the larger electrical potential. Based on the developed numerical method, we are now studying the 2D numerical solution of NCFET.

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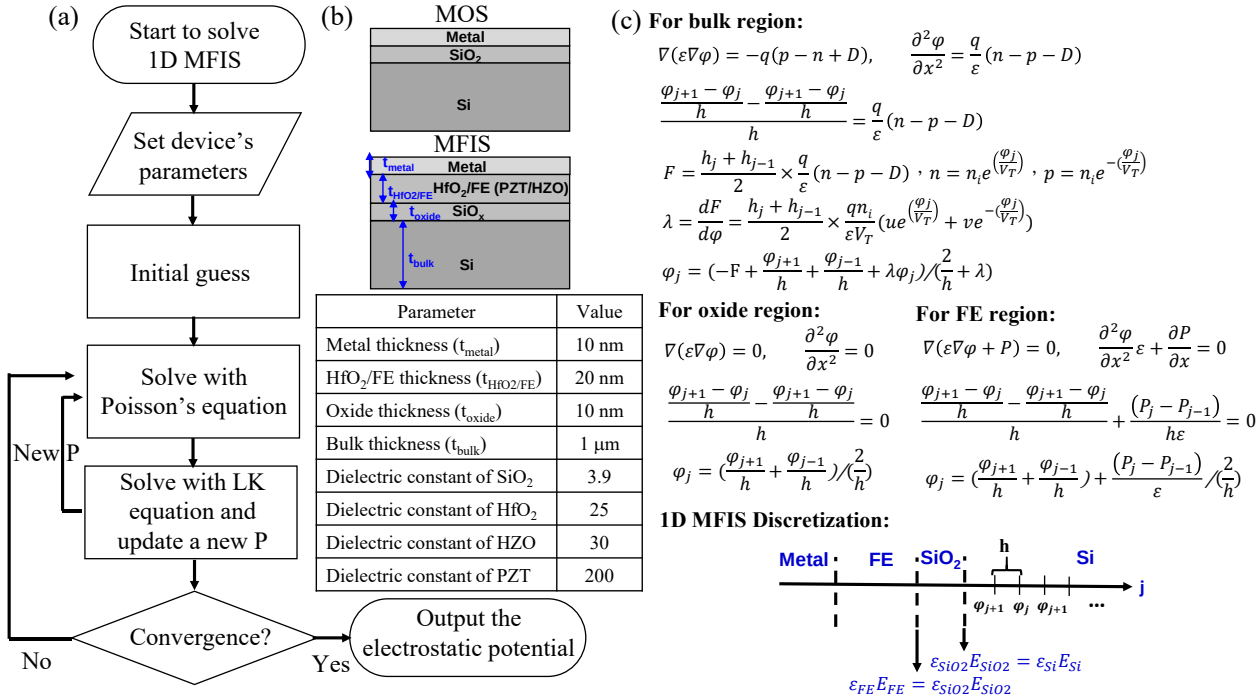

Parameter	Value
Metal thickness (t_{metal})	10 nm
HfO_2/FE thickness ($t_{HfO2/FE}$)	20 nm
Oxide thickness (t_{oxide})	10 nm
Bulk thickness (t_{bulk})	1 μm
Dielectric constant of SiO_2	3.9
Dielectric constant of HfO_2	25
Dielectric constant of HZO	30
Dielectric constant of PZT	200

Fig. 1 (a) The program flow chart for solving the 1D Poisson equation coupled with the LK equation. (b) The devices of metal-SiO_2-Si and metal-HfO_2/FE-SiO_2-Si. The devices' parameters are listed in the table. Notably, the FE material parameters are different in the PZT and HZO. In this study, we adopt the PZT layer for α is -1.35 x 10^8 m/F and the HZO layer α is -7.91 x 10^8 m/F which have been calibrated with the experimental data. (c) The discretized equations of the Poisson equation by using FBM over the uniform rectangular mesh in the bulk, insulator and FE region, respectively.

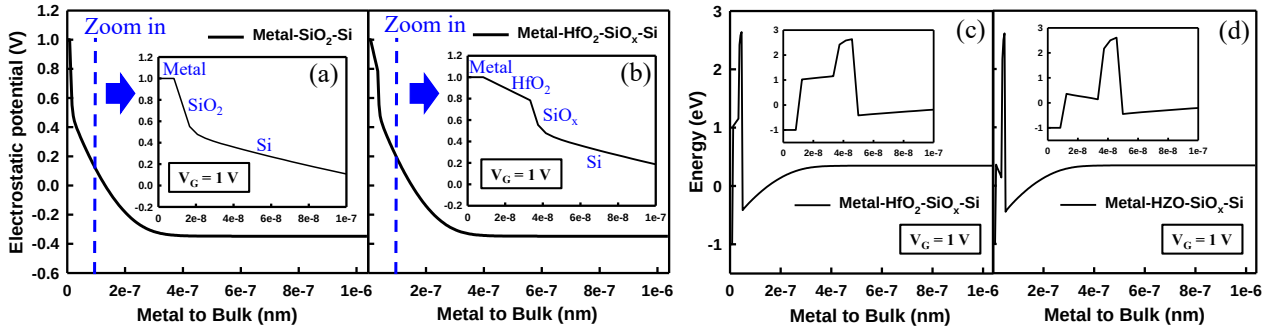

Fig. 2 (a) The electrostatic potential profile of metal-SiO_2-Si and (b) metal-HfO_2-SiO_2-Si under V_G is 1V. The larger voltage across the SiO_2 layer than that of the HfO_2 layer due to the different dielectric constant. (c) The band diagram of metal-HfO_2-SiO_2-Si and (d) metal-HZO-SiO_2-Si. The dipoles which in the FE layer will be rearranged due to occurring the polarization by applying the external voltage, the potential in the FE region and the insulator will drop in the opposite direction. Therefore, the surface potential of FE layer will be raised.

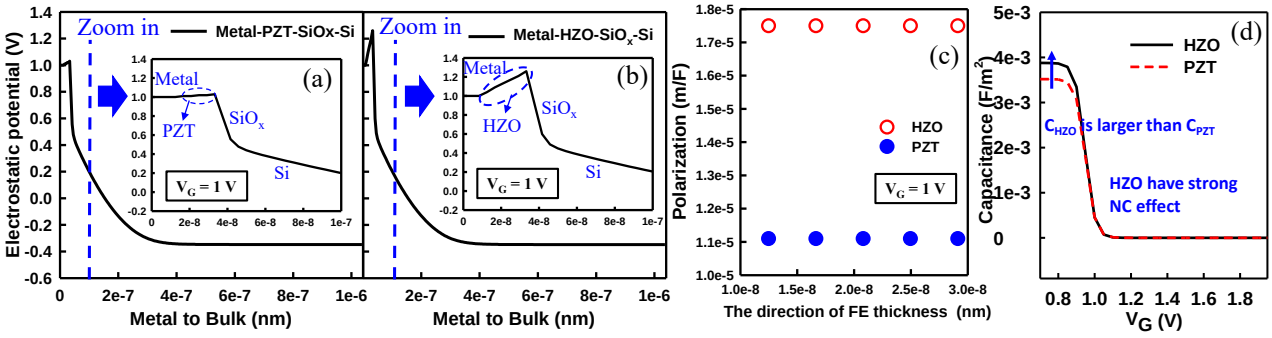

Fig. 3 The electrostatic potential profiles of (a) PZT and (b) HZO for FE layer, respectively. Compared with the PZT, the strong polarized occurs in the HZO; and, thus the surface potential will be increased in the HZO obviously. (c) The polarization of HZO and PZT along the FE layer. The FE layer will obtain the polarization term due to solving the LK equation. The result indicates that the HZO has higher polarization than the PZT. However, the variation of polarization at each grid points along the FE layer is much small. It means the FE polarization distribution is uniform in the 1D NC MOS simulation. (d) The capacitance comparison of PZT and HZO. The capacitance of NC MOS can be denoted by a series connection of FE, insulator and bulk capacitance. Notably, the FE capacitance can be simply described as $C_{FE} = 1/2\alpha t_{FE}$.When the stronger polarized occurs in the FE layer, the FE capacitance will be large and it will influence the total capacitance of NC MOS. We can obtain the higher capacitance due to HZO has the stronger NC effect.

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