Acceleration of three-dimensional device simulation with the 3D convolutional neural network

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Abstract—In this work, the 3D convolutional neural network, which generates an electrostatic potential profile, is used to accelerate three-dimensional device simulation. In the training phase, the deep neural network is trained with the simulation results for various 3D MOSFETs in a supervised manner. The generated potential profile is used as an initial guess at a non-equilibrium condition, while carrier densities are estimated by the frozen field simulation. By adopting the proposed method, the number of the Newton iterations can be reduced significantly.

I. INTRODUCTION

In the device simulation, we typically ramp up the bias to arrive the target bias point. The time cost is proportional to the number of intermediate bias points during the bias ramping. Therefore, when the target bias point is solved directly without the bias ramping, the computational efficiency can be greatly improved. A trained deep neural network can generate a good initial guess for the device simulator. In our previous works [1,2,3], the deep neural networks could generate good initial solutions for diodes, BJTs, and two-dimensional MOSFETs. In this work, our method is further expanded to three-dimensional MOSFETs.

II. NEURAL NETWORKS

Since the electron and hole continuity equations become linear or at most locally nonlinear under a fixed electrostatic potential profile, carrier densities can be easily evaluated once the electrostatic potential is given. For this reason, the proposed deep neural network is trained to generate the electrostatic potential profiles.

Fig. 1 shows a conceptual diagram for the proposed neural network. The gate length, gate width, trench length, trench depth, trench width, oxide thickness, and source/drain depth are used as the length input parameters, source/drain doping and substrate doping are used as the doping input parameters, and the gate bias and drain bias are used as the bias input parameters. The output images are generated electrostatic potential profiles.

Our deep neural network can generate the potential profile suitable for a tensor grid. On the other hand, a general device simulator adopts unstructured meshes. In order to address such difficulty, we perform the interpolation between a tensor grid of the deep neural network and an unstructured mesh of the device simulator.

To simulate the device with the drift-diffusion model, carrier densities are additionally required. These quantities will be provided by the frozen field simulation. To construct the neural network structure, the code written in PyTorch library is used [4]. The sampling and interpolation capability is implemented into our in-house device simulation framework, G-Device [5].

III. THREE-DIMENSIONAL MOSFETS

In this work, the 3D convolution layer, which has been applied to a generative neural network [6], is adopted. Fig. 2 shows the neural network structure employed in this work. The three-dimensional MOSFET simulated in this work is shown in Fig. 3. The training data set contains 1,000 instances of sampled electrostatic potential profiles. The size of each profile is 64-by-64-by-64. Table I shows ranges of each input parameter in the training dataset. The distributions of input parameters are shown in Fig 4. The training and validation losses are measured as functions of the learning epoch in Fig. 5. After the training phase, the trained convolutional network can generate an approximate potential profile in the inference phase. Fig. 6 shows an example of the electrostatic potential profile generated by the trained convolutional neural network when input parameters are $L_g = 0.20\mu\text{m}$, $W_g = 0.28\mu\text{m}$, $t_{ox} = 1.6\text{nm}$, $L_{trc} = 0.32\mu\text{m}$, $D_{trc} = 0.17\mu\text{m}$, $W_{trc} = 0.091\mu\text{m}$, $X_j = 0.13\mu\text{m}$, $N_{sd} = 1.39 \times 10^{19}\text{cm}^{-3}$, $N_{sub} = 8.80 \times 10^{16}\text{cm}^{-3}$, $V_{GS} = 1.1\text{V}$, and $V_{DS} = 1.1\text{V}$. Its error is shown in Fig. 7. Fig. 8 shows another example with a longer gate. Its input parameters are $L_g = 0.11\mu\text{m}$, $W_g = 0.1\mu\text{m}$, $t_{ox} = 1.2\text{nm}$, $L_{trc} = 0.2\mu\text{m}$, $D_{trc} = 0.1\mu\text{m}$, $W_{trc} = 0.05\mu\text{m}$, $X_j = 0.05\mu\text{m}$, doping parameters and bias parameters are same to Fig.6. Its error is shown in Fig. 9. The distribution of Newton iterations for 500 device simulation runs is shown in Fig. 10. Also Fig. 11 shows the convergence behavior when $V_{GS} = V_{DS} = 1.1$ V. Fig. 10 and Fig. 11 show our proposed method can accelerate the device simulation significantly.

Parameter	Minimum	Maximum
L_g	0.11μm	0.28μm
W_g	0.1μm	0.3μm
t_{ox}	1.2nm	3.0nm
L_{trc}	0.2μm	0.38μm
D_{trc}	0.1μm	0.3μm
W_{trc}	0.05μm	0.15μm
X_j	0.05μm	0.15μm
N_{sd}	$1.0 \times 10^{19}\text{cm}^{-3}$	$1.0 \times 10^{20}\text{cm}^{-3}$
N_{sub}	$5.0 \times 10^{16}\text{cm}^{-3}$	$6.0 \times 10^{17}\text{cm}^{-3}$
V_{GS}	0.0V	1.1V
V_{DS}	0.0V	1.1V

Table I. Input parameter range

IV. CONCLUSION

In conclusion, the trained convolutional neural network can generate the electrostatic potential profiles which are close to the numerical solutions of three-dimensional MOSFETs.

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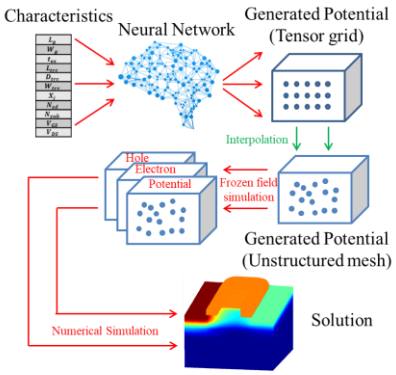

Fig. 1. Conceptual diagram for the proposed deep neural network.

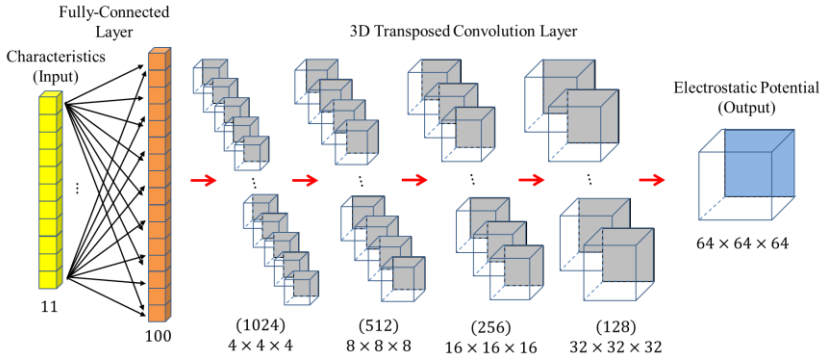

Fig. 2. Layer structure of the CNN structure adopted in the three-dimensional problem. The output layer generates a 64-by-64-by-64 matrix corresponding to the three-dimensional simulation domain.

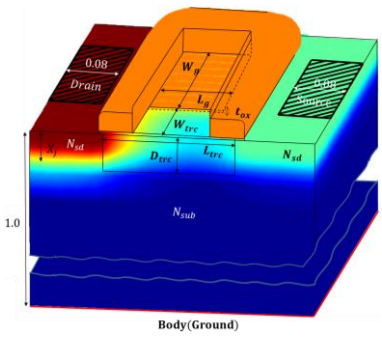

Fig. 3. Structures under consideration for 3D MOSFETs.

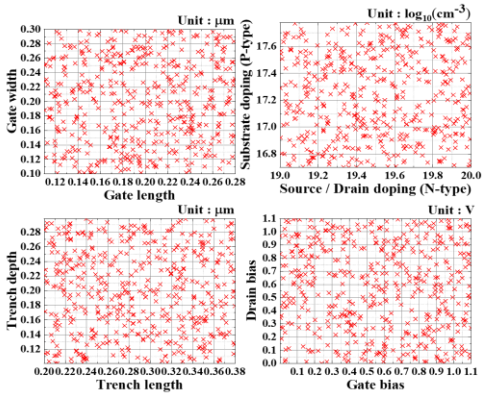

Fig 4. Distribution of parameters in the training dataset.

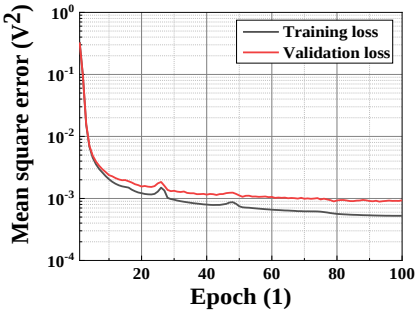

Fig. 5. Training and validation losses of a convolutional neural network, which is trained for the 3D MOSFETs.

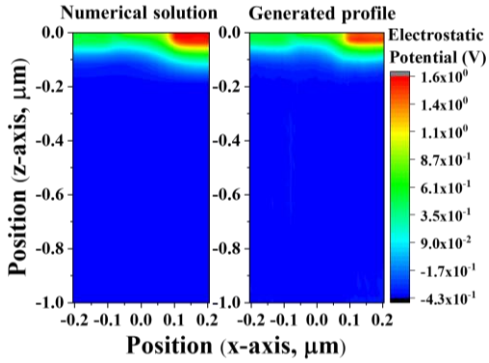

Fig. 6. Numerical solution (Left) and a generated potential profile by the 3D convolutional neural network (Right) when $V_{GS} = 1.1$ V and $V_{DS} = 1.1$ V. The two-dimensional cross-section in the xz-plane is made at the channel center position along the y-axis.

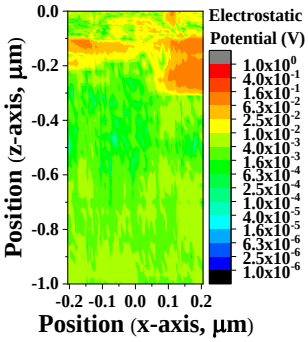

Fig. 7. Difference between two potential profiles in Fig. 6.

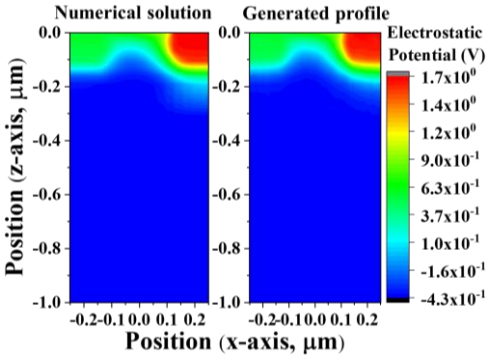

Fig. 8. Numerical solution (Left) and a generated potential profile by the 3D convolutional neural network (Right) when $V_{GS} = 1.1$ V and $V_{DS} = 1.1$ V. The MOSFET has a longer channel length than the one in Fig. 6.

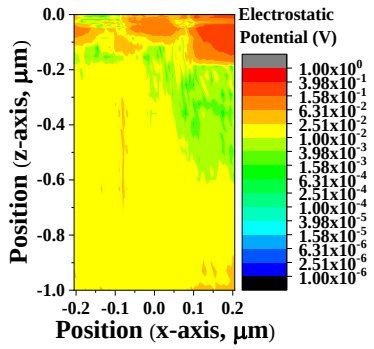

Fig. 9. Difference between two potential profiles in Fig. 8.

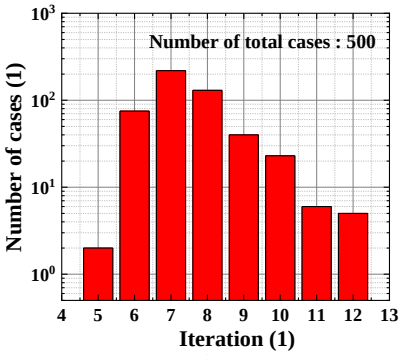

Fig. 10. Distribution of the Newton iterations when the generated potential profiles are used as initial solutions for 500 test cases.

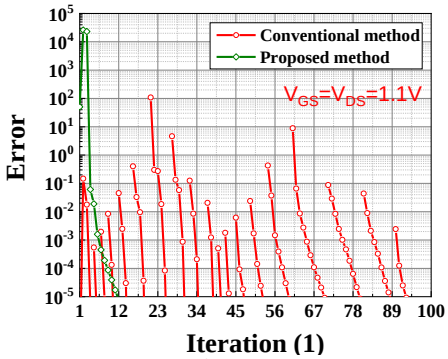

Fig. 11. Comparison of convergence behavior. The target bias condition is $V_{GS} = 1.1$ V and $V_{DS} = 1.1$ V.