Simulation of Hafnium-Based FinFET and Ferroelectricity of Related 2-Dimensional Hafnium-Based Materials

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Abstract. The application of MOSFET is constrained because $\boldsymbol{V_{DD}}$ cannot be successfully scaled down as the power density per unit area in an integrated circuit growing exponentially. Inserting ferroelectric layer can cause Complementary Metal-Oxide-Semiconductor (CMOS) to transit to Negative Capacitance CMOS (NCMOS), which presents steeper Subthreshold Swing (SS) and a higher $\boldsymbol{I_{on}/I_{off}}$ ratio. However, typical ferroelectric materials are not compatible with present CMOS production process. In this work, both Hafnium-based FinFET compatible with CMOS and normal Silicon-based FinFET are simulated to compare their electrical properties. The result shows that the drain current of Hafnium-based FinFET is 3.52 times larger than the Silicon-based one when gate voltage is 1.0V. In addition, the on/off current ratio also raises from $\boldsymbol{3.9 \times 10^5}$ to $\boldsymbol{1.5 \times 10^6}$. Other detailed electrical properties of Hafnium-based FinFET are also given out, including electric field distribution and valence band energy. Besides, through ab-initio calculation based on Density Functional Theory (DFT), 2-dimensional Hafnium dioxide which is different from bulk Hafnium dioxide is simulated to show its ferroelectricity.

Keywords: Negative capacitance, FinFET, Hafnium-based ferroelectric material, Ab-initio calculation, Density Functional Theory

1. Introduction

There are several reasons to choose FinFET devices over traditional MOSFET. More transistors are needed to increase computing power, which means that there will be increasing computing density. However, due to the limitation of transistors process accuracy, it is significant to keep this area roughly the same. As a result, the size of the transistor must be shrunken. But as transistors' size decrease, gate electrodes are not able to control the flow of current well, which is also known as the short-channel effects. Fortunately, after FinFET was created, this kind of problem was partly solved. With its shorter switching times, higher current densities and what is the most significant, the superior short-channel characteristics, FinFET is widely used in chip design. [1]

However, another problem arises here that the power density per unit area in an integrated circuit has grown exponentially because V_{DD} cannot be successfully scaled down. In order to solve this problem, a solution was proposed- the subthreshold slope (SS) should be increased[2]. There are two ways to reach this goal. First, employing a novel working principle instead of thermal electron emission process is a wise choice, which requires the technique revolution of the Field-effect transistor. The second method is to lower the sensitivity of V_G towards surface potential[2]. Negative capacity (NC) effect can be used in order to reach the second method, which requires insertion of a ferroelectric layer in the gate stack of conventional transistors[3-6]. The typical ferroelectric material such as BFO and PZT has been tested and they presented good performance- a high on/off ratio of 10^7 and a sub-20-mV/decade average subthreshold slope[7]. In addition, A. I. Khan et al. [8] demonstrates steep switching behavior in FinFET by using $BiFeO_3$ capacitors connected to the FET externally, which proves that steep switching mechanism based on negative capacitance is effective in 3D devices structures such as FinFET.

However, it is hard to use typical ferroelectricity materials as inserted layers in large-scale integrated circuit production because these kinds of materials are not compatible with current CMOS manufacturing processes. However, 2-dimensional HfO_2 is ferroelectricity material which is compatible with CMOS manufacturing process.[9-11]

In this work, Hafnium-based FinFET is studied using Silvaco TCAD. By introducing HfO_2, detailed electrical properties of Hafnium-based FinFET are given out, including drain current versus gate voltage, electric field distribution and valence band energy. To be compared, silicon-based FinFET is also simulated, which shows that the drain current of Hafnium-based FinFET is 3.52 times larger than the Silicon-based one when gate voltage is 1.0V. In addition, the on/off current ratio also raises from 3.9×10^5 to 1.5×10^6. These results show the excellent electrical properties of Hafnium-based FinFET. Besides, 2-dimensional Hafnium dioxide is simulated through VASP. Bulk hafnium dioxide is not ferroelectric, while 2-dimensioal Hafnium dioxide's ferroelectricity is shown in the simulation, which proves the significance of this material in Hafnium-based FinFET.

2. Methods

2.1. Ab-initio simulation of 2-dimensional Hafnium Dioxide

According to Q. Luo. et al[12], bulk Hafnium dioxide does not present ferroelectricity, but 2-dimensional Hafnium dioxide presents ferroelectricity because of $Pca2_1$ space group. STEM-HAADF and ABF technique is used to show the shift of oxygen atoms in hafnium dioxide, which intuitively confirms the non-centrosymmetric Pca21 structure in the hafnia ferroelectric material. Due to the fact that the inserted ferroelectric layer is about tens of nanometers thick, this kind of layer can be considered as 2-dimensional, which make it possible to use hafnium-based material as inserted layer which transit FinFET to NCFinFET.

Here, Density Functional Theory (DFT) is used to simulate the ferroelectric hysteresis loop implemented by Vienna Ab initio Simulation Package (VASP). The potential of electrons is considered as a unique functional of the electron density n(r) and the energy functional is derived [13].

$$E = \int v(r)n(r)dr + \frac{1}{2}\iint \frac{n(r)n(r\prime)}{|r-r\prime|} drdr' + T_s[n] + E_{xc}[n] \quad (1)$$

The DFT variational principle is then introduced which makes it possible for calculation.

Single layer structure is extracted from 2D material database and 3-layer structure is built through duplication in z-axis. Fig.1 shows the 3-layer hafnium dioxide structure, which is used in subsequent simulation. 3-layer model is used because the thickness is about 10 nanometers, which is an ideal inserted layer thickness. Electric field is exerted to examine the ferroelectricity, which will be discussed in detail in Result part.

Once the ferroelectricity of 2-dimentional hafnium dioxide is proved, hafnium dioxide layer can be inserted into FinFET to transit it to Negative Capacitance FinFET.

In order to understand of the mechanism of NCFET increasing SS, gate voltage divider capacitance C_{div} is given,

$$C_{div} = C_s + C_d + C_Q + C_{trap} + C_{dep} \quad (2)$$

in which C_s means source geometrical capacitance while C_d means drain geometrical capacitance. The quantum capacitance, interface capacitance and depletion capacitance are the last 3 terms on the right-hand side of this equation. And C_Q can be expressed,

$$C_Q = q^2 \sum_i \frac{DOS_i}{1+\exp\left(\frac{E_{c,i}-E_f}{kT}\right)} \quad (3)$$

where Fermi energy is expressed as E_f and $E_{c,i}$ is the energy level of i^{th} mode. In the Negative Capacitance FET, negative voltage drop occurs because of the negative C_NC, which reduces the Total gate voltage. According to W. Cao. et al [14], minimum SS without hysteresis is expressed,

$$SS_{min} = 60 \times \frac{C_Q}{C_Q + C_{div,<Vth}} \quad (4)$$

Considering this formula, lowering C_Q is a useful way to reduce SS_{min}. According to the relationship between DOS and C_Q, using low DOS material is a good choice. Inspired by this conclusion and the compatibility with CMOS, Hafnium dioxide is a suitable material to be used as inserted layer.

2.2. TCAD simulation of Hafnium-based FinFET

Silvaco TCAD is used to calculate the electric properties of this device. Normally there are two ways to insert ferroelectric layer: (a) connect ferroelectric layer directly towards the dielectric layer and (b)use a sandwich structure between the ferroelectric and dielectric layers. Here method (a) is used and Fig.2 shows the model built in Silvaco TCAD, whose results will be discussed in detail in Result part. Normally 2D simulation is enough for the survey, but when it comes to FinFET, the 3D fin makes it necessary to use 3D models and to include built-in Fermi Model.

3. Resulsts & Discussion

3.1. Ab-initio simulation of 2-dimensional Hafnium Dioxide

Bulk Hafnium does not present ferroelectricity. But when this material is very thin, which means only several layers in its z-axis, the ferroelectricity shows up. According to Q.Luo[12], the $Pca2_1$ phase of Hafnium Dioxide is the source of ferroelectricity. Here VASP is introduced to calculate the ferroelectricity of 2-dimensional Hafnium Dioxide.[15-24]. VASP, which is based on Density Functional Theory (DFT) theory, is highly reliable software to simulate and calculate atomic behavior.

In order to simulate the dipole moment of the Hafnium-dioxide layer inserted into FinFET, a model of 3-layer hafnium dioxide is built, which is showed in Fig.1. Considering the inserted layer is about several nanometer thick, 3 layers is a suitable case to study. Material Studio is used to copy the single-layer hafnium dioxide structure to build a multi-layer structure.

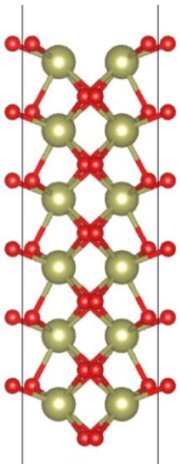


Figure 1. 3-layer Hafnium Dioxide structure before optimization

To reach a high-accuracy result, multiple structural optimizations is done using VASP. In structure optimization, atomic retardation and electron selection are nested, and in each step of atomic retardation, a limited force is applied to the atomic system, which determines how atoms move and how to optimize the positions of atoms. The atomic position is specified by using the quasi-Newton method or the conjugate gradient method, and the criterion for the convergence of the atomic relaxation is judged at the two positions before and after. Criteria for reaching atomic retardation stop retardation. In this process, if the parameters and convergence values are set properly, the atomic retardation can be made to reach the convergence standard within the maximum allowable number of steps, so that a relatively stable ground state structure of the system can be obtained. The convergence of atomic retardation and the convergence of electron self-consistent iteration need to be set to an appropriate value, so as to ensure that the system has reached a relatively stable state when the maximum number

of steps is reached, but the convergence value should not be too small, because it will increase the number of calculations. There are generally two choices for the criterion of structural relaxation: energy and force. The two are related, ideally, the energy should converge to the ground state, and the force should also converge to the equilibrium state. However, the difference in the numerical calculation process leads to a large difference in the convergence speed based on the two criteria, and the force convergence speed is generally slower than the energy convergence speed in most cases. This is because force calculations are performed on the basis of energy, and the first derivative of energy with respect to the coordinates gives the force. The increase in computation and the transfer of errors result in slow force convergence [25, 26]. The energy criterion of 10^{-6} eV is used here because the data that is ultimately required to be used is the magnetic dipole moment, which is related to energy. The following Fig.2 shows the optimized structure after 3 times optimization.

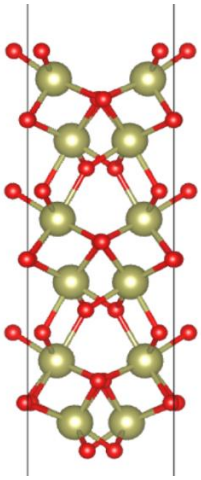


Figure 2. 3-layer Hafnium Dioxide structure after optimization

After optimization it comes to self-consistent calculation. Static self-consistent calculation is based on structural optimization, fixing the position coordinates of atoms when the system energy is low and the system is relatively stable, and then adjusting the electrons in the system to achieve the lowest energy of the system. Therefore, before the static self-consistent calculation, it is necessary to provide the lattice structure information of the relatively stable system, so that the Fermi level and the wave function of the electron in the ground state of the system can be completely calculated by electronic self-consistent calculation (that is, solving the Schrödinger equation through self-consistent iteration), charge density, etc. In this step of calculation, K-mesh is set to $5 \times 5 \times 1$ because it is a 2D structure. The EDIFF is set to 1×10^{-4} eV to reach a high accuracy.

Then, the non-self-consistent calculation is carried out after high-symmetry k points are found. Non-self-consistent calculation is to change parameters such as k point (regenerate k point) on the basis of self-consistency, select energy or potential function or electron density as the initial value according to different needs, and perform non-self-consistent iterative calculation, which can be used to solve DOS, Band or other properties such as optics. Fig.3 shows the band structure and the density of states of the 3-layer hafnium dioxide inserted layer.

Finally, electric field is exerted gradually towards the structure. And the ferroelectricity shows up in Fig.4 The electric field exerted on the material varies from 0 to $-0.01V/m$ then from $-0.01V/m$ to $0.01V/m$ and finally back to $-0.01V/m$, completing a whole loop of changes.

Fig.4 (a) is the experimental data extract from the simulation and the trend line of the ferroelectric loop is shown Fig.4 (b). Through Fig.4, the ferroelectric loop of this 3-layer hafnium dioxide inserted layer can be clearly identified, which, proves the correctness to use 2D Hafnium Dioxide to insert in the FinFET to reach Negative Capacity (NC), which is useful to reach higher Subthreshold Swing (SS).

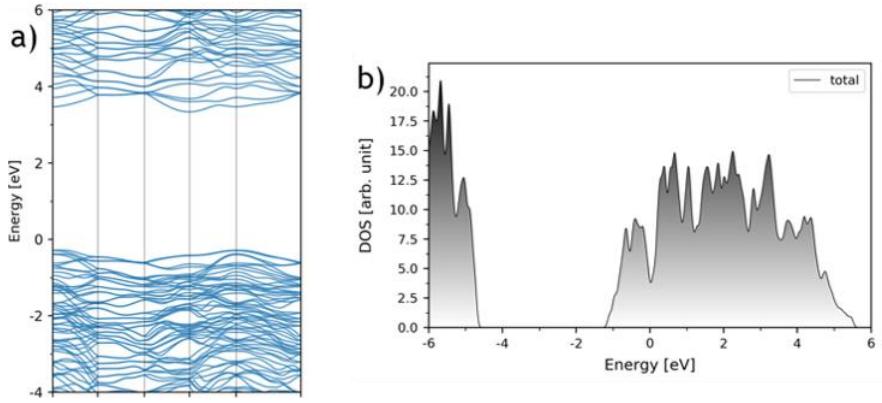


Figure 3. a) Band Structure of 2D Hafnium Dioxide b) DOS of 2D Hafnium Dioxide

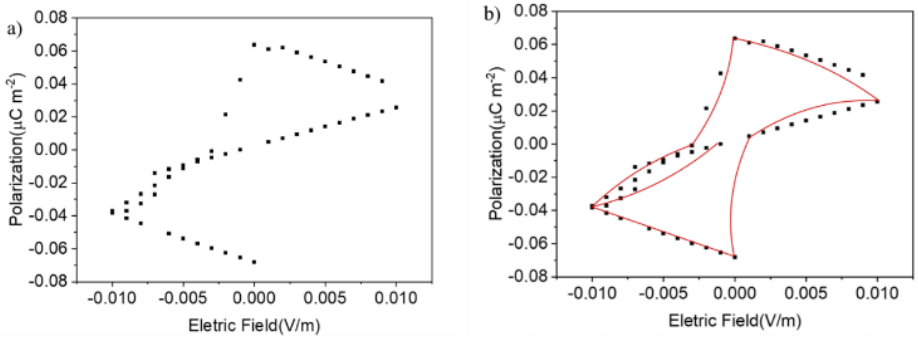


Figure 4. Polarization versus Voltage of 2D Hafnium Dioxide a) data distracted directly from simulation b) Original data and trend line of ferroelectric loop

3.2. TCAD simulation of Hafnium-based FinFET

Here Silvaco TCAD is used to do this simulation. The first step is to build the FinFET structure and the mesh. The basic structure is shown in Fig.5. The mesh is set denser in particular area to reach a more reliable result. A hafnium dioxide layer is set inside the model. And in order compare, a silicon dioxide model with the same shape parameter is also built.

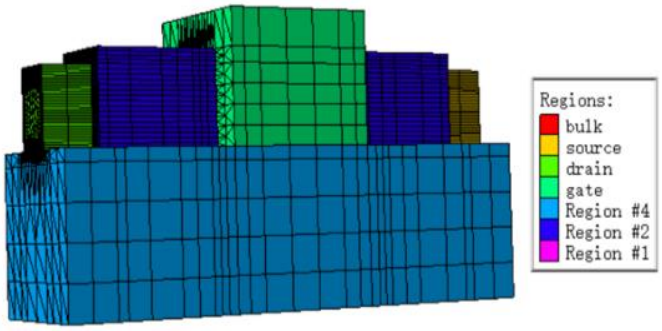


Figure 5. Model and mesh of FinFET built in TCAD

The plot of drain current versus gate voltage is shown in Fig.6. Through this simulation, it shows that the drain current of the Silicon-based FinFET is $7.41 \times 10^{-6}\ A$ when gate voltage is 1.0V, while it is $2.14 \times 10^{-6}\ A$ when it comes to Hafnium-based FinFET. And the drain current of Hafnium-based FinFET is 3.52 times larger than the Silicon-based one. In addition, the on/off current is 3.9×10^{5} in normal Silicon-based FinFET and this value rises to 1.5×10^{6} in hafnium dioxide inserted layer FinFET. These results show that the hafnium dioxide can not only make it possible for NCFinFET to be compatible to present production process, but also increase the performance of FinFET- steeper subthreshold swing and higher On/Off ratio.

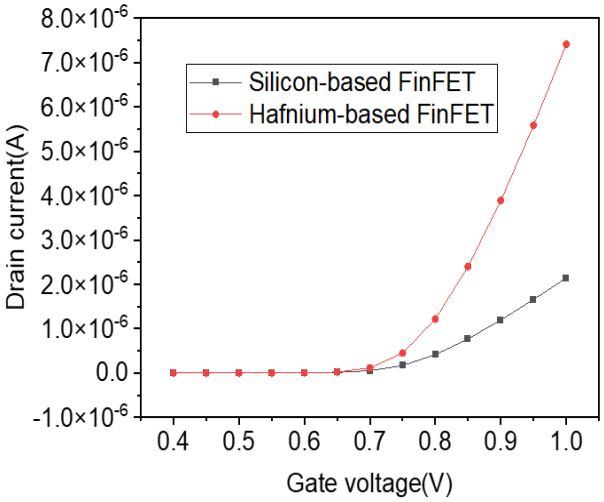
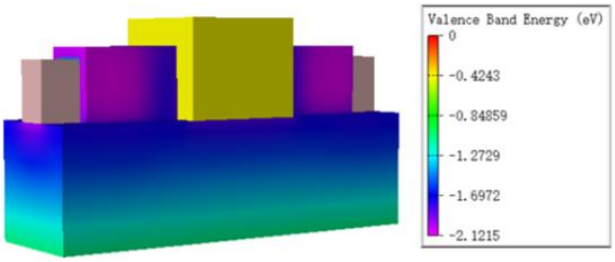


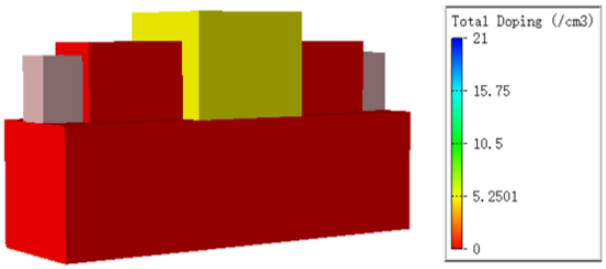
Figure 6. Drain current versus Gate voltage of Hafnium-based FinFET and Silicon-based FinFET

Other electric properties are also shown in Fig.7. Fig.7(a) shows the electric field distribution, Fig.7(b) shows the Valence Band Energy and Fig.7(c) shows the total doping.

(a)



(b)



(c)

Figure 7. Electric properties: a) Electric field distribution of Hafnium-based FinFET b) Valence band energy of Hafnium-based FinFET c) total doping of Hafnium-based FinFET

4. Conclusion

Using Silvaco TCAD to simulate the FinFET model shows the advantage of Negative Capacitance Hafnium-Based FinFET -high I_{on}/I_{off} ratio and steeper subthreshold swing. The result shows that the drain current of Hafnium-based FinFET is 3.52 times larger than the Silicon-based one when gate voltage is 1.0V. In addition, the on/off current ratio also raises from 3.9×10^5 to 1.5×10^6. Other electric properties, including electric field distribution, valence band energy and total doping of Hafnium-based FinFET are also shown in the previous discussion. In addition, the 2D hafnium dioxide inserted layer is also simulated to show the ferroelectricity by using VASP, which proves the correctness of using 2D Hafnium Dioxide inserted layer to reach Negative Capacity FinFET.

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