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Comparison of Atomic Level Simulation Studies of MOSFETs Containing Silica and Lantana Nanooxide Layers

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The intense downscaling of a Metal Oxide Semiconductor Field Effect Transistor (MOSFET) to nano range for improving the device performance requires a high-k dielectric material instead of conventional silica (SiO_2) as to avoid Quantum Mechanical Tunneling towards the gate terminal which leads to unnecessary gate current. Out of all the rare earth oxide materials, since lanthana (La_2O_3) has significantly high dielectric constant (*k*) and bandgap, we've chosen it as oxide layer for one of the MOSFETs. In this work, we simulated two MOSFETs – one with nano SiO_2 oxide layer and other with nano La_2O_3 oxide layer in the atomic level to analyze and compare the transmission spectra, I-V characteristics and Channel conductance of both the MOSFETs.

Keywords: MOSFET, Nano oxide layer, Quantum mechanical tunneling, Transmission spectra, I-V characteristics, Channel conductance.

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1. INTRODUCTION

The most important electronic device is a Complementary Metal Oxide Semiconductor (CMOS) transistor which has been widely used in all the electronic gadgets like cellular phones, digital computers, digital cameras, data processing systems, etc. For the fast performance of these electronic devices, the MOSFETs used to build them play a very prominent role and hence the downscaling of transistors has been started over a fifty year time span as per Moor's law of scaling which states that the number of devices on an integrated circuit increases exponentially with the time [1]. Out of all other components and layers present in a MOSFET, downscaling of oxide layer has lead to a large leakage current from source to gate regions due to Quantum Mechanical Tunnelling when the oxide layer is in nano range (especially for less than 1.4 nm) [2].

Since the conventional oxide layer material SiO_2 has the dielectric constant of 3.9 which is much less compared to other dielectric materials, it is replaced with lanthana (La_2O_3) in *n*-type MOSFET. The material La_2O_3 is chosen due to it's high dielectric constant (*k*) and significantly large bandgap [3]. In this work, two MOSFETs – one with nano silica oxide layer and other with nano lanthana oxide layer were atomically built in QuantumWise ATOMISTIX TOOLKIT (ATK) 12.8 version software package and were simulated for the analysis and comparison of Transmission spectra, I-V characteristics and conductance.

ATOMISTIX TOOLKIT (ATK) 12.8 version software package is commercially provided to the users all over the world in various research institutes and organizations. Using this software we've built two MOSFETs in atomic scale. The simulations are done using the combination of Density Functional Theory (DFT) and Non-Equilibrium Green's Function (NEGF) technique [4].

2. ATOMIC SCALE MODELING OF MOSFET

For modeling of *n*-type MOSFETs, silicon is selected as substrate, antimony (Sb) is selected for N-well and interfaced with silicon on either sides. Among the N-type materials (phosphorous, arsenic, antimony and bismuth), antimony (beta) possess a very strong adhesion with silicon (alpha) and it also have the advantage of high evaporating temperature compared to that of the others. For the MOSFET containing nano SiO_2 oxide layer, the SiO_2 is interfaced with antimony on the either side as shown in Fig. 1. Similarly for the other MOSFET containing nano La_2O_3 oxide layer, the La_2O_3 layer is interfaced on the upper side of the silicon which is interfaced with antimony on either sides as shown in Fig. 2. For each MOSFET, a metal contact is placed on the interfaced oxide layer and electrodes are placed on either side of the structure built for the electrical contacts of gate, source and drain. Now this completes the designing of both MOSFETs in atomic level.

The ATOMISTIX TOOLKIT software implements Non-Equilibrium Green's Function (NEGF) for simulation of MOSFET as it can handle strong external fields and electron – electron interactions are considered by infinite summations [5]. For the optimization of device geometry, the software implements Density Functional Theory (DFT) as it deals with multi – component systems with electronic pairing mechanism, molecular dynamics, etc. [6].

3. MATERIAL DETAILS

3.1 Silicon (Alpha)

1. Face Centered Cubic (FCC)
2. Lattice Constant, *a* = 5.4306 Å
3. Space Group: 227
4. Crystal System: Cubic

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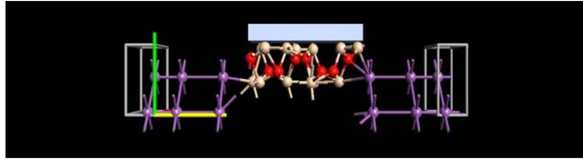

Fig. 1 – MOSFET built using SiO_2 oxide layer

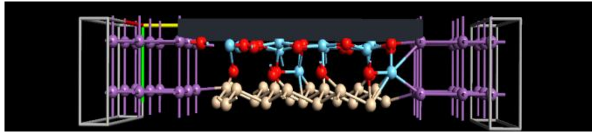

Fig. 2 – MOSFET built using La_2O_3 oxide layer

3.2 Antimony (Beta)

1. Simple Cubic
2. Lattice Constant, $a = 2.992$ Å
3. Space Group: 221
4. Crystal System: Cubic

3.3 Silica

1. Chemical Formula: SiO_2
2. Crystal System: Cubic
3. Lattice Constant, $a = 3.9299$ Å
4. Space Group: 205

3.4 Lanthana

1. Chemical Formula: La_2O_3
2. Crystal System: Hexagonal
3. Lattice Constants: a, $b = 4.057$ Å, $c = 6.430$ Å
4. Space Group: 194

4. RESULTS AND DISCUSSIONS

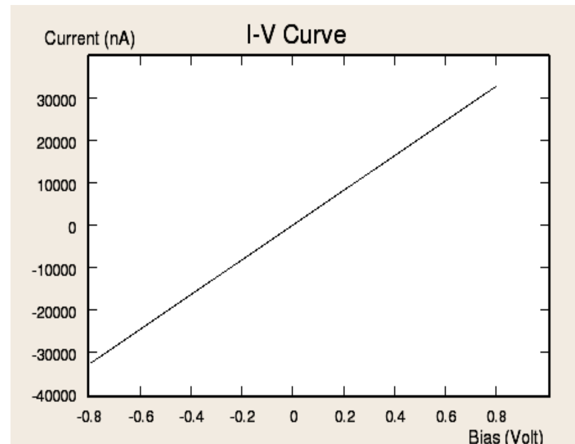

Fig. 3 – I-V Characteristics of MOSFET containing SiO_2 insulator layer

From the above figures (Fig. 3 and Fig. 4), for the same bias voltage i.e., 0.8 V, the source to drain current flow is higher for the MOSFET containing La_2O_3 oxide layer (66697.2 nA) compared to the MOSFET containing SiO_2 oxide layer (32897.7 nA).

From the above figures (Fig. 5 and Fig. 6), we can analyze that the electron transport between the source and drain electrodes is higher in MOSFET containing La_2O_3 insulator layer compared to that of MOSFET containing SiO_2 insulator layer. Here, the electron transport represents the sum of transmission

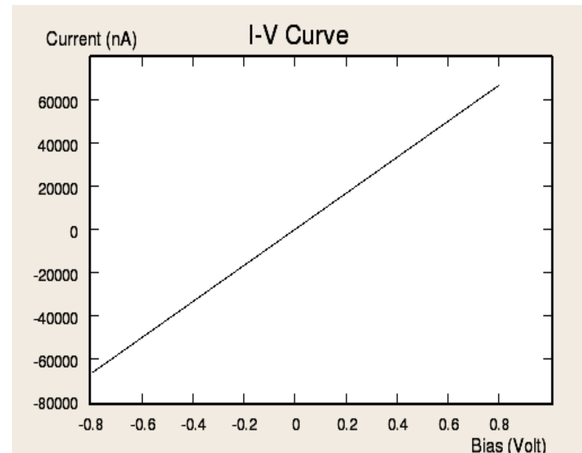

Fig. 4 – I-V Characteristics of MOSFET containing La_2O_3 insulator layer

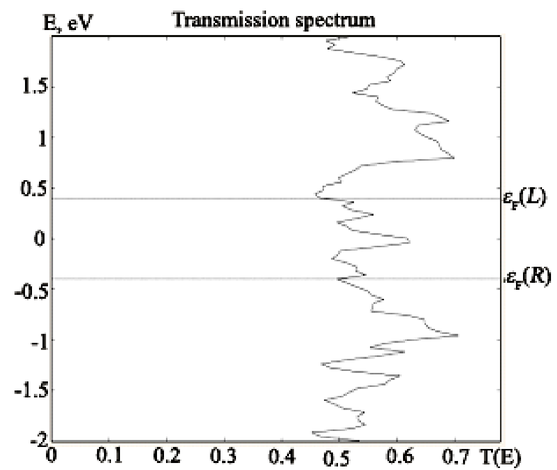

Fig. 5 – Transmission spectrum of the MOSFET using SiO_2 insulator layer along with Fermi levels of the electrodes

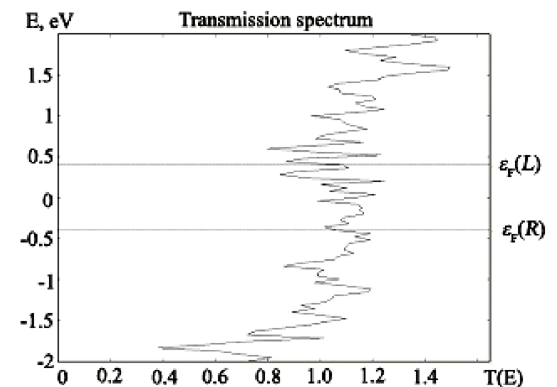

Fig. 6 – Transmission spectrum of the MOSFET using La_2O_3 insulator layer along with Fermi levels of the electrodes

probabilities of the electrons in the complete molecular system. The sum of transmission probabilities between the electrodes is less for the SiO_2 oxide layer MOSFET due to the Quantum Mechanical Tunneling effect occurring at the oxide layer when the thickness of the oxide layer is less than approximately 1.5 nm. When the oxide layer is scaled to nano level, the energy bands

become more discrete and close to each other and hence the electrons which are ought to travel from drain to source tunnel towards the gate terminal which often leads to unnecessary gate current. This tremendously effects the power consumption and switching speed of the MOSFET. When nano SiO_2 is used as oxide layer, the tunneling (leakage) current is too large exceeding 1 A/cm^2 for 1 V gate voltage and hence the electron transport is less between the electrodes (from Fig. 5). The maximum transmission between the electrodes for the MOSFET containing SiO_2 insulator layer is 0.62 but for the other MOSFET the maximum transmission between the electrodes is 1.24 which is much larger compared to the MOSFET containing SiO_2 oxide layer. This implies that electron transport from drain to source has increased in MOSFET containing La_2O_3 oxide layer which is desirable.

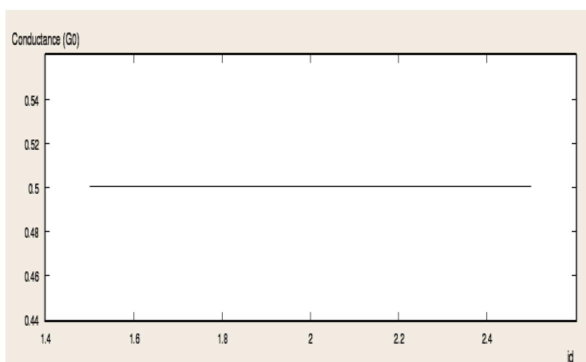

Fig. 7 – Conductance vs drain current for MOSFET containing SiO_2 oxide layer

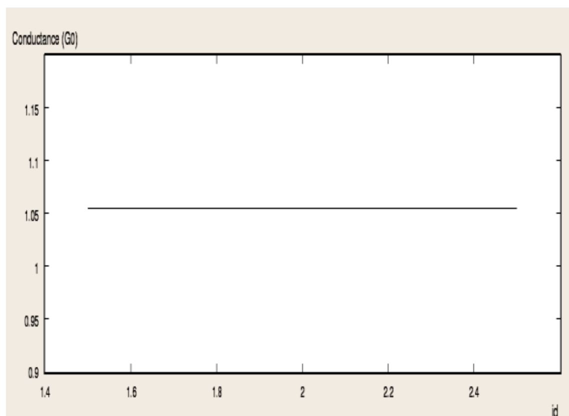

Fig. 8 – Conductance vs Drain current for MOSFET containing La_2O_3 oxide layer

From the above figures (Fig. 7 & Fig. 8), we can analyze that the channel conductance (G0) in the MOSFET containing La_2O_3 oxide layer (1.05 S) is increased compared to that of the other (0.5 S).

The conductance in the molecular system is given by Landauer formula which is given by,

$$G(E) = G_0 \sum T_n(E),$$

where G indicates electrical conductance, G_0 is given by $e^2 / \pi\hbar \sim 7.75 \times 10^{-5}℧$ and is referred as 'Quantum Conductance'. $T_n(E)$ indicates the transmission eigen values and E indicates the energy of electrons. The electron transition rate is given by,

$$\Gamma(E_{b,a}) = 2\pi / (\hbar)^2 \, | V |^2 \, \rho(E_{b,a}),$$

where $E_{b,a}$ indicates the energy of electron which goes from state a to state b when a potential V is applied to the atom. ρ indicates the charge density of the corresponding electron.

For the first transition of an electron, the transmission probability is given by,

$$T(E) = \Gamma_{1L}(E)\Gamma_{1R}(E) / ((E - E_1)^2 + (\Gamma_1(E) / 2)^2)$$

(maximum = 1).

The relation between conductance and transmission probability is given by,

$$G = (e^2 / \pi\hbar) T(E)$$

5. CONCLUSION

In this paper, comparison between MOSFETs using nano SiO_2 and La_2O_3 oxide layers is done by simulating both the MOSFETs using ATOMISTIX TOOLKIT. From the simulation results, we can conclude that the MOSFET containing nano La_2O_3 oxide layer is showing high output current, high channel transmission and high channel conductance. The output i.e., the drain current of La_2O_3 contained MOSFET is increased by a value of 67.871 % compared to that of nano SiO_2 contained MOSFET. The major device aging problems including Hot-Carrier Injection (HCI) and Positive Bias Temperature Instability (PBTI) for n-type MOSFETs can be enormously reduced. Hence we conclude that nano La_2O_3 oxide layer contained MOSFET is efficient compared to nano SiO_2 oxide layer contained MOSFET.

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