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Hole Tunnel Currents in TiN/HfSiO$_x$N/SiO$_2$/p-Si(100) MOS Capacitors

Khairurrijal[1], Fatimah A. Noor[1], Mikrajuddin Abdullah[1], Sukirno[1], Akio Ohta[2], and Seiichi Miyazaki[2]

[1]Physics of Electronic Materials Res. Div., Fac. of Math. & Natural Sci., Institut Teknologi Bandung
Jalan Ganesa 10, Bandung 40132, Indonesia
Phone: +62-22-250-0834 E-mail: krijal@fi.itb.ac.id
[2]Graduate School of Advanced Sciences of Matter, Hiroshima University
1-3-1 Kagamiyama, Higashi-Hiroshima 739-8530, Japan

1. Introduction

Silicon-based metal-oxide-semiconductor field effect transistors (MOSFETs) that are continuously scaled down to the sub-micrometer regime and below to enhance speed, to increase density, and to lower operation voltage cause the shrinking of the SiO$_2$ gate-dielectric thickness down to sub-nm region [1]. When the SiO$_2$ gate-dielectric thickness is less than 1.5 nm, considerable leakage current occurs and power dissipation becomes significantly high [2]. Hf-based silicates, which are high dielectric constant (k) materials, are more promising to replace SiO$_2$ due to high thermal stability, improved threshold instability, good leakage characteristics and low mobility degradation [3]. Noting that an ultrathin interfacial SiO$_2$ often forms during the fabrication process, a gate oxide expected to substitute SiO$_2$ is a stack of ultrathin SiO$_2$ and Hf-based silicate layers.

Very recently, electron tunnel current in SiO$_2$/high-k-based MOS capacitors have been theoretically studied under an anisotropic mass approach and with considering a coupling effect between transverse and longitudinal motions [4] following a model developed for a SiGe-based heterojunction bipolar transistor [5]. This model has been applied to TiN/HfSiO$_x$N/SiO2/p-Si(100) MOS capacitors. It has been found that the measured tunnel currents are well fitted by the calculated ones only for high oxide voltages. In addition, it is suggested that, for low oxide voltages, the measured currents are contributed by holes tunneling from the p-Si substrate [6,7].

Here, we present hole tunnel currents in the TiN/HfSiO$_x$N/SiO2/p-Si(100) MOS capacitors calculated by using the model. The calculated tunnel currents are compared to the measured ones. The hole effective mass in the HfSiO$_x$N will be discussed.

2. Theoretical Model

An energy band diagram of a TiN/HfSiO$_x$N/SiO$_2$/p-Si MOS capacitor in a flatband condition is shown in Fig. 1.(a). Here, the metal work function φ_m is 4.50 eV, the electron affinity of Si χ is 4.03 eV, E_c and E_v are the conduction and valence bands of Si, respectively, and E_{Fs} is the Fermi level of Si, and $E_{g,a}$, $E_{g,b}$, and $E_{g,S}$ are the band gaps of HfSiO$_x$N, SiO$_2$, and Si, respectively. E_{cm} and E_{cs} are the conduction band edges of TiN and Si, respectively. The valence band differences between HfSiO$_x$N and Si, SiO$_2$ and Si are $\Phi_{a,h}$= 2.60 eV, $\Phi_{b,h}$= 4.43 eV, respectively. The difference between the Si valence band and the TiN conduction band is Γ= 0.59 eV. All the values were obtained from measurement [7]. Figure 1.(b) gives a potential profile under the application of a negative bias to the TiN metal gate.

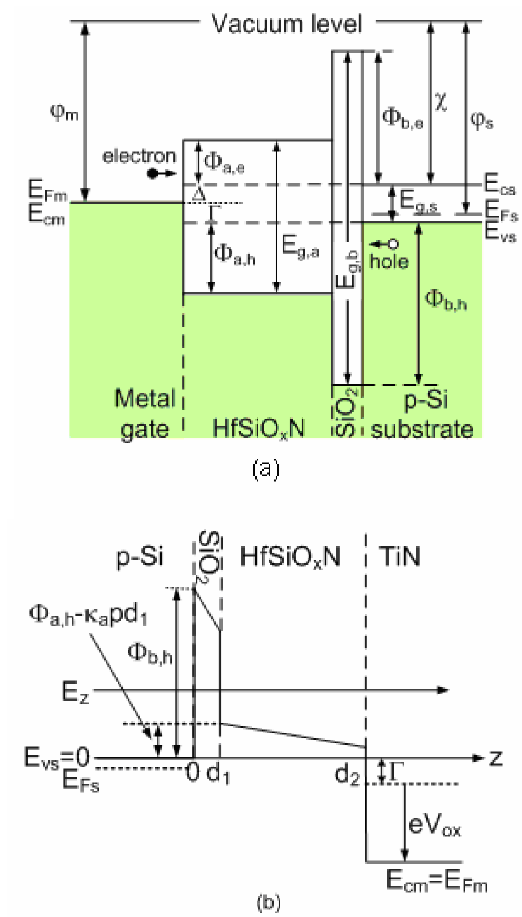

Fig. 1.(a) Energy band diagram of a TiN/HfSiO$_x$N/SiO$_2$/p-Si MOS capacitor and (b) a potential profile for holes tunneling from p-Si into TiN.

Using a simple electrostatic analysis, the potential profile shown in Fig. 1.(b) is mathematically expressed as

$$V(z)=\begin{cases}0 & z<0\\ \Phi_{b,h}-\kappa_a pz & 0\le z<d_1\\ \Phi_{a,h}+pd_1(\kappa_b-\kappa_a)-\kappa_b pz & d_1\le z<d_2\\ -(eV_{ox}+\Gamma) & z\ge d_2,\end{cases} \quad (1)$$

where $p = \dfrac{eV_{ox}}{\kappa_a(d_2 - d_1) + \kappa_b d_1}$, e is the electronic charge, V_{ox} is the oxide voltage which is the voltage across the barrier, d_1 and (d_2-d_1) are the thicknesses of $HfSiO_xN$ and SiO_2, respectively, and κ_a and κ_b are the dielectric constants of $HfSiO_xN$ and SiO_2, respectively.

3. Calculated Results and Discussion

We used the following parameters to calculate hole tunnel currents. The dielectric constants of $HfSiO_xN$ and SiO_2 are 13.5 and 3.9. The hole effective masses in the TiN metal gate and SiO_2 are considered to be isotropic and taken as m_0 and 0.8 m_0. The hole effective mass in the Si substrate is 0.29 m_0 [8]. The hole effective mass in the $HfSiO_xN$ layer, m_h, and the substrate hole velocity, v_h, are the only two parameters to compare the measured tunnel currents with the theoretical ones. The results are given in Fig. 2. The calculated tunnel currents fit well the measured ones.

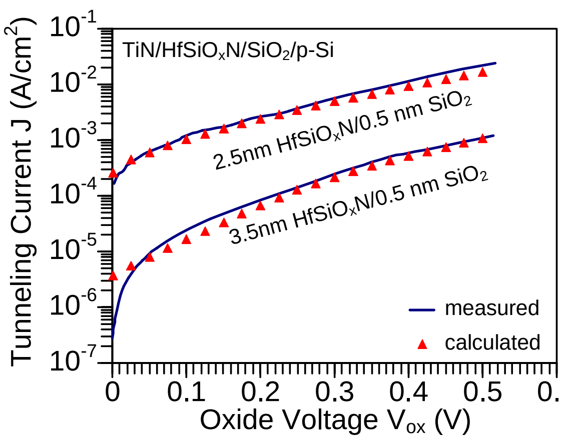

Fig. 2. Measured and calculated hole tunnel current densities in TiN/HfSiOxN/SiO2/p-Si(100) MOS capacitors.

The fitted values of m_h and v_h are 0.27 m_0 and 1×10^5 m/s, respectively, for the 2.5 nm-thick $HfSiO_xN$ layer. For the 3.5 nm-thick $HfSiO_xN$ layer the fitted values of m_h and v_h are 0.165 m_0 and 1×10^5 m/s, respectively. These results suggest that the hole effective mass in the $HfSiO_xN$ layer tends to increase as the $HfSiO_xN$ thickness decreases. This finding is also observed for ultrathin SiO_2 layer as reported in Refs. [9] and [10].

From the fitting process, it was found that the substrate hole velocity is 1×10^5 m/s independent of the $HfSiO_xN$ thickness.

4. Conclusions

The hole tunnel current in the $TiN/HfSiO_xN/SiO_2$/p-Si(100) MOS capacitor has been studied theoretically. It has been shown that the theoretical tunnel current densities fit to the measured ones by employing the hole effective mass in the $HfSiO_xN$ layer and the substrate hole velocity as fitting parameters. It has been found that the hole effective mass in the $HfSiO_xN$ tends to increase with decreasing the $HfSiO_xN$ thickness and the substrate hole velocity is 10^5 m/s.

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