Hole Tunnel Currents in TiN/HfSiO\textsubscript{x}N/SiO\textsubscript{2}/p-Si(100) MOS Capacitors

Khairurrijal\textsuperscript{1}, Fatimah A. Noor\textsuperscript{1}, Mikrajuddin Abdullah\textsuperscript{1}, Sukirno\textsuperscript{1}, Akio Ohta\textsuperscript{2}, and Seiichi Miyazaki\textsuperscript{2}

\textsuperscript{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

\textsuperscript{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\textsubscript{2} gate-dielectric thickness down to sub-nm region [1]. When the SiO\textsubscript{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\textsubscript{2} due to high thermal stability, improved threshold instability, good leakage characteristics and low mobility degradation [3]. Noting that an ultrathin interfacial SiO\textsubscript{2} often forms during the fabrication process, a gate oxide expected to substitute SiO\textsubscript{2} is a stack of ultrathin SiO\textsubscript{2} and Hf-based silicate layers.

Very recently, electron tunnel current in SiO\textsubscript{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\textsubscript{x}N/SiO\textsubscript{2}/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\textsubscript{x}N/SiO\textsubscript{2}/p-Si MOS capacitors calculated by using the model. The calculated tunnel currents are compared to the measured ones. The hole effective mass in the HfSiO\textsubscript{x}N will be discussed.

2. Theoretical Model

An energy band diagram of a TiN/HfSiO\textsubscript{x}N/SiO\textsubscript{2}/p-Si MOS capacitor in a flatband condition is shown in Fig. 1.(a). Here, the metal work function \( \phi_m \) is 4.50 eV, the electron affinity of Si \( \chi \) is 4.03 eV, \( E_c \) and \( E_v \) are the conduction and valence bands of Si, respectively, and \( E_{F_S} \) is the Fermi level of Si, and \( E_{g,a} \), \( E_{g,b} \), and \( E_{g,S} \) are the band gaps of HfSiO\textsubscript{x}N, SiO\textsubscript{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\textsubscript{x}N and Si, SiO\textsubscript{2} and Si are \( \Phi_{a,h}=2.60 \text{ eV} \), \( \Phi_{b,h}=4.43 \text{ eV} \), respectively. The difference between the Si valence band and the TiN conduction band is \( \Gamma=0.59 \text{ eV} \). 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.

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

\[
V(z) = \begin{cases} 
0 & z < 0 \\
\Phi_{p,h} - \kappa_p z & 0 \leq z < d_1 \\
\Phi_{p,h} + pd_1 (\kappa_p - \kappa_s) - \kappa_s z & d_1 \leq z < d_2 \\
-(eV_{cm} + \Gamma) & z \geq d_2,
\end{cases}
\] (1)

Fig. 1.(a) Energy band diagram of a TiN/HfSiO\textsubscript{x}N/SiO\textsubscript{2}/p-Si MOS capacitor and (b) a potential profile for holes tunneling from p-Si into TiN.
where \( p = \frac{eV_{ox}}{\kappa^o(d^2 - d^1) + \kappa^s d^1} \), \( e \) 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\(_x\)N and SiO\(_2\), respectively, and \( \kappa^o \) and \( \kappa^s \) are the dielectric constants of HfSiO\(_x\)N and SiO\(_2\), respectively.

3. Calculated Results and Discussion

We used the following parameters to calculate hole tunnel currents. The dielectric constants of HfSiO\(_x\)N 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\(_x\)N 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/HfSiO\(_x\)N/SiO\(_2\)/p-Si(100) MOS capacitors.](image)

The fitted values of \( m_h \) and \( v_h \) are 0.27 \( m_0 \) and \( 1 \times 10^5 \) m/s, respectively, for the 2.5 nm-thick HfSiO\(_x\)N layer. For the 3.5 nm-thick HfSiO\(_x\)N layer the fitted values of \( m_h \) and \( v_h \) are 0.165 \( m_0 \) and \( 1 \times 10^5 \) m/s, respectively. These results suggest that the hole effective mass in the HfSiO\(_x\)N layer tends to increase as the HfSiO\(_x\)N 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 \( 1 \times 10^5 \) m/s independent of the HfSiO\(_x\)N thickness.

4. Conclusions

The hole tunnel current in the TiN/HfSiO\(_x\)N/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\(_x\)N layer and the substrate hole velocity as fitting parameters. It has been found that the hole effective mass in the HfSiO\(_x\)N tends to increase with decreasing the HfSiO\(_x\)N thickness and the substrate hole velocity is \( 10^5 \) m/s.

Acknowledgements

One of the authors (F.A.N) would like to thank the Habibie Center Foundation, Indonesia, for the domestic doctoral scholarship at Institut Teknologi Bandung. The authors would like to acknowledge Drs. H. Murakami and S. Higashi of the Graduate School of Advanced Sciences of Matter, Hiroshima University for their arrangement to make electrical measurements. The authors also wish to thank the members of the research project “High-k Network” to characterize the samples prepared by Drs. T. Kawahara and K. Torii and Y. Nara in Semiconductor Leading Edge Technologies, Inc. (Selete), Japan.

References