

Evidence for a Very Small Tunneling Effective Mass ($0.03m_0$) in MOSFET High- k (HfSiON) Gate Dielectrics

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Abstract—We have recently conducted experimental and modeling tasks on TaC/HfSiON/SiON n-type MOSFETs, leading to an effective mass of $0.03m_0$ for 2-D electrons tunneling in high- k HfSiON dielectrics. In this letter, we present extra evidence obtained from complementary MOSFETs undergoing the same TaC/HfSiON/SiON processing, which shows that such a very small tunneling effective mass is existent not only for 3-D electrons but also for 2-D holes. This new finding is very important because it can substantially enhance the current understanding of gate tunneling leakage suppression in metal-gate high- k MOSFETs.

Index Terms—Effective mass, effective oxide thickness (EOT), HfO₂, HfSiON, high- k , metal gate, MOSFETs, tunneling.

I. INTRODUCTION

HIGH- k GATE dielectrics are currently largely employed in advanced MOSFET manufacturing. Thus, understanding the fundamental properties of high- k dielectrics is crucial. Relative to conventional SiO₂ and SiON counterparts, high- k dielectrics feature two fundamentally distinct properties: a narrower energy bandgap and a lower optical phonon energy [1]. Concerning electrons or holes tunneling in high- k dielectrics, their tunneling effective masses should, in principle, differ fundamentally from those of gate oxide. More recently, we have conducted experimental and modeling tasks on TaC/HfSiON/SiON n-MOSFETs and found that 2-D electrons in a HfSiON dielectric have a tunneling effective mass of around $0.03m_0$ [2]. This value is quite unusual because it is far below that of gate oxide and is the smallest of high- k dielectrics to date. On the other hand, a countertrend with increasing effective oxide thickness (EOT) was experimentally observed [3]–[5]: HfO₂ gate tunneling leakage with respect to the SiO₂ one does not decrease as intuitively expected. To elucidate this, an intermixing action between a high- k dielectric and an interfacial layer was proposed [3], [4]; however, tunneling effective masses as responsible origins were not mentioned there.

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The aim of this letter is to provide extra evidence to confirm the existence of a very small tunneling effective mass and make it one of the fundamental properties of the high- k HfSiON dielectric. In a sense, the current understanding of the observed gate tunneling leakage suppression [3]–[5] is able to be significantly enhanced.

II. EXPERIMENT

TaC/HfSiON/SiON n- and p-MOSFETs were fabricated in a manufacturing process detailed elsewhere [6]. A TEM picture of the underlying TaC/HfSiON/SiON/Si system is shown in Fig. 1. The corresponding energy band diagram is together plotted for a p-MOSFET in flatband condition. All relevant material and process parameters are labeled in Fig. 1, along with the corresponding values. By performing a quantum mechanical numerical fitting of gate capacitance C_g - V_g measured from the p-MOS device in inversion, we obtained TaC work function = 4.48 eV, EOT = 1.5 nm, and n-type substrate doping concentration = 1×10^{17} cm⁻³. Evidently, the p-MOS gate stack is slightly larger than the n-MOS one (1.4 nm) [2]. We attributed this to the different nitrogen concentrations encountered. To meet the same EOT (1.5 nm), ϵ_{IL} in the interface layer (IL) was changed to $6.2\epsilon_0$. The corresponding φ_{ILC} and φ_{ILV} were 2.54 and 3.06 eV, respectively [7].

The carrier separation method in inversion condition was employed. The measured terminal currents are shown in Figs. 2 and 3 for n- and p-MOSFETs, respectively. Fig. 2 reveals the following: 1) The source/drain current $I_{S/D}$ dominates the gate current I_g due to 2-D electron tunneling, and 2) owing to 3-D valence-band electron tunneling to the gate, separated holes flow down the substrate and constitute the substrate current I_b . In the inset of the figure, the carrier separation measurement setup is shown. In Fig. 3, one can see that I_g comprises two distinct components: 1) $I_{S/D}$ due to hole tunneling from the inversion layer and 2) I_b due to 3-D electron tunneling from the metal side. In Fig. 3, we inserted experimental C_g - V_g for p-MOSFET in inversion, along with the aforementioned curve fitting. The corresponding energy band diagrams and tunneling paths are shown in Fig. 4.

III. CALCULATION AND FITTING

A quantum gate tunneling simulator [2], [8] was used. Given the known material and process parameters ($m_k^* = 0.03m_0$,

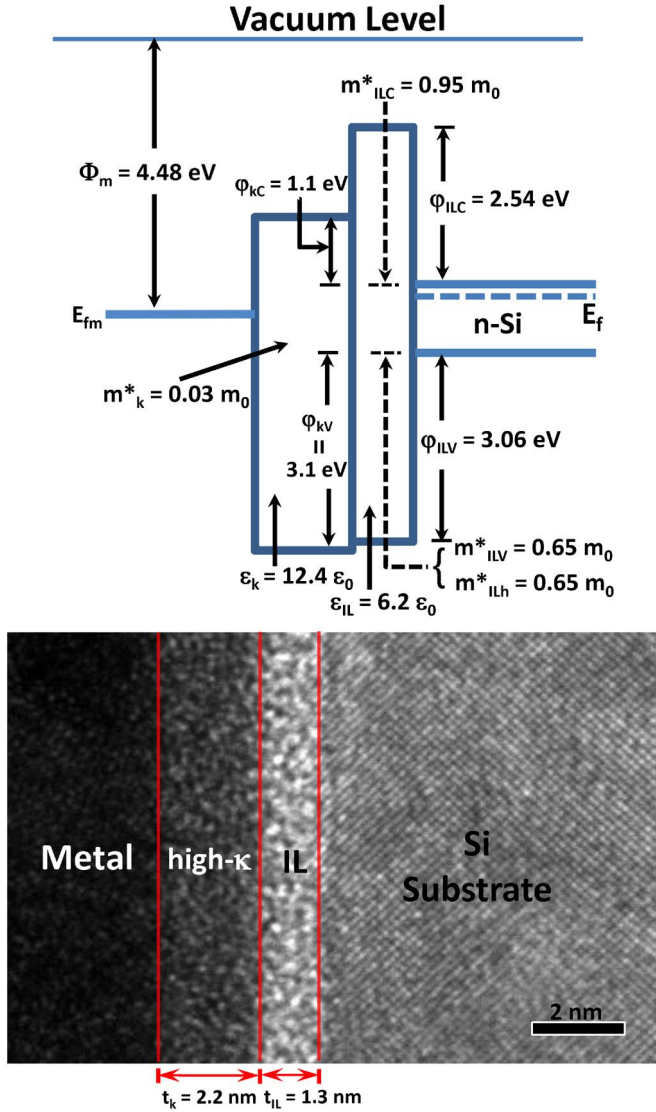


Fig. 1. Schematic of the energy band diagram in a metal-gate/high- k /IL/Si system for a p-MOSFET in flatband condition, along with a high-resolution TEM picture. The relevant material and process parameters are as follows: 1) the TaC metal work function Φ_m ; 2) for the HfSiON high- k part, its physical thickness t_k , permittivity ϵ_k , tunneling effective mass m_k^* , conduction-band offset φ_{kC} , and valence-band offset φ_{kV} ; and 3) for the SiON IL part, its physical thickness t_{IL} , permittivity ϵ_{IL} , conduction-band electron tunneling effective mass m_{ILC}^* , valence-band electron tunneling effective mass m_{ILV}^* , hole tunneling effective mass m_{ILh}^* , conduction-band offset φ_{ILC} , and valence-band offset φ_{ILV} .

$\varphi_{kC} = 1.1$ eV, $\epsilon_k = 12.4\epsilon_0$, $m_{ILC}^* = 0.95m_0$, $\epsilon_{IL} = 7\epsilon_0$, and $\varphi_{ILC} = 2.36$ eV [2], the calculated $I_{S/D}$ of the n-MOSFET and, hence, its $d\ln(I_g)/dV_g$ are shown in Fig. 2. The opposite tunneling case, namely the I_b of the p-MOSFET in inversion, should encounter the same tunneling parameters. To testify to this, we quoted an existing formula [9], and thereby, the underlying I_b can be written as

$$I_b = \frac{4\pi q m_M^*}{h^3} \int_0^{E_{\max}} ET_{\text{WKB}}(E) dE \quad (1)$$

where m_M^* ($= 1.0m_0$) is the metal electron mass; E is the allowed electron energy, as shown in Fig. 4 for the p-MOSFET,

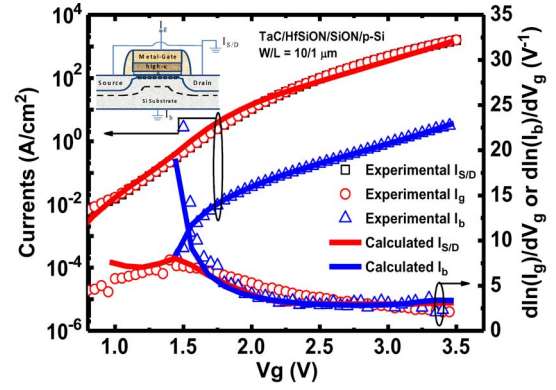


Fig. 2. (Symbols) Experimental I_g , $I_{S/D}$, and I_b , as well as the corresponding $d\ln(I_g)/dV_g$ and $d\ln(I_b)/dV_g$, plotted versus V_g for n-MOSFET in inversion. The (lines) calculated results are given. For $I_{S/D}$ calculation, $\varphi_{kC} = 1.1$ eV, $\varphi_{ILC} = 2.36$ eV, $m_k^* = 0.03m_0$, $m_{ILC}^* = 0.95m_0$, and $\epsilon_{IL} = 7\epsilon_0$. For I_b calculation, $m_k^* = 0.03m_0$, and $m_{ILV}^* = 0.65m_0$. The inset schematically shows the current separation measurement.

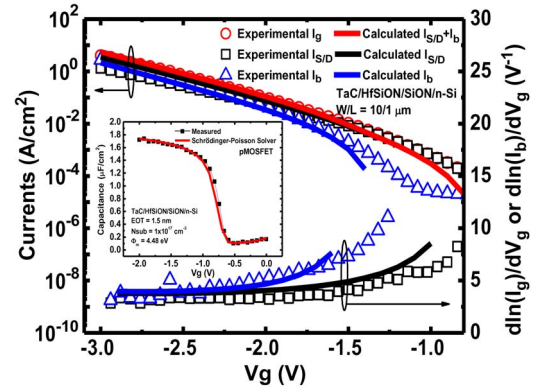


Fig. 3. (Symbols) Experimental I_g , $I_{S/D}$, and I_b , as well as the corresponding $d\ln(I_{S/D})/dV_g$ and $d\ln(I_b)/dV_g$, plotted versus V_g for p-MOSFET in inversion. The (lines) calculated results are given. For I_b calculation, $\varphi_{kC} = 1.1$ eV, $\varphi_{ILC} = 2.54$ eV, $m_k^* = 0.03m_0$, and $m_{ILC}^* = 0.95m_0$. For $I_{S/D}$ calculation, $\varphi_{kV} = 3.1$ eV, $\varphi_{ILV} = 3.06$ eV, $m_k^* = 0.03m_0$, and $m_{ILh}^* = 0.65m_0$. The inset shows a comparison of the (symbol) experimental and (line) simulated C_g versus V_g for TaC/HfSiON/SiON-gate-stack p-MOSFET in inversion.

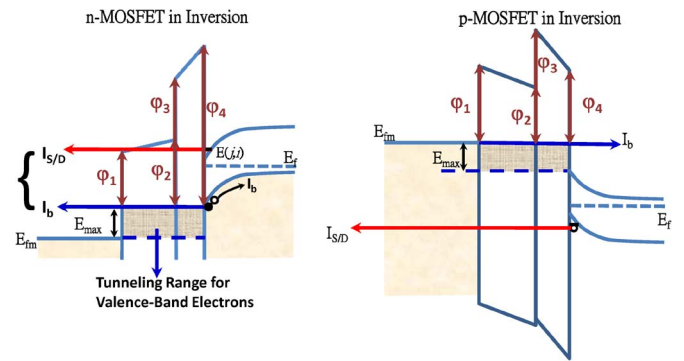


Fig. 4. Schematics of the energy band diagrams and tunneling paths for n- and p-MOSFETs.

for tunneling between metal Fermi level and conduction-band energy at the Si/IL interface; and E_{\max} is the corresponding energy difference. The WKB transmission probability T_{WKB} in (1) can make use of existing analytic expressions (i.e., [2, eq. (2)]) as long as the tunneling criteria (i.e., φ_1 , φ_2 , φ_3 , and

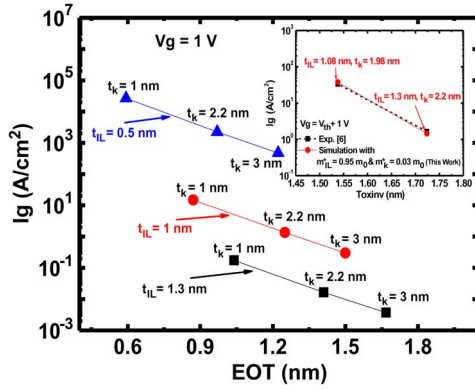


Fig. 5. Simulated I_g due to electron tunneling from the inversion layer versus EOT with t_{IL} as a parameter. The corresponding t_k values are labeled. The material parameters used in the simulation are the same as those in Fig. 2. The inset shows a comparison of the simulated I_g with experimental values [6] in the same TaC/HfSiON/SiON process, plotted versus electrical gate oxide thickness in inversion. V_{th} is the threshold voltage.

φ_4 therein) are modified according to the energy band diagram in Fig. 4. Strikingly, the resulting I_b appears to match the experimental data well, as shown in Fig. 3. This was achieved without changing any parameters.

Next, the values of $m_k^* = 0.03m_0$ and $m_{ILV}^* = 0.65m_0$ were drawn from a fitting of the experimental I_b of the n-MOSFET in inversion. This was done by using (1) but with the following changes: m_M^* was replaced by a valence-band electron effective mass of $0.65m_0$ [9], E_{max} was redefined as the difference between metal Fermi level and silicon valence-band edge, and the corresponding criteria (φ_1 , φ_2 , φ_3 , and φ_4) for T_{WKB} were altered, in accordance with the energy band diagram in Fig. 4. The fitting quality is fairly good, as shown in Fig. 2.

Physically speaking, m_{ILh}^* in IL should be equal or close to m_{ILV}^* . In this work, we made $m_{ILh}^* = 0.65m_0$. To calculate the hole tunneling component $I_{S/D}$ of the p-MOSFET, a hole tunneling simulator [8] was utilized. T_{WKB} can be easily modified accordingly. Then, a comparison of the calculated $I_{S/D}$ with the experimental one led to $\varphi_{kV} = 3.1$ eV. As shown in Fig. 3, good fitting holds again.

IV. DISCUSSION

To see the individual effects of varying t_k and t_{IL} , we show in Fig. 5 the simulated I_g due to electron tunneling from the inversion layer, plotted versus EOT for three t_{IL} values. The simulation points are also labeled with corresponding t_k . In addition, the simulated I_g was found to match existing data in the same manufacturing process [6], as shown in the inset of the figure for two different combinations of t_k and t_{IL} .

From Fig. 5, we can see the following: 1) the gate leakage increases with decreasing EOT, in agreement with [3]–[5], and 2) an increase in t_{IL} can suppress I_g more significantly than t_k . We also show in Fig. 5 that reducing t_{IL} will seriously increase I_g until it is intolerably high. This seems to be inconsistent with recent experiments [5]: I_g through HfO₂ is tolerable even for the case of t_{IL} approaching zero. However, one of the fundamental differences should be kept in mind: HfO₂

permittivity is higher than that of HfSiON, and as a consequence of maintaining the same EOT, the HfO₂ dielectric is much thicker. Indeed, this is the fact since a fair comparison of experimental I_g between HfSiON and HfO₂ has been published in the literature [6].

As corroborated earlier, a fundamental very small tunneling effective mass is existent. In this sense, a tunneling effective mass point of view is able to enhance current understanding of the observed I_g suppression [3], [4]. First, the HfO₂ dielectric is featured by a very small m_k^* while the interfacial layer can have a much higher m_{IL}^* . Next, as stated in [3] and [4], extra annealing treatments increase t_{IL} while simultaneously making more hafnium atoms appear in the regrown interfacial layer. Thus, the corresponding m_{IL}^* is likely to be lowered according to this work. Consequently, the gate leakage suppression ability relative to the SiO₂ gate oxide is degraded, as experimentally observed [3], [4].

V. CONCLUSION

Characterization and modeling of gate tunneling components of TaC/HfSiON/SiON complementary MOSFETs in inversion have been carried out. A fundamental tunneling effective mass featuring a very small value has been corroborated in the HfSiON dielectric. Current understanding of gate leakage suppression has been substantially enhanced.

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