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Determination of Physical Parameters for $HfO_2/SiO_x/TiN$ MOSFET Gate Stacks by Electrical Characterization and Reverse Modeling

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Outline of Talk

- *Introduction*
- *Details of Experimental Samples*
- *Simulation Model for I-V Response*
- *MOS: Experimental and Simulated I-V*
- *MOS: Experimental and Simulated C-V*
- *MOSFET: Experimental and Simulated I-V*
- *Conclusions*
- *Acknowledgements*

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Introduction

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TABLE I. Comparison of relevant properties for high-κ candidates.

Material	Dielectric constant (κ)	Band gap E_G (eV)	ΔE_C (eV) to Si	Crystal structure(s)
SiO_2	3.9	8.9	3.2	Amorphous
Si_3N_4	7	5.1	2	Amorphous
Al_2O_3	9	8.7	2.8[a]	Amorphous
Y_2O_3	15	5.6	2.3[a]	Cubic
La_2O_3	30	4.3	2.3[a]	Hexagonal, cubic
Ta_2O_5	26	4.5	1–1.5	Orthorhombic
TiO_2	80	3.5	1.2	
HfO_2	25	5.7	1.5[a]	
ZrO_2	25	7.8	1.4[a]	

[a]Calculated by Robertson (See Ref. 153).

[b]Mono.=monoclinic.

Wilk, Wallace, Anthony, *JAP* **89** (10), 5243 (2001).

- High-*k* oxides, such as HfO_2, are now incorporated into the gate stacks of silicon-based MOSFETs.
- The high-*k* oxide is used in conjunction with a metal gate electrode.
- Deposition on silicon creates an interfacial SiO_x layer during processing.
- High leakage for thin SiO_2 < ~2nm, & EOT rule gives same capacitance for a physically thicker high-*k* oxide layer.

Wu, Zhao, White, *Solid State Elec.* **50**, 1164 (2006).

- Leakage current dependent on:- tunnelling mechanism (ECB/HVB), tunnelling barrier height ($\Delta E_{(c/v)}$, ϕ_b), tunnelling effective mass {m_{eff} (m_0)}.
- $\phi_b = \chi_{Si} - \chi_{HfO2}$ (χ = electron affinity).

Material	La_2O_3	Al_2O_3	HfO_2	Si_3N_4	SiON	SiO_2
Tunneling mechanism	ECB	ECB	ECB	HVB	ECB	ECB
ϕ_b (eV)	2.3	2.8	1.13	1.9	3.04	3.10
m_{eff} (m0)	0.26	0.35	0.22	0.41	0.21	0.4
α	0.1	0.6	0.8	1	0.4	0.6
K	27	10	20	7	5.08	3.9

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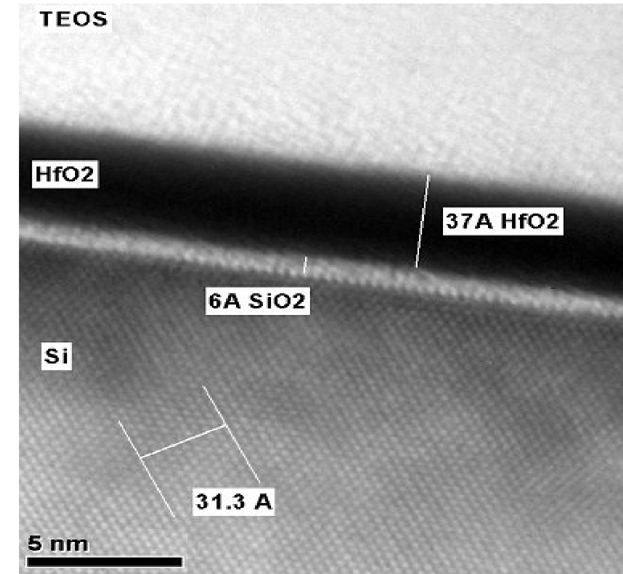
Details of Experimental Samples

- n-Si(100)/SiO_x/HfO_2/Ni MOS capacitors.
  - Samples with FGA at 400°C for 30 min → low D_{it}.
  - HR-TEM determination of SiO_x and HfO_2 thicknesses (accurate to ±2 Å).
  - In this study: HfO_2 ~ 35 Å, SiO_x ~ 6 Å.
- MOSFETs on Si(100) and ALD HfO_2/TiN gate stacks (D_{it}~$4x10^{10}cm^{-2}$ from charge pumping).
  - Gate dimensions are 10 μm x 10 μm.
  - Parameter fit in this study for all devices in the table (right).

M. A. Negara *et al.*, *Microelectronic Eng.* **84**, 1874 (2007).



Wafer	A	B	C	D
t-HfO_2 [Å]	16	20	24	30
t-SiO_x [Å]	10	10	10	10
$C_{ox\ eff}$ [F/cm^2]	$2.43x10^{-6}$	$2.35x10^{-6}$	$2.25x10^{-6}$	$2.16x10^{-6}$
V_{FB} [V]	-0.49	-0.51	-0.58	-0.6
E_{OT} [Å]	10.6	11.4	12.1	12.5
Na [x 10^{17} /cm^3]	3	3	3	3
μ_{peak} [cm^2/V.s]	225	212	195	178

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Simulation Model: I-V Response

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$$j_n = -\frac{g_n A_0 T}{k_B} \int_{0^-}^{\infty} du\, \mathcal{T}_n \left[u, 0^-, E_c(u)\right] \left| \frac{dE_c}{du}(u) \right| \Theta \left[\frac{dE_c}{du}(u) \right] \times$$
$$\times \ln \left\{ \frac{\exp\left[\frac{E_{F,n}(u) - E_c(u)}{k_B T}\right] + 1}{\exp\left[\frac{E_{F,n}(0^-) - E_c(u)}{k_B T}\right] + 1} \right\} . \qquad (1)$$

- 1D Schrödinger equations solved along straight lines connecting the channel to the gate contact. These are incorporated into a 2D drift-diffusion simulator.
- Special purpose grid (SPG) generated for solutions of 1D Schrödinger-Poisson system.
- SPG details: straight lines at semiconductor vertex connect to points on the gate contact. Angle and two length parameters include regions not directly within the gate stack.
- The 1D Schrödinger equations are solved in the one-band effective mass approximation (EMA) using the scattering matrix approach (SMA).
- The tunnelling probability (T_n) - from the SMA solution of the 1D Schrödinger equation - can be calculated for the gate stack barrier *and* any possible substrate potential barrier.

Synopsys Inc., *Sentaurus Device User Guide*, Version Z-2007.03, Mountain View, California, 2007.

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Simulation Model: I-V Response

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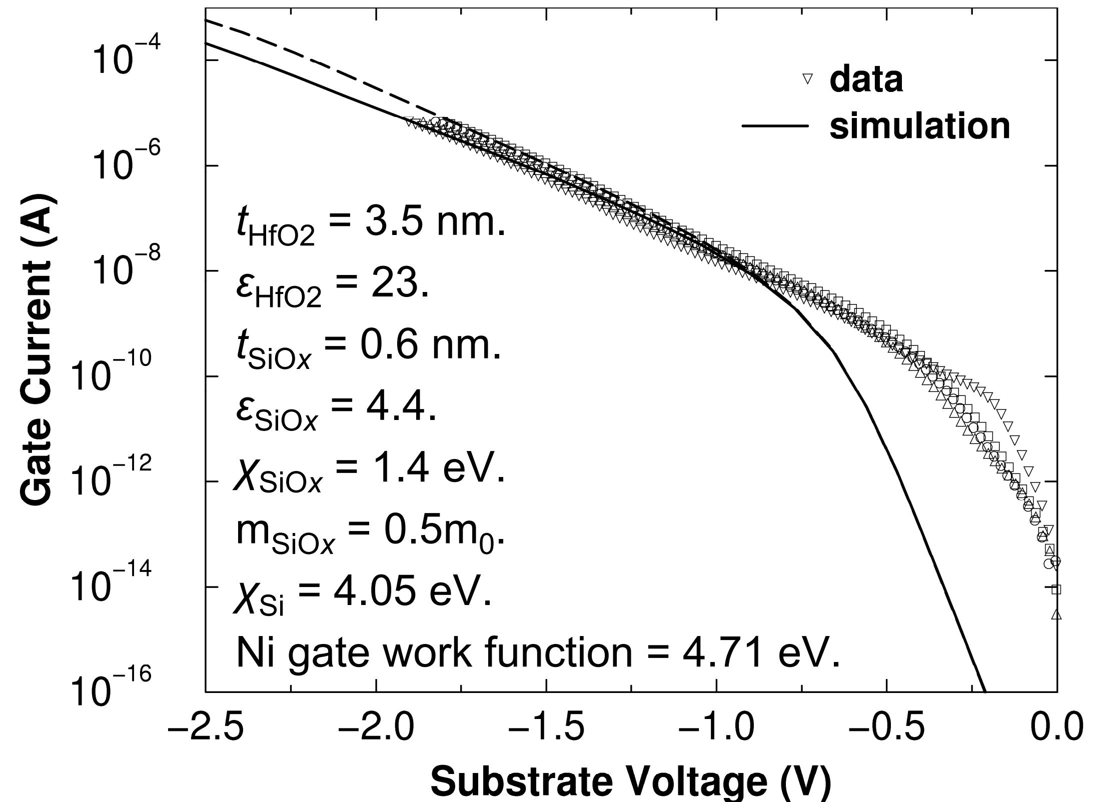
$$j_{\rm n} = -\frac{g_{\rm n} A_0 T}{k_{\rm B}} \int_{0^-}^{\infty} du\, \mathcal{T}_{\rm n}\left[u, 0^-, E_{\rm c}(u)\right] \left|\frac{dE_{\rm c}}{du}(u)\right| \Theta\left[\frac{dE_{\rm c}}{du}(u)\right] \times$$
$$\times \ln\left\{\frac{\exp\left[\frac{E_{\rm F,n}(u)-E_{\rm c}(u)}{k_{\rm B}T}\right]+1}{\exp\left[\frac{E_{\rm F,n}(0^-)-E_{\rm c}(u)}{k_{\rm B}T}\right]+1}\right\}. \quad (1)$$

- Line coordinates of the SPG are denoted by u, with the origin at the metal contact.
- $A_0 = 4\pi m_0 k_B^2 q/h^3$ is the Richardson constant for free electrons, T denotes the temperature (drift-diffusion model, no carrier heating), k_B the Boltzmann constant, $E_c(u)$ the position-dependent conduction band edge, $E_{F,n}(u)$ the quasi-Fermi energy. The parameter g_n can be used to change the effective DOS mass (m_0) in the Richardson constant.
- For tunnelling across a (100)-oriented interface, a reasonable choice is $g_n = 2m_t/m_0$ for the valley pair perpendicular to the interface, and $g_n = 4(m_t m_l)^{1/2}/m_0$ for the two valley pairs parallel to the interface. Separate simulations of the current for these pairs were performed in order to account for the variability of the Si effective mass entering the tunnelling probability, T_n.

Synopsys Inc., *Sentaurus Device User Guide*, Version Z-2007.03, Mountain View, California, 2007.

MOS: Exp. & Simulated I-V

- Measured (circles) and simulated (lines) I-V responses for e-beam MOS devices.
- Excellent fits for $V_s < -0.7$ eV.
- Direct tunnelling is the dominant leakage mechanism.
- The Ni gate area is 55 μm x 55 μm.
- The best lower fit (solid line) has an electron effective mass and electron affinity for HfO_2 of $m_{HfO2} = 0.11m_0$ and $\chi_{HfO2} = 1.75$ eV.
- The best upper fit (dashed line) has an electron effective mass and electron affinity for HfO_2 of $m_{HfO2} = 0.135m_0$ and $\chi_{HfO2} = 2.0$ eV.



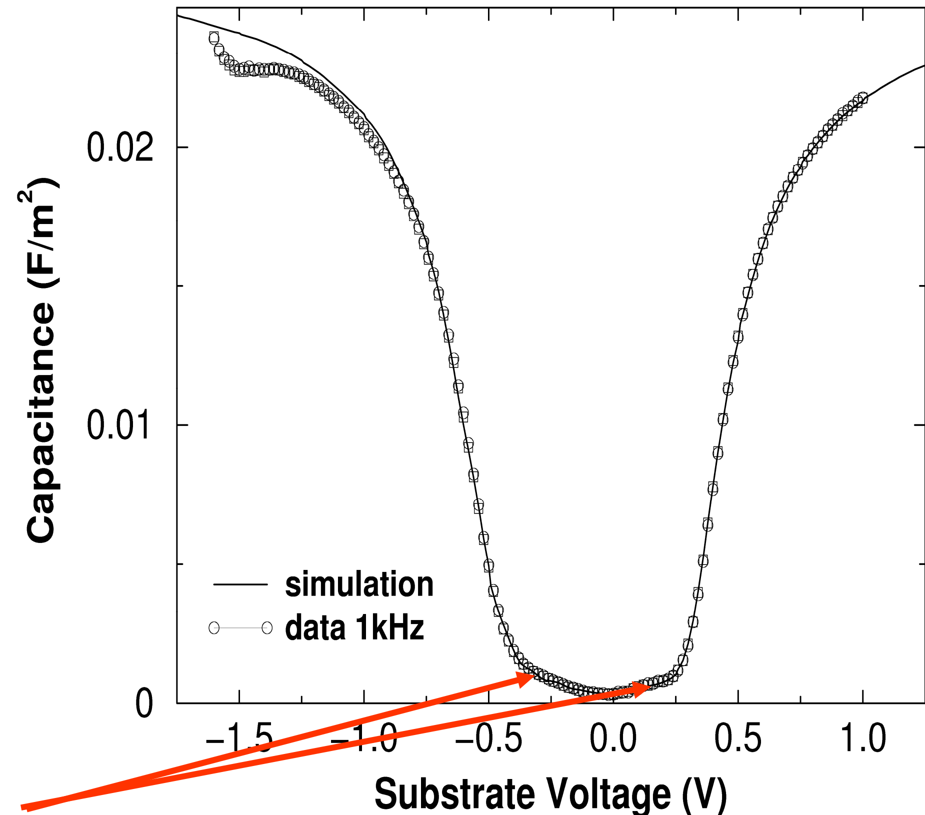
MOS: Exp. & Simulated C-V

- Measured (circles) and simulated (line) CV for e-beam MOS devices, using the same parameters as those for the I-V results.

- The simulated CV exhibits an excellent fit to the measured CV response, from the low frequency response in strong inversion (V_s = 1 V) through depletion and into strong accumulation (V_s = -1.25 V).

- Quasi-static CV simulation method used: QV (charge-voltage) curves calculated from the 1D Schrödinger-Poisson system and differentiated over the voltage bias range.

- Region of CV showing effects of acceptor-like interface traps (U-shaped region) is simulated with the inclusion of a Gaussian density of interface trap states method (2-3 x 10^{11} cm^{-2} near the mid gap energy).



MOSFET: Exp. & Simulated I-V

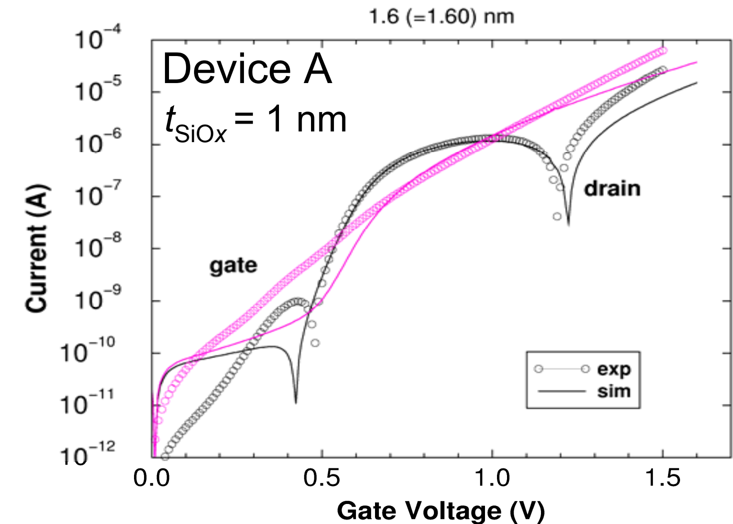
- Series of simulations: (i) varying t_{HfO2}; (ii) varying t_{SiOx}; (iii) varying electron effective masses and affinities.

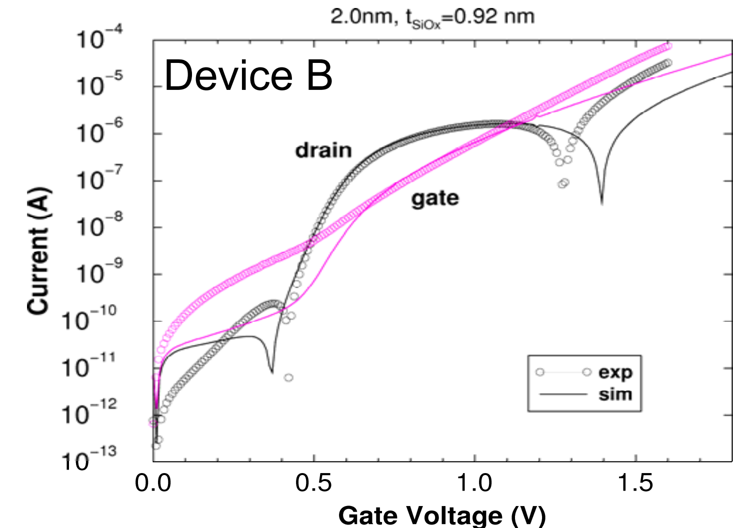
- Simulation results are compared to measurements and best fits are determined over voltage range 0 V - 1.5 V.

- Experimental (circles) and simulated (solid) gate and drain currents for MOSFET devices A, B, C, and D (V_{ds} = 10 mV) are shown.

- The best fit electron effective mass and electron affinity parameters for HfO_2 are $m_{HfO2} = (0.11 \pm 0.03)m_0$, χ_{HfO2} = (2.0±0.25) eV. The equivalent SiO_x parameters are $m_{SiOx} = 0.5m_0$, χ_{SiOx} = 1.4 eV.

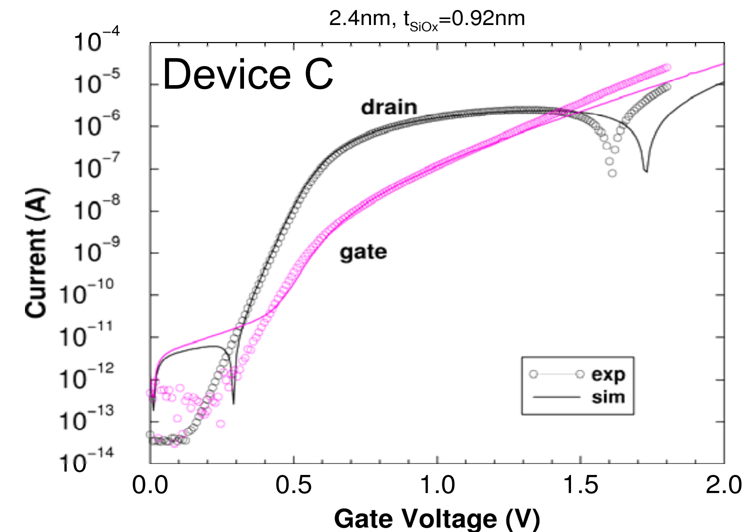
- Sign changes in I_d: 1st is at 10 mV drain bias before onset $r_{Ch} > r_{TB}$ in sub-V_{th} regime; 2nd is at V_{th} (when channel conductivity > tunnel barrier); 3rd is when $r_{Ch} > r_{TB}$.

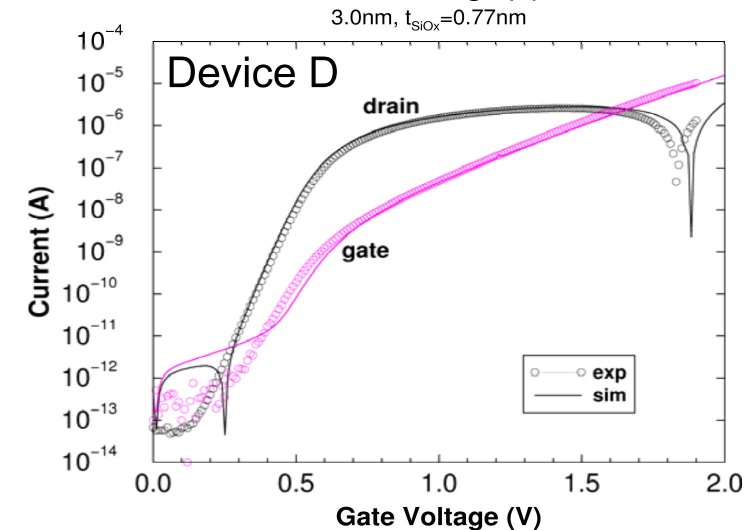




MOSFET: Exp. & Simulated I-V

- No partition correction is applied to the measured drain current, so that the leakage current density at the gate effects the measured (terminal) drain current.
- Best I-V fits requires that t_{SiOx} reduces (1 nm to 0.77 nm) as t_{HfO2} increases (1.6 nm to 3 nm), which is indicative of a stoichiometric change in the SiO_x layer as t_{HfO2} increases.
- Device area is chosen to obtain comparable values of I_g and I_d over voltage range 0 V - 1.5 V.
- Accurate simulation for V_g less than ~0.6 V not possible due to doping profile variations under gate corners and unknown gate overlap conditions.
- The TiN gate work function is 4.6 eV, with a negligible change of ±0.03 eV over all devices.





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Conclusions

- Experimental and simulated tunnelling currents for e-beam deposited, and atomic layer deposited (ALD), metal-gate/HfO_2/SiO_x/Si(100) structures.

- We have extended on previous studies by:-

  - Applying the self-consistent 1D-Schrödinger-Poisson solver to the entire gate stack, including the SiO_x region, ***and*** the adjacent Si-substrate.

  - Combining experimental and simulated tunnelling currents for MOS and MOSFET devices, ***and*** incorporating the correlated drain and gate currents.

- The electron effective mass in HfO_2 (m_{HfO2}) is $(0.11 \pm 0.03)m_0$.

- The electron affinity in HfO_2 (χ_{HfO2}) is (2.0 ± 0.25) eV, corresponding to a conduction band offset between Si and HfO_2 of $\Delta E_c = (2.05 \pm 0.25)$ eV.

- Gate metal selection, and HfO_2 deposition method, do not strongly alter the electron effective mass or the electron affinity in HfO_2.

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