Contact Model Based on TCAD-Experimental Interactive Algorithm

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***Abstract*—This work demonstrated a novel method utilizing Sentaurus Technology Computer Aided Design simulation along with experiments to intermediately extract Schottky barrier height and contact resistance in FinFETs. The proposed algorithm can automatically calibrate contact model based on measurement data. This interactive contact model is also capable of prediction of contact resistance sensitivity including key process features such as implant energy, dose and thermal process based on a design of experiment splits. This robust, physical and efficient contact model provides insightful understandings of the metal-semiconductor contact in FinFETs. It can be easily implemented in simulation tools for device design in state-of-art semiconductor technology development.**

Keywords—Schottky Contact, Barrier Height, FinFET, TCAD, Interactive Algorithm

I. Introduction

With the scaling of MOSFET transistors, the source and drain (S/D) contact size is aggressively reduced and the contact silicide formation faces many process challenges. Due to the small effective contact area and the difficulties in lowering the silicide resistivity, the S/D contact resistance R_C is becoming one of the major bottlenecks limiting device performance for future technology node 3-D devices [1-4]. To drive the FinFET transistor performance following Moore's law, a robust and physical contact model and good understanding of the metal-semiconductor Schottky barrier is crucial in the early stage technology development to capture R_C sensitivity to process flow towards device performance optimization [5]. However, it is a difficult task to estimate the Schottky barrier height (SBH) in the device level with conventional contact model due to the very complex nature of the S/D interfaces [6]. And the barrier lowering model, accounting for image force and tunneling effects, can cause convergence issues in 3-D transistors simulations. In addition, the conventional contact model lacks an automatic calibration technique to hardware data.

In this study, we present a novel method which utilizes Sentaurus Technology Computer Aided Design (TCAD) simulation along with experiments to extract SBH in FinFETs. The proposed algorithm can automatically calibrate contact model based on measurement data and then predicts contact resistance. TCAD simulation results show that the interactive contact model is able to reproduce R_C sensitivity by intended design of experiment (DoE) splits.

II. Algorithm

As shown in Fig. 1, S/D contact resistance R_C^{Exp} is obtained with a normalized value around 40 Ω·μm by Kelvin contact resistance measurement in the first step. Then, the calibrated process simulation extracts the surface doping density N_C^{TCAD} over the contact area A^{TCAD}. Fig. 2 illustrates that TCAD dopant profile is consistent with as-implanted phosphorus dopant data from SIMS measurement. It should be noted that during the silicide contact formation, more than 5-nm-thick silicon will be consumed and therefore a small doping concentration variation over the contact surface can be considered after silicidation.

Next, an iterative computation of ρ_C^{TCAD} via device simulation is performed until that a match of the TCAD result R_C^{TCAD}, which is a product of ρ_C^{TCAD} and A^{TCAD}, to the experimental data R_C^{Exp} is obtained.

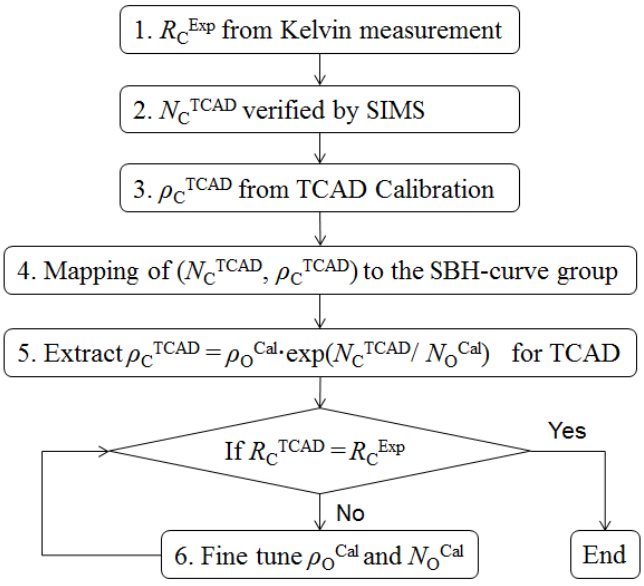

Fig. 1. The flow chart of the TCAD-Experimental contact model algorithm extracts the resistivity dopant dependent equation for TCAD simulations.

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Having obtained ρ_C^{TCAD} and N_C^{TCAD}, SBH is extracted in the fourth step using the theoretically calculated ρ_C characteristics. For this calculation, one-dimensional non-self-consistent Schottky barrier potential profile at a given barrier height in the semiconductor region is assumed. The current density across the barrier is calculated using the Tsu-Esaki formula wherein barrier tunneling probability is evaluated by the transfer matrix method [6-7]. Then, the contact resistivity is obtained from the current voltage characteristics at a very small applied bias. By repeating the procedure above, the doping dependent ρ_C characteristics are computed at different SBH values. With the theoretical calculated SBH-curve group, one can map the interested NFET and PFET contact data **N** (N_C^{TCAD}, ρ_C^{TCAD}) and **P** (N_C^{TCAD}, ρ_C^{TCAD}) to extract their contact interface barrier height. The examples are shown in Fig. 3.1 and 3.2, NFET SBH is estimated to be 0.2 eV while PFET 0.6 eV.

In the fifth step, a simple dopant concentration dependent ρ_C fitting equation, suitable for device electrical simulation, is extracted within specific range of doping density related to contact surface doping level. The equation follows the form:

$$\rho_C = \rho_O \cdot \exp\left(\frac{N_C}{N_O}\right)$$

where ρ_O and N_O are fitting parameters. The automatic interactive fine tuning to ensure R_C^{TCAD} equal to R_C^{Exp} will be performed on those two parameters to obtain calibrated ρ_O^{Cal} and N_O^{Cal} through the equation below in the sixth step:

$$\rho_C^{TCAD} = \rho_O^{Cal} \cdot \exp\left(\frac{N_C^{TCAD}}{N_O^{Cal}}\right)$$

The TCAD-experimental interactive analytic equation described above directly captures the sensitivity of resistivity to contact surface doping concentration. Furthermore, the implementation of this simple equation in TCAD eliminates convergence challenges from the direct modeling consideration of image force, tunneling and dipole effects.

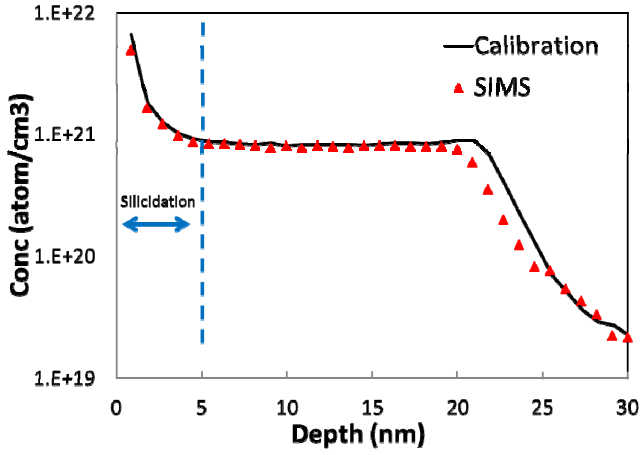

Fig. 2. Calibrated as-implanted phosphorus profile in Epi region matches SIMS data; The silicidation consumes around 5nm thick silicon at the Epi surface and therefore the kink can be ignored for contact modelling.

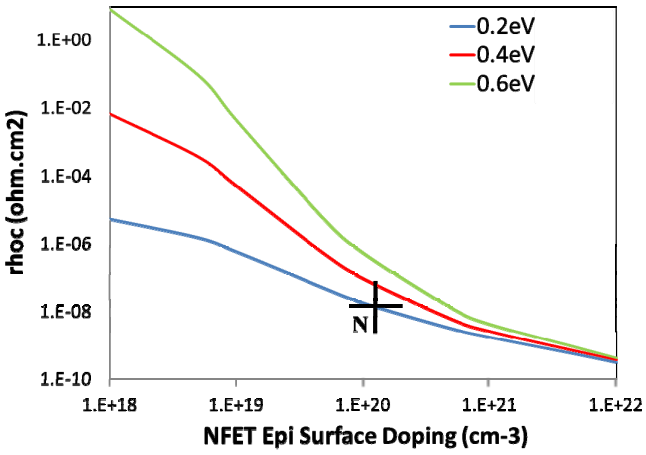

Fig. 3.1 Map the calibrated the NFET coordinate **N** (N_C^{TCAD}, ρ_C^{TCAD}) to theoretically computed SBH curve group and then extract NFET SBH as 0.2 eV.

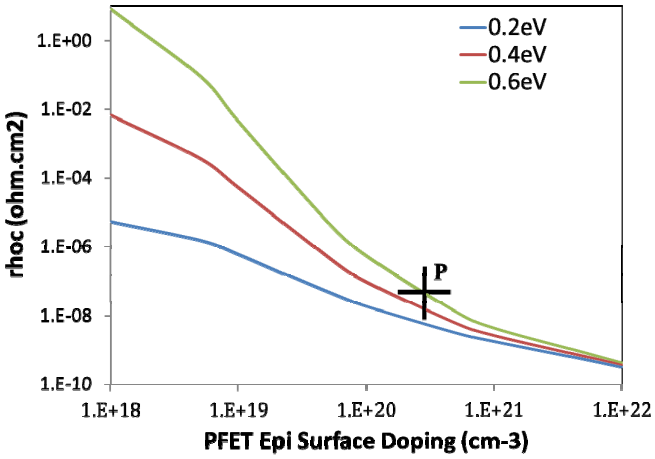

Fig. 3.2 Map the calibrated the PFET coordinate **P** (N_C^{TCAD}, ρ_C^{TCAD}) to theoretically computed SBH curve group and then extract PFET SBH as 0.6 eV.

III. Results

Fig. 4 shows the TEM of the Epi (the diamond) structure and the contact interface in the FinFET. TCAD process simulation mimics the silicide shape (green region) and the contact surface doping concentration, which is of the order of 1e20 cm^{-3}.

An average surface doping concentration, by finite element analysis method over the contact surface, is extracted instead of local doping density to determine N_C^{TCAD}. This is due to the fact that (1) the contact surface doping level can be fairly approximated as a uniform distribution around the contact area as stated previously and (2) the simplification can improve simulation efficiency and robustness.

Experimental results are used as a reference to interact and verify the proposed model. The DoEs are on S/D implantation

with dose and energy variation, and S/D diffusion thermal budget to examine the contact sensitivity to contact interface doping concentration. For the DoEs, the S0 transistors are the standard NFET and PFET devices which are calibrated in TCAD to hardware data for both linear and saturation operation region (see Fig. 5.1 and 5.2) with their contact resistance matching measurement results. Subsequently, the analytic contact model with certain SBH is accurately extracted based on the S0 transistor.

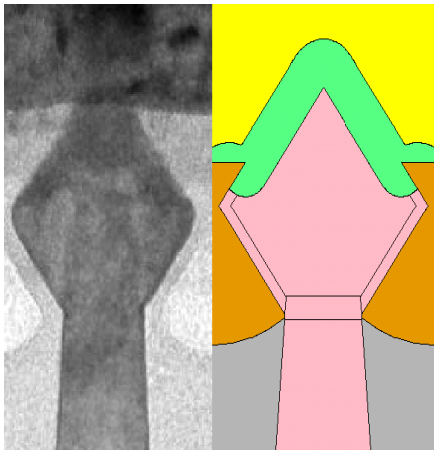

Fig. 4. TCAD process simulation mimic TEMs Epi and Contact; the diamond pink region is for S/D Epi region, the green for silicide, the yellow for metal, the grey for STI, and the brown for nitride.

Table 1.1 and Table 1.2 summarize results of NFET and PFET front end of line (FEOL) DoEs, where SBH can be treated as a constant. This assumption is valid as long as the contact electrode materials do not change, and the contact surface doping density is higher than 1e20 cm^{-3} allowing significant tunneling current through the contact interface according to the criterion comparing the thermal energy kT with E_{00} defined as:

$$E_{00} = \frac{q\hbar}{2}\sqrt{\frac{N_D}{\varepsilon_S m_T}}$$

where q is the electron charge, ħ the reduced Plank's constant, ε_S the silicon dielectric constant and m_T the tunneling effective mass [8].

The review of the table shows that the predicted TCAD extracted contact resistance values not only shows a consistent trend among experiments but also well match experimental data with an error less than 2%.

The DoE sensitivity provides device design guideline for FinFETs. It suggests that (1) shallow implant retains peak concentration around the contact interface to reduce the resistance, (2) contact surface doping level is proportional to S/D implant dose, and (3) increased thermal budget alters doping distribution and lowers contact surface doping concentration. The reliable simulated contact resistivity sensitivity reminds the designer of the trade-off among the contact, the junction, and other device factors.

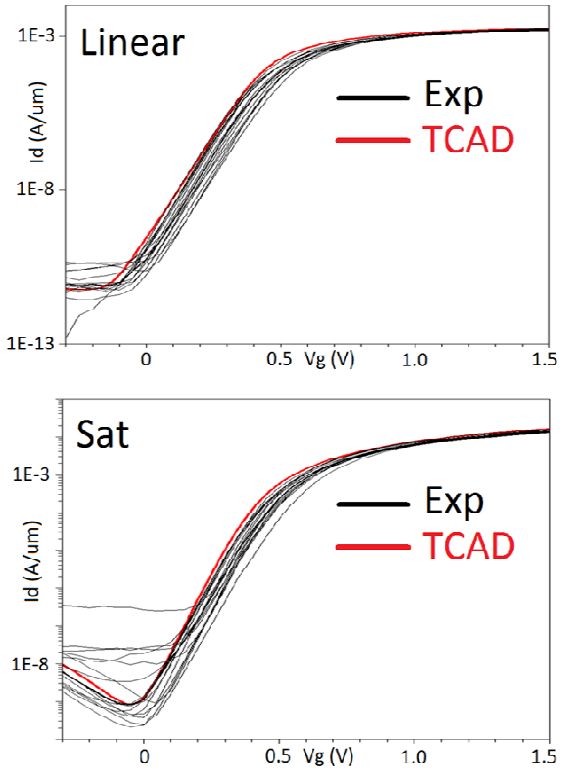

Fig.5.1 Calibrated NFET simulation results agree with electrical data.

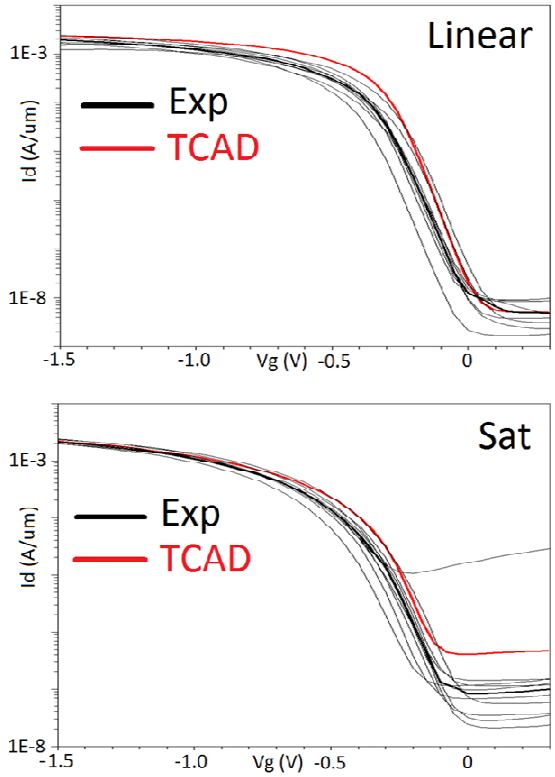

Fig.5.2 Calibrated PFET simulation results agree with electrical data.

NFET	Contact Related Condition	TCAD	Exp
S0 Standard	As 3e15cm^{-2} 3keV Imp w/ RTA	40.1	40.2
S1 Energy	As 3e15cm^{-2} 2keV Imp w/ RTA	39.5	39.6
S2 Dose	As 5e15cm^{-2} 3keV Imp w/ RTA	35.3	35.0
S3 Thermal	As 3e15cm^{-2} 3keV Imp w/o RTA	37.1	37.7

Table 1.1 NFET DoE comparison results show that TCAD simulation capture experimental sensitivity on Epi implantation dose and energy, and rapid thermal anneal (RTA); the normalized contact resistance result has a unit of Ω·μm;

PFET	Contact Related Condition	TCAD	Exp
S0 Standard	B 4e15cm^{-2} 2keV Imp w/ RTA	47.3	47.7
S1 Energy	B 4e15cm^{-2} 1.5keV Imp w/ RTA	46.2	46.8
S2 Dose	B 5e15cm^{-2} 2keV Imp w/ RTA	43.5	42.8
S3 Thermal	B 4e15cm^{-2} 2keV Imp w/o RTA	40.0	39.2

Table 1.2 PFET DoE comparison results show that TCAD simulation capture experimental sensitivity on Epi implantation dose and energy, and rapid thermal anneal (RTA); the normalized contact resistance result has a unit of Ω·μm;

IV. Conclusion

We have demonstrated a novel contact model based on TCAD-Experimental interactive algorithm with theoretical analysis and DoE results verification. The proposed model is capable of extracting SBH and it accurately predicts sensitivity of contact resistivity to variation in doping concentration. By interactive calibration method in the model, our TCAD simulation results accurately agree with hardware data based on FinFET technology. The implementation of the model is simple and will improve both simulation efficiency and robustness. This model can be extended to nanowire and future 3-D devices.

Acknowledgment

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References

[1] E. Yu, L. Chang, S. Ahmed, H. Wang, S. Bell, C. Yang, C. Tabery et al, "FinFET scaling to 10 nm gate length," *Electron Devices Meeting, 2002. IEDM'02. International,* pp. 251-254. IEEE, 2002.

[2] "International technology roadmap for semiconductors," 2013. [Online]. Available: http://www.itrs.net

[3] P. Feng, "Design, Modeling and Analysis of Non-classical Field Effect Transistors," (2012).

[4] S. Narayanan et al, "Extraction of Parasitic and Channel Resistance Components in FinFETs using TCAD tools," *Electron Devices, IEEE Transactions on,* to appear.

[5] R. T. Tung, "The physics and chemistry of the Schottky barrier height," *Applied Physics Reviews,* vol. 1, no. 1 (2014): 011304.

[6] B. Jonsson, and S. T. Sverre, "Solving the Schrodinger equation in arbitrary quantum-well potential profiles using the transfer matrix method," *Quantum Electronics, IEEE Journal of,* vol. 26, no. 11 (1990): 2025-2035.

[7] J. Kim, B. Lee, Y. Park, K. Murali, and F. Benistant, "Specific contact resistivity of n-type Si and Ge M-S and M-I-S contacts," *Simulation of Semiconductor Processes and Devices (SISPAD), 2015 International Conference on*, Sep. 2015.

[8] F. A. Padovani, and R. Stratton, "Field and thermionic-field emission in Schottky barriers," *Solid-State Electronics,* vol. 9, no. 7 (1966): 695-707.