MARS: a Multiscale *Ab initio* Reliability Simulator for Advanced Si and 2D Material Based MOSFETs

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2024 IEEE International Electron Devices Meeting (IEDM) | 979-8-3503-6542-9/24/$31.00 ©2024 IEEE | DOI: 10.1109/IEDM50854.2024.10873591

***Abstract*—**We propose an accurate reliability simulator, MARS (short for Multiscale *Ab initio* Reliability Simulator), that works for both industrial Si MOSFET and emerging two-dimensional (2D) material FET. It is composed of three blocks, namely the *ab initio* database of defects and defect-precursors, the physical calculator of charge trapping rates and defect creation rates, and the compact simulator of device parameter shift which is largely inspired by the open-source code Comphy. It has the following features and advantages: (1) All the defect fingerprints are obtained by *ab initio* calculations on atomistic interfaces models, including $Si/SiO_2/HfO_2$ and WSe_2/SiO_2. (2) The Marcus charge transfer theory is adopted to calculate the charge trapping/de-trapping rates, and no empirical parameter or approximation is used. (3) It is able to simulate both BTI and HCD issues in Si MOSFETs, and the hysteresis issue in 2D FETs. (4) Excellent agreements between simulation and experimental data are presented.

I. Introduction

Reliability simulation and design is becoming more and more important with the continuous shrinking of device size, advancing of device architecture, and introducing of new channel materials. However, traditional simulation tools are not catching up with the increasing demanding on accuracy and universality due to the reliance on empirical/fitted parameters and phenomenological or oversimplified models. It is highly anticipated to improve the traditional tools by integrating with more physical models and more accurate atomistic simulations for various devices and reliability issues.

One pioneering tool emerged specially for reliability simulation is the Comphy package [1,2], which is developed by TU Wien and imec. It is designed to improve the calculation of oxide charge trapping by adopting the non-radiative multi-phonon (NMP) theory, and then combine it with compact frameworks to realize the efficient simulation of BTI and gate leakage current etc. The adoption of NMP theory is a big advance since it is much more physical and powerful than the usually used SRH model. Nevertheless, a current dilemma of NMP application is the difficulty in calculating the phonon spectrum of device models with both amorphous interfaces and defects, and thus the important term, namely phonon-assisted electronic coupling, has to be estimated by the WKB approximation at the current stage. The approximation is definitely very helpful, but still waiting for replacement by accurate phonon calculations.

To leap over the current dilemma, we propose to use another accurate charge transfer theory, namely Marcus theory, to deal with the charge trapping in devices. We have proved that the combination of Marcus theory with full *ab initio* calculations, *i.e.* no empirical parameters or WKB approximation, can study the charge trapping of high-k gate stacks well [3]. Now we push it forward to be an accurate reliability simulator, namely multiscale *ab initio* reliability simulator (MARS), that can go straight from *ab initio* defect data to measurable reliability data. We prove that it works for both Si MOSFET and 2D FET, and excellent agreements with experimental data are presented. Moreover, we integrate a module for HCD simulation based on our successive works on defect generation [4,5]. With all these features, we believe MARS will be very helpful to promote the reliability study of advanced Si MOSFETs and emerging 2D FETs.

II. Workflow of the Simulator

As is shown in **Fig. 1**, the simulator starts with atomic level interface models, and goes through first-principles calculations, Marcus theory and trap generation model, compact framework, and ends up with experimentally measurable degradation curves.

A. Ab initio calculation

The first feature of MARS is the full *ab initio* calculation of semiconductor-oxide interfaces and oxide defects. It begins with the building of atomistic interfaces such as $Si/SiO_2/HfO_2$, where the SiO_2 and HfO_2 are amorphous, as is shown in **Fig. 2**. This is realized by bond switching Monte Carlo simulation and molecular dynamics simulation. Then first-principles calculations are carried out on these large models (>500 atoms) with the PWmat package [6], which is compiled on GPUs for acceleration, as is shown in **Fig. 3**. The computational-expensive HSE hybrid functional is used to obtain correct band gaps and band alignments, as is shown in **Fig. 4**. Systematic defect calculations are conducted in sequence, and one typical defect level is also shown in **Fig.4.**

B. Physical calculator of charge trapping

Charge trapping theory is the indispensable bridge between defect information and BTI issue. The second feature of MARS is the adoption of Marcus theory, which does not require empirical parameter or approximation, and had been successively applied to high-k gate stacks by us earlier [3]. The theory gave birth to the charge transfer rate formula that is shown in **Fig. 5**, where V_C is the coupling constant between initial state and final states, ΔG is the total energy change before and after charge

trapping, and λ is the reorganization energy that reflects the magnitude of structural relaxation. All these parameters can be obtained from first-principles calculations, and the detailed formulas are also given in **Fig. 5**.

C. Compact framework for BTI

While charge trapping and emission rates are obtained, the charge occupation of each defect and its evolution with time can be calculated by solving the master equation, as is shown in **Fig. 6**. Then the occupation can be converted into the threshold voltage shift by treating the defect as a charge sheet and by calculating the capacitance between the charge sheet and the gate electrode. One important fact is that the oxide electric field will influence the charge trapping rates of defects, and in turn, the trapped charges will affect the oxide field. Therefore, an iteration between Marcus theory and the compact framework is required.

D. Defect creation model for HCD

One well-recognized model was provided by Tyaginov and Grasser et al. in 2014 [7,8]. Based on that model, as is shown in **Fig. 7**, we changed the Keldysh-like reaction cross section by the energy dependent projected density of states (PDOS) of hydrogen atoms at a real Si-SiO_2 interface, which is obtained by first-principles calculations. The most significant feature of the PDOS is that it presents peaks at both low energy range and high energy range, which making it capable to manifest the important role of low-energy carriers on defect creation [4,5].

III. RESULTS AND DISCUSSION

A. Ab initio database of defect fingerprints

Considering the complexity of amorphous oxides, we think it necessary to calculate four kinds of defects, namely the oxygen vacancy (V_O) inside SiO_2, the hydroxyl defect inside SiO_2, the V_O at SiO_2/HfO_2 interface, and the V_O inside HfO_2. Moreover, to make the data statistically valid, the three kinds of bulk defects are sampled at ~50 different positions, respectively, and the SiO_2/HfO_2 interface defects are sampled at ~30 different positions. The calculated defect properties, typically defect levels (E_t), turn out to be quasi-Gaussian distributions, as are show in **Fig. 8.** The different defects present very distinct defect levels with respect to the band edge of Si, and this largely determines their relative activeness in charge trapping. The statistical results of λ and V_C are shown in **Fig. 9**, and the combination of $\{E_t, \lambda, Vc\}$ of all defects forms the *ab initio* database of defect fingerprints in a MOSFET. Note that the concentrations of defect are very difficult to calculate because they depend greatly on the growth process. So as most simulation tools do, they are treated as a tunable parameter within the range of $10^{17} \sim 10^{19}$ cm^{-3}.

B. BTI simulation of 28nm high-k MOSFET

To verify the accuracy of MARS, we first simulate the NBTI of foundry 28nm MOSFET. The device setup and the experiment data are referred to Comphy [1]. By calling the *ab initio* defect database, the first output is the charge trapping/emission rates and the resulted charge occupation of each defect, as are shown in **Fig. 10**. Obviously, the $V_O@SiO_2$ is not active in trapping holes, while the $V_O@HfO_2$ captures the largest number of holes. Both hydroxyl defect and interface defect contribute notably to hole trapping. The simulated evolution of ΔV_{th} under pulse-like stress and relax voltages are shown in **Fig.11**. It can be seen that the simulation results match with the experimental data (red circles) very well at every time period. This strongly demonstrates the accuracy of our *ab initio* simulator.

C. HCD simulation of 14nm Si FinFET

To further show the capability of MARS, we simulate the HCD degradation of 14nm FinFET. The key task is calculating the defect generation rate, which is decided by two factors, namely the bond breaking barrier and the electron-phonon resonance cross section, as is shown in **Fig. 12**. We have new insights into both factors through *ab initio* calculations. First, different breaking barriers with a certain ratio should be used because the barrier depend greatly on the breaking process, as is shown in **Fig. 13**. Second, the projected density of states (PDOS) of H atoms should be used as the cross section. The carriers whose energy coincides with the PDOS peak, as is shown in **Fig. 14**, will contribute most to the bond breaking. By integrating these new insights into the defect generation framework, MARS exports a series of HCD degradation curves that agree well with experimental data, as is shown in **Fig. 15.** This proves the capability of MARS for a second time.

D. Hysteresis simulation of 2D WSe_2 MOSFET

2D semiconductors have drawn huge attentions due to their great potential in realizing extremely scaled devices and circuits [9-11], and the reliability study of them are coming to the spotlight recently [12-14]. We are excited to show that MARS also works for those MOSFETs with 2D material channel. We fabricated the WSe_2 FET with amorphous SiO_2 as gate dielectric, as is shown in **Fig. 16**. Such a device shows typical hysteresis in transfer characteristics, as can be seen in **Fig. 17**. Interestingly, the positive shifts of V_{th} are more significant than the negative ones. We think the phenomenon should be related to the interface defects between WSe_2 and SiO_2. Thus, we constructed atomistic WSe_2/SiO_2 interface models with various defects, as is shown in the insets of Fig. 16, and calculated their defect fingerprints and put them into MARS to simulate the V_{th} shift under different voltages. To our delight, it produces very consistent results with the measured ones, as is shown in **Fig. 18**, which demonstrates the accuracy and reliability of MARS for a third time.

IV. CONCLUSION

In summary, we have developed a satisfying reliability simulator that based on *ab initio* calculations and Marcus charge transfer theory. It is proved to be applicable to both industrial Si MOSFETs and emerging 2D FETs, and is demonstrated to be accurate for BTI, HCD and even hysteresis simulations. Moreover, the *ab initio* database of MARS will be enriched further in following days. We believe this simulator will be a very useful tool to the understanding and simulation of reliability issues in different semiconductor devices in the near future.

ACKNOWLEDGMENT

Y.Y. Liu, R. Wang and L.W. Wang were supported by the National Key Research and Development Program of China (Grant No. 2022YFF0605800), NSFC (62174155, 61927901, T2293702), and CAS Project for Young Scientists in Basic Research (No. YSBR-056).

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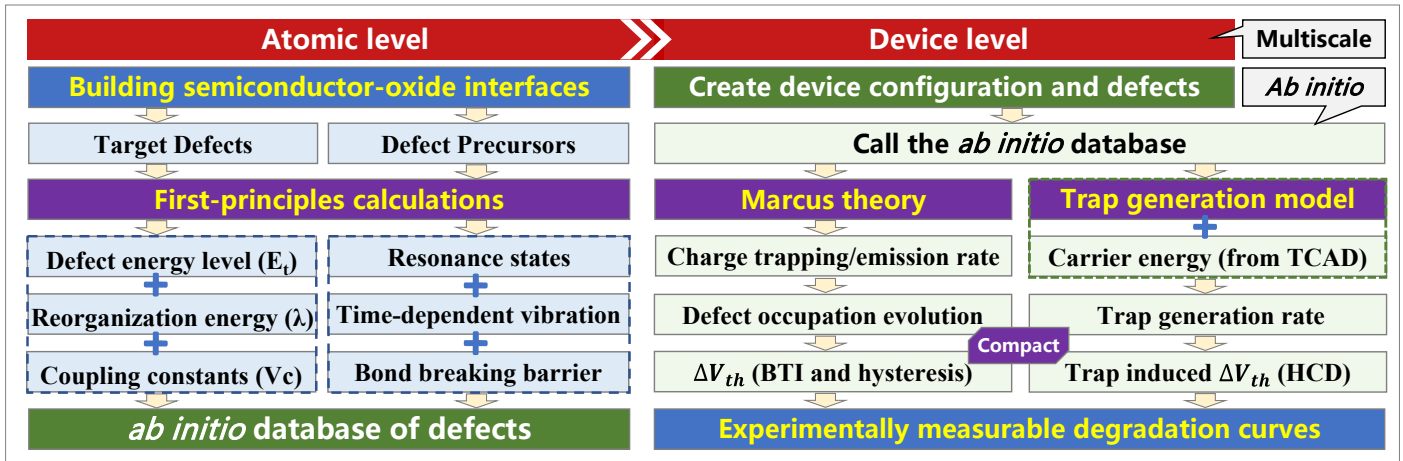

Fig. 1 The main components and workflow of the MARS package. It starts with atomic level interface models, and goes through first-principles calculations, Marcus theory, trap generation model, compact frameworks, and finally ends up with measurable degradation curves.

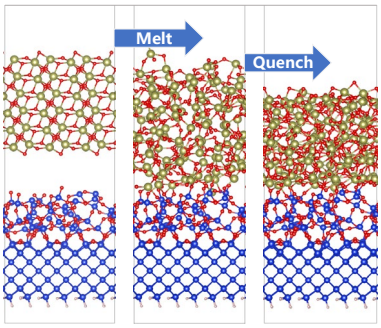

Fig. 2 The building process of atomistic $Si/SiO_2/HfO_2$ interface.

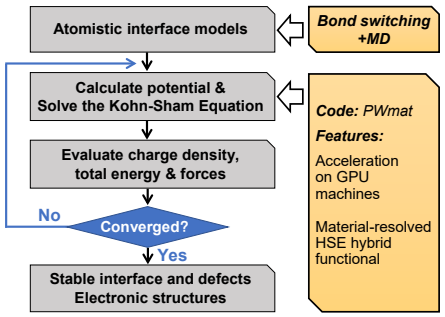

Fig. 3 The principle, workflow and features of our *ab initio* calculations.

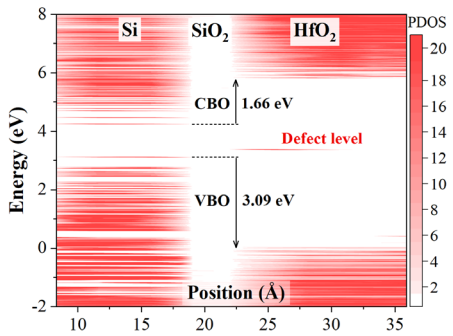

Fig. 4 The clear band alignment and defect level manifested by the local density of states contour.

$$k_{12}=\frac{2\pi}{\hbar}|V_C|^2\sqrt{\frac{1}{4\pi\lambda k_BT}}\exp\left[-\frac{(G_2-G_1+\lambda)^2}{4\lambda k_BT}\right]$$

$$G_2=E_0-(E_t\pm qx_tE_{ox})-\lambda_{defect}$$

$$G_1=E_0-E_{VBM}-\lambda_{VBM}$$

$$\lambda=E(R_0,N\text{-}1)-E(R_1,N\text{-}1)$$

$$\hat{H}=\begin{pmatrix}-\frac{\Delta\varepsilon_0}{2}+eF\cdot\frac{d}{2} & V_C\\ V_C & \frac{\Delta\varepsilon_0}{2}-eF\cdot\frac{d}{2}\end{pmatrix}$$

$$\Delta\varepsilon=2\sqrt{V_C^2+\left(\frac{\Delta\varepsilon_0}{2}-eF\cdot\frac{d}{2}\right)^2}$$

Ab initio

Fig. 5 The formulas of Marcus theory. All the parameter are obtained by *ab initio* calculations.

$$\frac{dp_2(t)}{dt}=(1-p_2)\sum_{r=1}^{N}k_{12,r}-p_2\sum_{r=1}^{N}k_{21,r}$$

$$p_2(t)=\frac{k_{12}}{k_{12}+k_{21}}+\left(p_2(t-dt)-\frac{k_{12}}{k_{12}+k_{21}}\right)e^{-(k_{12}+k_{21})dt}$$

$$\Delta V_{th,traps}=\frac{1}{\varepsilon_0\varepsilon_r WL}\sum_{i=1}^{n_t}(t_{ox}-x_{t,i})(-e\cdot p_{t,i})$$

$$Q_s=\pm\frac{\sqrt{2}k_BT}{qL_D}\left[(e^{-\varphi_s/k_BT}+\varphi_s/k_BT-1)+\frac{n_0}{p_0}(e^{\varphi_s/k_BT}-\varphi_s/k_BT-1)\right]^{1/2}$$

$$\frac{Q_s(\varphi_s)WL}{C_{ox}}+\varphi_s-V_G+\Delta E_{W,0}/q+\Delta E_{F,0}/q+V_{traps}=0$$

$$E_{ox}=\frac{V_G-\Delta E_W/q-\varphi_s}{t_{ox}}$$

Fig. 6 The compact framework of ΔV_{th} referred to Comphy. An iteration with Marcus theory is required.

$$\frac{dN_{it}}{dt}=(N_0-N_{it})R_a-N_{it}^2R_p\qquad R_p=u_p\exp(-E_p/k_BT)$$

$$R_a=\frac{1}{k}\sum_i R_{a,i}\left(\frac{P_u}{P_d}\right)^i\qquad R_{a,i}=\omega_{th}\exp[-(E_b-E_i)/k_BT]+I_{SVE,i}$$

$$I_{SVE,i}=\int f(E)g(E)v(E)\sigma(E)(E-E_b+E_i)^{\sigma(E)}dE$$

$$P_u=I_{MVE}+(1/\tau)\exp(-\hbar\omega/k_BT)\qquad P_d=I_{MVE}+1/\tau$$

$$I_{MVE}=\int f(E)g(E)v(E)\sigma(E)dE$$

$$\sigma(E)=nPDOS(E)\qquad E_b=[E_{b1},E_{b2},E_{b3}]$$

$$\Delta V_{th}=\sum_{x,y,z}\eta(x,y,z)\cdot N_{it}\cdot S_{mesh}\qquad \eta \text{ and } S \text{ are from TCAD}$$

Fig. 7 The trap generation model that originates from Ref. [7] and modified in Ref. [5]. We propose critical changes to $\sigma(E)$ and E_b.

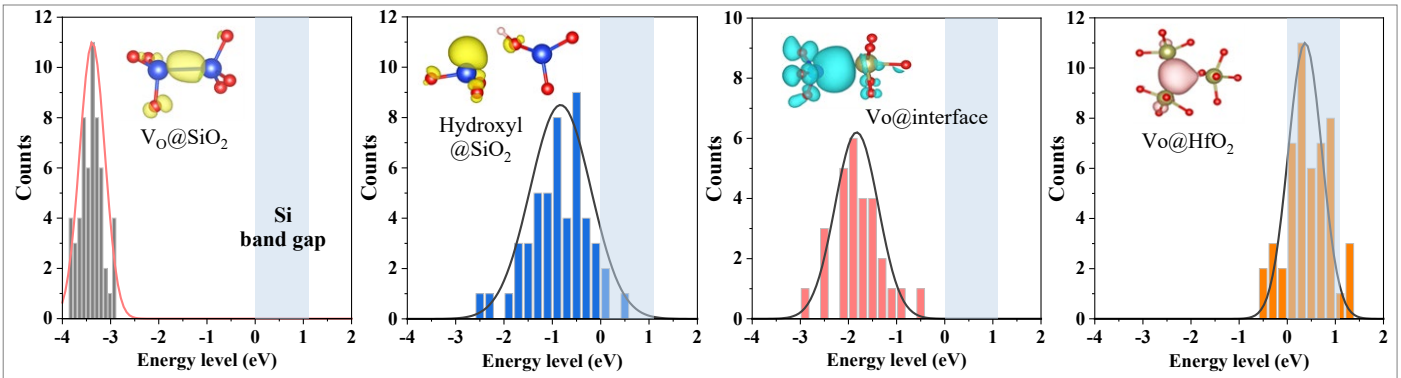

Fig. 8 The defect level (E_t) distribution of four kinds of important defects, namely the oxygen vacancy (V_O) inside SiO_2, hydroxyl defect inside SiO_2, V_O at SiO_2/HfO_2 interface, and V_O inside HfO_2. The data can be fitted by Gaussian distributions, and the parameters are shown in Fig. 9.

	Et: μ	Et: σ	λ: μ	λ: σ	Vc
Vo@SiO_2	-3.38	0.26	0.84	0.3	0.337×exp(-0.66*d*)
Hydroxyl@SiO_2	-0.83	0.63	3.0	0.5	1.368×exp(-0.77*d*)
Vo@interface	-1.83	0.45	1.3	0.5	0.07×exp(-0.58*d*)
Vo@HfO_2	0.37	0.35	0.90	0.2	0.07×exp(-0.58*d*)

Fig. 9 The *ab initio* database of defect's fingerprints. The defect levels (Et) and reorganization energy (λ) are presented by Gaussian distributions, and the coupling constant (Vc) between defect states and channel is a curve that decays with defect distance (*d*).

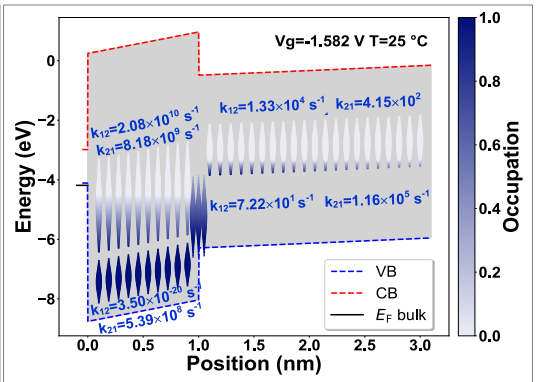

Fig. 10 The charge occupation of all defects calculated by the charge trapping/emission rates of Marcus theory.

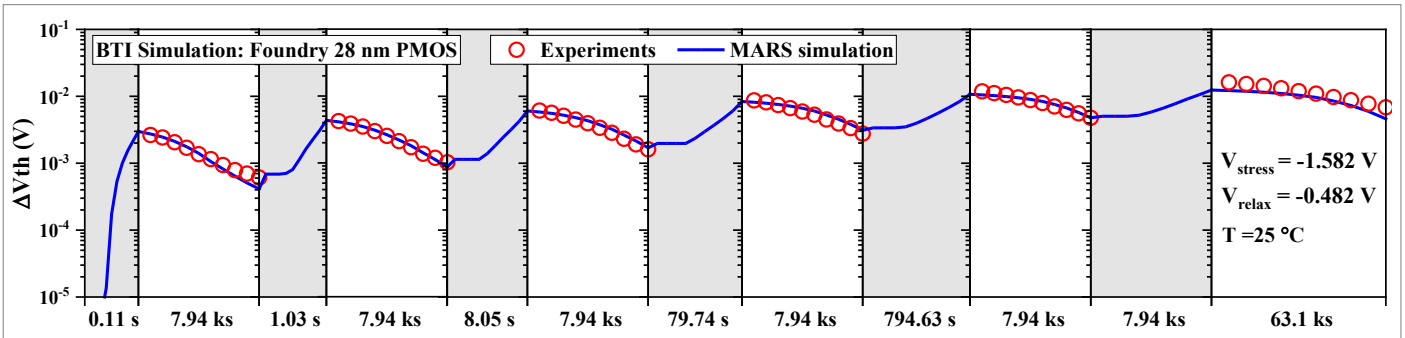

Fig. 11 The simulated ΔV_{th} evolution and its comparison with experimental measurements. An excellent agreement can be seen at every time period, which strongly demonstrates the accuracy of MARS.

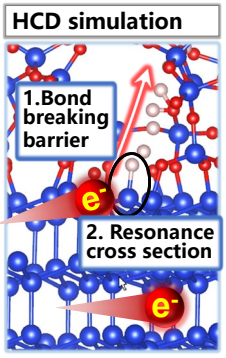

Fig. 12 The two key factors required in HCD simulation.

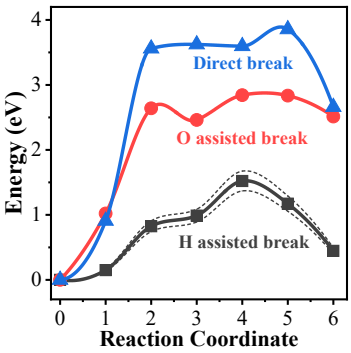

Fig. 13 The process-dependent bond breaking barriers obtained by *ab initio* calculations.

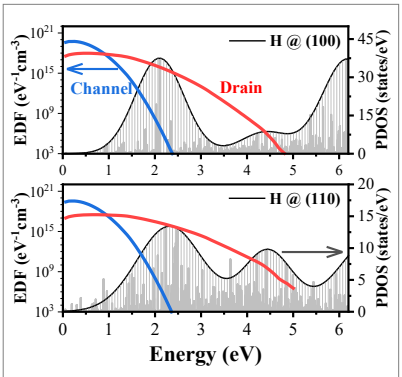

Fig. 14 The overlap of carrier EDF with PDOS of H. It manifests the necessity of using PDOS as cross section.

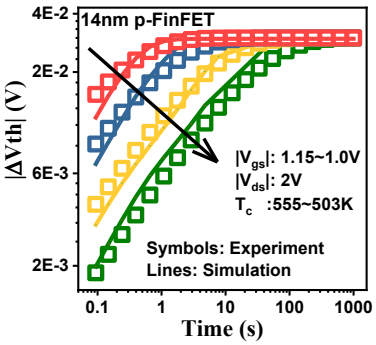

Fig. 15 The HCD simulation results and the comparison with measured data. Again, good agreement is obtained.

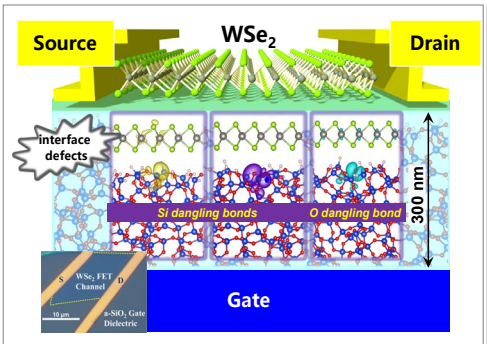

Fig. 16 The experimental setup of WSe_2 2D FET, in which a 300 nm-thick amorphous SiO_2 is used as gate dielectric. In simulation, different kinds of interface defects along with bulk defects are taken into consideration.

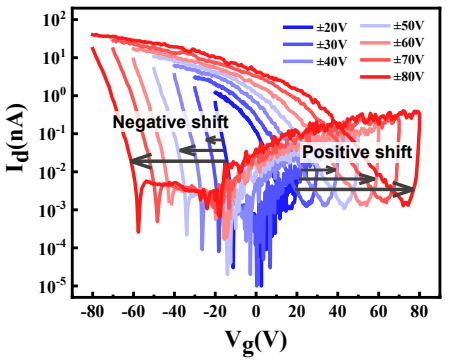

Fig. 17 The experimentally measured transfer characteristics of the WSe_2 FET, which shows an obvious hysteresis. The V_{th} shifts are extracted from each curve for comparison with simulation.

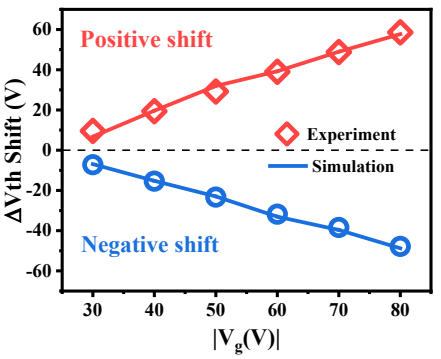

Fig. 18 The simulation results of MARS, which matches the measured data very well. This triply demonstrates the accuracy and advance of our reliability simulator.