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Hierarchical modeling for TCAD simulation of short-channel 2D material-based FETs

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ABSTRACT

An integrated hierarchical modeling flow for fast analysis and prototyping of 2D material-based field-effect transistors (FETs) is presented. Advanced transport simulators using *ab initio* atomistic density functional theory (DFT) and continuum effective mass non-equilibrium Green's Functions (NEGF) consistently provide TCAD tools with device material and component parameters and reference curves for physical model selection and calibration. We validate each step of the hierarchical flow, and we show that the simulations performed with the resulting TCAD setup accurately predict 2D-FETs device characteristics.

1. Introduction

2D-FETs fabricated with transition metal dichalcogenide (TMD) materials are promising candidates to replace silicon technology at 15 nm channel length and below [1]. However, 2D material technology is still facing several challenges, such as forming good source/drain contacts to TMDs [2] and variability issues [3]. The design of short-channel 2D-FETs requires the investigation of atomic-scale phenomena and the accurate analysis of quantum–mechanical effects. At the same time, the traditional drift–diffusion (DD) model used in TCAD is infused with more rigorous approaches to maintain accuracy, while still affording the fast turnaround time and flexibility required by modern development in the semiconductor industry [4].

In this work, we present a hierarchical modeling simulation platform, integrated in Sentaurus Materials Workbench tool of QuantumATK software package by Synopsys [5], for fast analysis and prototyping of 2D-FETs. It allows to investigate the impact on device characteristics of different channel materials, number of channel monolayers (ML), source/drain contact material and orientation, device doping and geometry. The fully comprehensive approach allows consistent comparisons of different solutions. The parameter extractions and exchanges between simulation tools in the hierarchy are automatized.

2. Simulation method

A detailed scheme of the implemented method is shown in Fig. 1. As a first step, atomistic DFT calculations of the chosen 2D channel material are performed with QuantumATK. The material parameters extracted from the results are given as input to Sentaurus Device QTX (indicated with QTX below) [6] to simulate device characteristics using a continuum effective mass (EM) NEGF transport model.

The choice of EM NEGF instead of QuantumATK atomistic full-band NEGF to simulate 2D-FET characteristics is justified by a significant advantage in terms of simulation time and memory consumption. Ballistic EM NEGF simulations run in only a few minutes.

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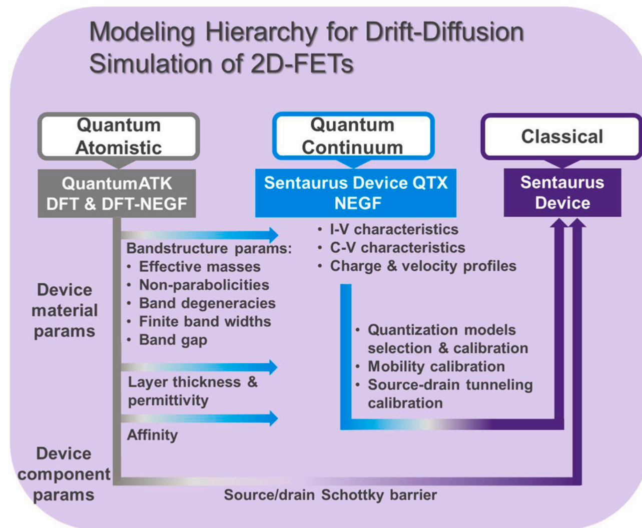


Fig. 1. Schematic of the two-step hierarchical modeling approach implemented in Sentaurus Materials Workbench, with the details of the parameter exchanges.

The calculated curves are used as reference for the calibration of quantum-corrected carrier density, ballistic mobility and source-to-drain tunneling models in Sentaurus Device [7]. The device component parameters extracted from QuantumATK, that is, the source/drain Schottky barriers, are instead given as input directly to the Schottky contact model in Sentaurus Device. The resulting calibrated model setup can be used for TCAD design of short-channel 2D-FETs.

3. Results and discussion

3.1. Device material and component parameters extraction from ab initio calculations

The electronic properties of 2D-FET channels depend on the chosen material and its thickness or number of monolayers [8]. MoS_2 monolayer (1ML), MoS_2 bilayer (2ML) and WS_2 1ML channels are considered here as showcases. However, the method is applicable to other TMDs and number of monolayers.

To simulate the 2D material unit cell we considered GGA and GGA-1/2 exchange–correlation functionals using linear-combination-of-atomic-orbitals (DFT-LCAO) basis set [9]. The implemented code scans the k-space for band minima. The two lowest conduction bands are considered. Their effective mass parameters (effective masses, non-parabolicity coefficients and bandwidths) are automatically extracted by fitting the local band structure. In Fig. 2, MoS_2 1ML DFT band structure is shown. In Table 1, we report the selected band structure parameters that are used in the hierarchical flow (when two values are given for a parameter, they correspond to minima at different locations in the k-space).

In order to extract layer thickness and permittivity of the 2D material to be used in continuum models, we implemented a methodology that first extracts the layer thickness from the projected average *ab initio* electron density. The corresponding dielectric constant is found by matching the electrostatic response of a continuum dielectric region with that thickness to *ab initio* results. An example is shown in Fig. 3. The results for the three different channel configurations are reported in Table 2. For simplicity, the extracted dielectric constant value is used as isotropic permittivity in QTX and Sentaurus Device. We plan to include 2D materials anisotropic permittivity in a future extension of the project.

To calculate the electron affinity, the density of states (DOS) is calculated using plane-wave (DFT-PW) basis set [9] with absolute reference to find the valence band maximum. The band gap previously calculated with DFT-LCAO is then added to the valence band maximum

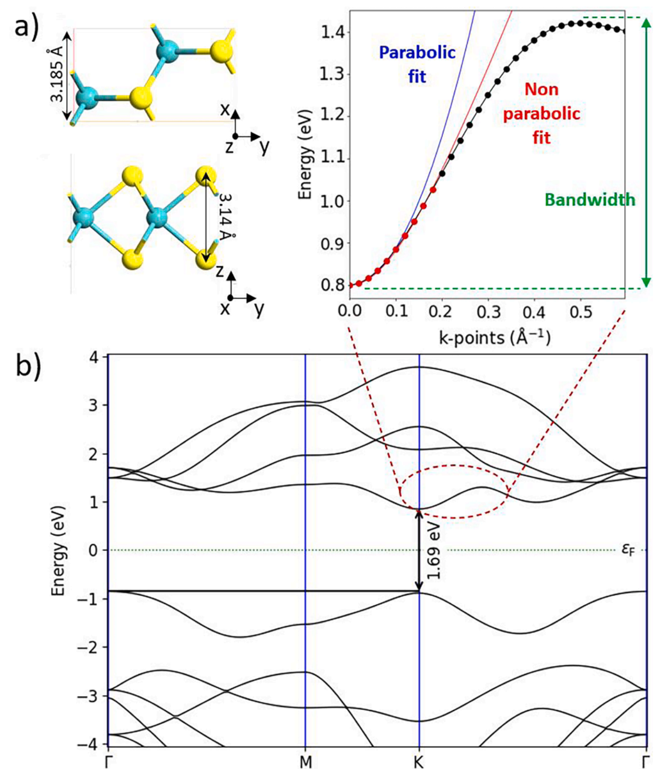


Fig. 2. (a) Relaxed monolayer MoS_2 rectangular unit cell. (b) DFT band structure of monolayer MoS_2. The effective mass parameters are extracted for each valley minima along the two free directions.

to obtain the affinity (Table 2).

The Schottky barrier height (SBH) formed between channel and source/drain contacts is extracted from the calculation of the projected bands of the TMD-metal atomic system (Fig. 4). The simulated structure is chosen to minimize metal strain and system size. The TMD-metal distance is relaxed keeping the unit cell and the relative atom position within each material fixed.

3.2. Validation of EM NEGF simulation approach

In Fig. 5, 2D-FETs ballistic Id-Vg curves calculated with QTX EM NEGF, using the parameters in Tables 1 and 2, and with QuantumATK full-band atomistic DFT NEGF are compared. EM NEGF tends to overestimate the current due to narrow bandwidth of TMDs. We implemented a solution that uses the finite bandwidth extracted from DFT calculation as cut-off for the density of states (DOS) in EM NEGF simulations. A good match between EM NEGF and DFT NEGF Id-Vg characteristics is obtained with the finite bandwidth correction, which validates the first step of the model hierarchy.

Moreover, we have verified that EM NEGF results are in line with full-band results from the literature. For instance, MoS_2 1ML-FET performs better than MoS_2 2ML-FET. Id-Vg curves show smaller subthreshold slope due to a better electrostatic control [8]. We have also seen that WS_2 1ML-FET shows larger ballistic ON current than MoS_2, due to smaller transport mass (not shown here) [10].

3.3. Setup and calibration of Sentaurus Device models

The Sentaurus Device setup for carrier density used to reproduce QTX characteristics includes a multi-valley description, as well as the 2D DOS and the density gradient (DG) models to account for quantum confinement in the transverse direction. The DG parameter *gamma* [7] is modeled as a linear function (with calibrated coefficient) of the 2D layer

Table 1
Effective masses (m_l and m_t), non-parabolicity coefficient (α), band degeneracy (d), bandwidth (BW), band splitting (ΔE) and band gap (BG) of TMDs extracted from *ab initio* calculation.

	First band					Second band					
	ml [m_0]	mt [m_0]	α [eV^{-1}]	d	BW [eV]	ml [m_0]	mt [m_0]	α [eV^{-1}]	d	ΔE [eV]	BG [eV]
MoS_2 1ML	0.48	0.48	1.21	2	0.48	0.8/1.31	1.08/0.71	0.43/1.15	6	0.14	1.69
MoS_2 2ML	0.48/0.48	0.48/0.48	1.47/0.98	4	0.45/0.53	0.78/1.13	1/0.73	2/0.8	6	0.08	1.54
WS_2 1ML	0.32	0.32	0.95	2	0.65	0.73/0.79	0.77/0.7	0.08/0.43	6	0.06	1.88

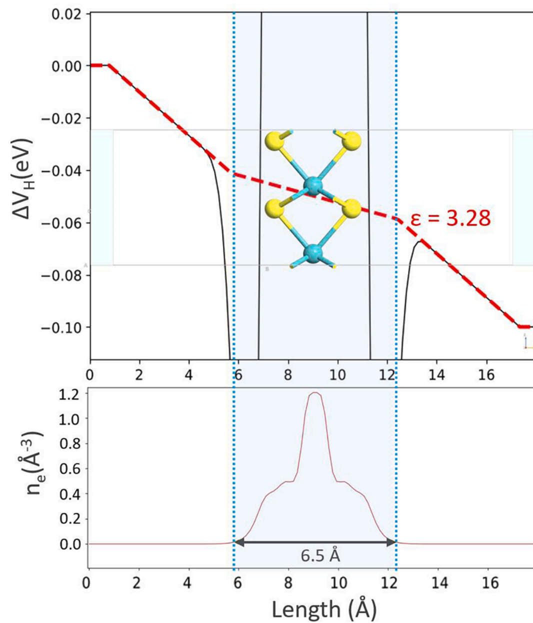


Fig. 3. Top: Hartree Difference Potential of *ab initio* model (black solid line) and continuum model (red dashed line) for MoS_2 1ML. Bottom: *ab initio* electron density for the layer thickness extraction. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 2
Layer thickness, dielectric constant and affinity of TMDs extracted from *ab initio* calculation.

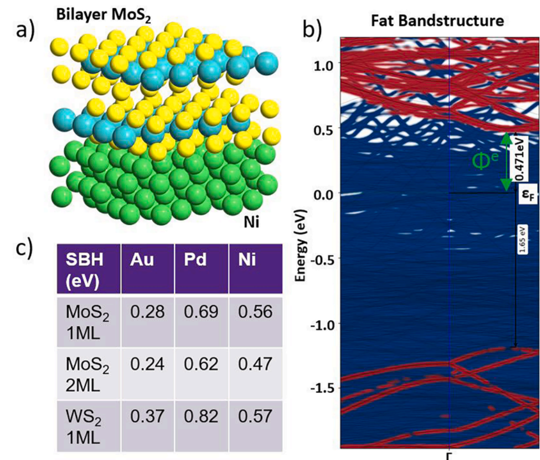
	Layer thickness [nm]	Dielectric constant [ε_0]	Affinity [eV]
MoS_2 1ML	0.6516	3.28	4.25
MoS_2 2ML	1.338	3.38	4.2
WS_2 1ML	0.6521	3.28	3.82

thickness. In Fig. 6, the Sentaurus Device density profile for MoS_2 1ML and 2ML are compared to the corresponding QTX curves. As a result of the good match of the density profiles, the C-V characteristics of Sentaurus Device and QTX are in good agreement too, as illustrated in Fig. 7.

The Kinetic Velocity Model (KVM) is used for the ballistic mobility, accounting for both thermionic emission and free carrier acceleration terms. The source-to-drain tunneling is modeled as non-local tunneling based on WKB approximation [7].

An automatic calibration of the parameters of the ballistic mobility model and the source-to-drain tunneling model is performed to match the QTX linear and saturation Id-Vg characteristics for different channel lengths down to 5 nm. The results for WS_2 1ML-FET are reported in Fig. 8, together with density and velocity profiles along the channel. Sentaurus Device well reproduces QTX characteristics, which validates the second step of the hierarchical model.

The fully automatized parameter extraction and calibration flow runs in a few hours.



SBH (eV)	Au	Pd	Ni
MoS_2 1ML	0.28	0.69	0.56
MoS_2 2ML	0.24	0.62	0.47
WS_2 1ML	0.37	0.82	0.57

Fig. 4. (a) Simulated atomistic MoS_2 2ML-Nickel system. (b) The Schottky barrier height (SBH) is extracted from the fat band structure as the distance between the Fermi energy and the lowest energy conduction band with significant projection weight (0.75). (c) SBH results for different TMD-metal systems are reported. Metals are (1 0 0) oriented.

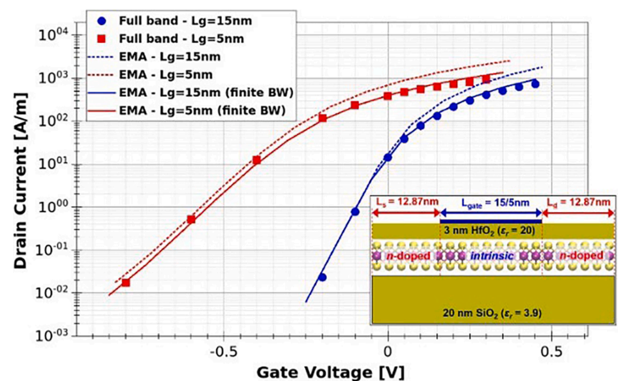


Fig. 5. Id-Vg curves for two different channel lengths (15 and 5 nm) calculated with atomistic full-band NEGF (symbols) and continuum EM NEGF (lines) with and without accounting for the finite bandwidth correction. The simulated structure is also shown (for the continuum case the atomistic channel is replaced by a continuum semiconductor region of thickness from Table 2).

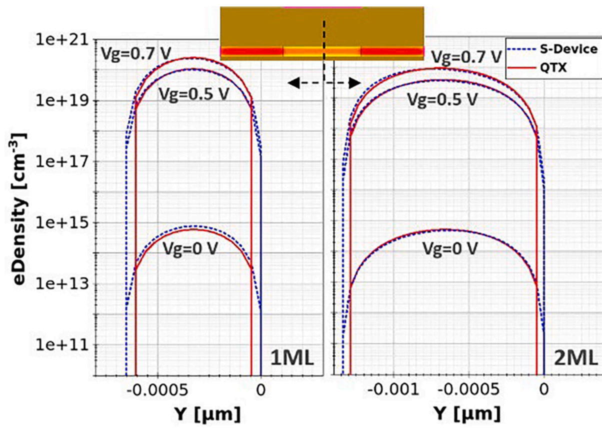


Fig. 6. Comparison between electron density profiles in a device cross-section as a function of the gate voltage calculated with EM NEGF (QTX) and quantum-corrected DD (Sentaurus Device).

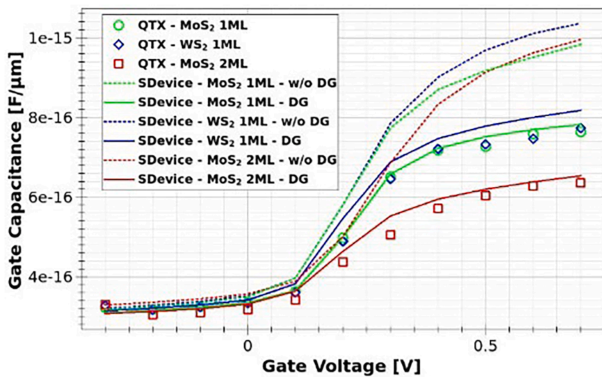


Fig. 7. Cg-Vg curves for three different channels (MoS_2 1ML and 2 ML and WS_2 1ML) calculated with EM NEGF (symbols) and DD (lines) with and without accounting for the density gradient correction.

3.4. Validation of the Sentaurus Device calibrated setup

In the final calibrated Sentaurus Device deck, source and drain contacts are modeled as Schottky contacts with non-local tunneling through the Schottky barrier [7]. QuantumATK provides with the Schottky barrier value for the specific 2D material/metal configuration.

The scattering-limited mobility calculation is not included in the hierarchical flow. Its complexity and sensitivity to device architectural and non-ideal factors in 2D-FETs [11] makes it unpractical for such an automatized flow. However, the Sentaurus Device bulk phonon-limited mobility μ_{max} [7] can be used to model the scattering-limited mobility, as a user input. It represents the measured mobility of a long channel device for the specific 2D-FET technology under investigation. Such mobility value is combined with the KVM ballistic mobility by means of the Frensley formula [7].

The calibrated Sentaurus Device TCAD setup has been tested by comparing the simulation results with measurements from the literature. An example is illustrated in Fig. 9, where we compare experimental Id-Vg characteristics of the 10 nm channel 2D-FET from [12] with the corresponding simulated curves. The simulated structure, that mimics the fabricated 2D-FET device from [12] is shown in Fig. 9. The device materials, the geometrical and doping parameters and the scattering-limited mobility, as measured in [12], are also reported. All the parameters are extracted from the modeling flow or taken from [12]. No parameter fitting has been performed, apart from the threshold voltage, that is adjusted to the experiments. It is known that Al_2O_3 insulator used in [12] introduces a threshold voltage shift [13]. However, the modeling

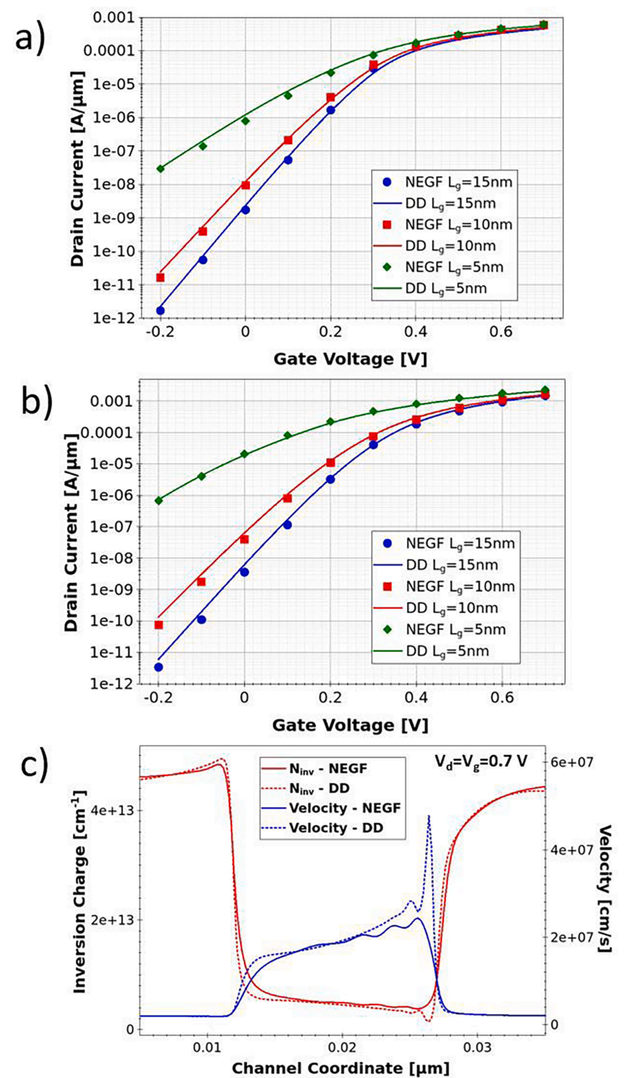


Fig. 8. Id-Vg curves at a) Vd = 0.05 V and b) Vd = 0.7 V for three different channel lengths of WS_2 1ML calculated with EM NEGF (symbols) and DD (lines). c) Inversion charge and velocity profiles along the channel at Vg = Vd = 0.7 V.

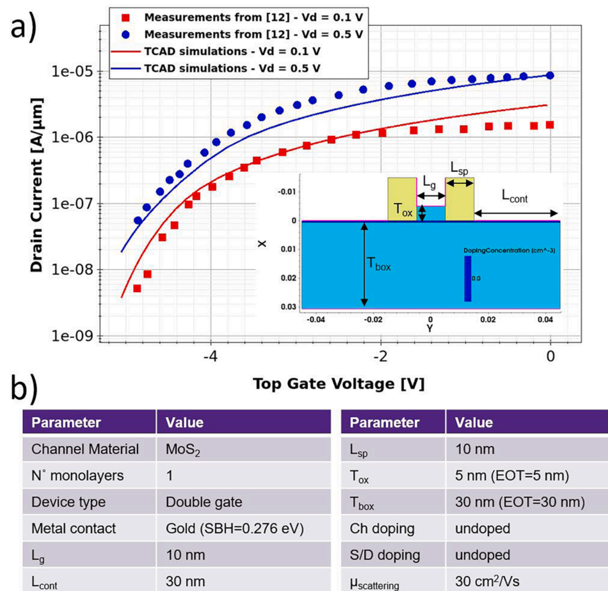
of such effect has not been considered here and needs further investigation.

4. Conclusions

We implemented an integrated example of hierarchical modeling of 2D materials-based FETs, that uses *ab-initio* atomistic DFT, continuum effective mass NEGF and TCAD simulations. The fully automatized parameter extraction and calibration allows to perform fast and consistent comparisons of different solutions for 2D-FETs. A calibrated TCAD deck is provided in an overnight run, which allows flexible device design and can be used to generate reference curves for the development of compact models for Design Technology Co-Optimization (DTCO) of 2D-FETs.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.



Parameter	Value	Parameter	Value
Channel Material	MoS_2	L_{sp}	10 nm
N° monolayers	1	T_{ox}	5 nm (EOT=5 nm)
Device type	Double gate	T_{box}	30 nm (EOT=30 nm)
Metal contact	Gold (SBH=0.276 eV)	Ch doping	undoped
L_g	10 nm	S/D doping	undoped
L_{cont}	30 nm	$\mu_{scattering}$	30 cm^2/Vs

Fig. 9. (a) TCAD Id-Vg simulation results compared with the experimental curves from [12]. The simulated structure is also shown. (b) Device parameters used in the simulation.

Data availability

The code developed is part of Synopsys commercial tools

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