

Interface Modeling for TCAD Simulations of 2D Semiconductor Transistors

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Abstract—In two-dimensional (2D) semiconductor transistors, interfaces such as metal contacts and oxide dielectrics play a critical role in determining the I-V characteristics. Therefore, modeling of interface physics is essential for technology TCAD simulations. In this work, we present a TCAD framework incorporating key interface phenomena in 2D devices, including Schottky contacts, van der Waals (vdW) contacts, and interface traps. Particular attention is paid to vdW contacts, where carrier injection is strongly influenced by image-force barrier lowering (IFBL). The impact of these interface models on the simulated I-V characteristics is demonstrated, highlighting the importance of interface-aware device simulation for the design and optimization of next-generation 2D semiconductor transistors.

Index Terms—TCAD simulations, 2D semiconductors, Schottky contacts, van der Waals contacts

I. INTRODUCTION

Two-dimensional (2D) semiconductors, represented by transition metal dichalcogenides (TMDCs) such as MoS₂ and WSe₂, have attracted significant attention as channel materials for next-generation electronic devices owing to their atomically thin body structure, excellent electrostatic gate controllability, and scalability beyond conventional silicon technologies [1].

Because of their atomically thin body structure, interfaces play a central role in determining the electrical characteristics of 2D semiconductor devices. In particular, interfacial phenomena occurring at metal contacts [3], dielectric interfaces [4], and defect states [5] strongly influence carrier transport and device performance. Accurate modeling of these interface-related effects is therefore indispensable for technology computer-aided design (TCAD) simulations.

Among the various interface effects, carrier injection at metal contacts plays a particularly important role. The carrier injection mechanism strongly depends on the contact structure. In direct metal-semiconductor contacts, carrier injection is mainly determined by the Schottky barrier and contact electrostatics. In contrast, vdW contacts contain a finite van der Waals (vdW) gap between the metal and the semiconductor, which introduces an additional tunneling barrier. Consequently, the current transport mechanism in vdW contacts differs from that in direct contacts, even when identical Schottky barrier heights are assumed. Different physical models are therefore required to describe carrier injection in direct and vdW contact structures.

In addition to Schottky barrier formation, image-force barrier lowering (IFBL) is an important factor affecting carrier injection across metal-semiconductor interfaces [6], [7]. Because IFBL is governed by the local electrostatic environment near the contact, its magnitude and spatial distribution strongly depend on the contact geometry. Accurate evaluation of IFBL therefore often requires numerical electrostatic analysis, particularly for realistic two-dimensional device structures.

Another important issue is the presence of interface states. These states can cause Fermi-level pinning, carrier trapping, threshold-voltage shifts, and degradation of transport properties. Consequently, defect-induced interface states can affect both contact characteristics and channel transport in 2D semiconductor devices.

To achieve predictive TCAD simulations of 2D semiconductor transistors, these interface-specific phenomena must be appropriately incorporated into device models. In particular, physical descriptions of Schottky contacts, vdW contacts, IFBL, and interface trap states are important for understanding and reproducing the electrical characteristics of 2D semiconductor devices.

In this paper, we introduce the basic concepts and modeling approaches for incorporating interface physics into TCAD simulations of 2D semiconductor devices. Physical models for Schottky contacts, vdW contacts, IFBL, and interface trap states are presented, and their roles in determining device characteristics are discussed from the viewpoint of physics-based device modeling.

II. CONTACT MODELING

First, we introduce a drift-diffusion (DD) model for 2D semiconductor transistors with Schottky or vdW contacts. Here, we consider n-type transistors. Since charge carriers are confined in the thin MoS₂ layer, carrier transport is treated as one-dimensional along the channel direction (x -direction). The device is assumed to have an infinite width in the transverse (y) direction, so that variations along the y -axis can be neglected. In the drift-diffusion equation, the current density is described as

$$J(x) = -q\mu_{\text{eff}}n(x)\frac{d\Phi}{dx} + qD_n(x)\frac{dn(x)}{dx}, \quad (1)$$

where n is the sheet electron density, μ_{eff} is the mobility, and Φ is the electrostatic potential. The diffusion coefficient is evaluated using the generalized Einstein relation,

$$D_n = g_n \frac{k_B T}{q} \mu_{\text{eff}}, \quad (2)$$

with

$$g_n = \frac{1}{k_B T} n \left[\frac{\partial n}{\partial E_{F,n}} \right]^{-1}. \quad (3)$$

Here, $E_{F,n}$ is the quasi-Fermi energy, k_B is the Boltzmann constant, and T is the temperature. The continuity equation is given by

$$\frac{1}{q} \frac{dJ(x)}{dx} - R(x) = 0, \quad (4)$$

where $R(x)$ is the carrier injection rate. For a 2D semiconductor, the carrier density is

$$n(x) = \frac{2\pi g_s g_v m^* k_B T}{h^2} \ln \left[1 + \exp \left(\frac{E_{F,n} - E_C}{k_B T} \right) \right], \quad (5)$$

where $g_{s(v)}$ denotes the spin (valley) degeneracy factor. The electrostatic potential is obtained from

$$\nabla \cdot (\epsilon \nabla \Phi) = -qC, \quad (6)$$

where C represents the net charge concentration in the MoS₂ layer.

A. Schottky Contacts

First, we consider the case where the metal is directly connected to the 2D semiconductor, forming a Schottky contact at the metal edge [8], [9]. The carrier injection through the Schottky contact is incorporated into the continuity equation via the injection rate defined in Eq. (4) [10]. The Schottky contribution is expressed as

$$R_{\text{SB}}(x) = \frac{1}{q} \frac{dI_{\text{SB}}(x)}{dx}, \quad (7)$$

where I_{SB} is the current injected from the metal–semiconductor junction. The current per unit width at a metal–2D semiconductor junction is given by

$$I_{\text{SB}} = \int q v_x D(E) [f_M(E) - f_S(E)] T_{\text{SB}}(E_x) dE, \quad (8)$$

where $D(E)$ is the density of states, f_M and f_S are the Fermi-Dirac distribution functions in the metal and semiconductor, respectively, and T_{SB} is the transmission probability through the Schottky barrier. For thermionic emission, electrons above the injection threshold are assumed to be fully transmitted,

$$T_{\text{SB}}(E_x) = 1, \quad E_x > E_{C,0}, \quad (9)$$

where $E_{C,0}$ is the conduction band edge at the top of the Schottky barrier. Electrons with energies below the barrier may tunnel through the Schottky barrier. Approximating the barrier by a triangular potential,

$$E_C(x) = E_F + q\Phi_B - qFx, \quad (10)$$

where Φ_B is the Schottky barrier height and F is the local electric field.

The tunneling probability is evaluated using the WKB approximation. For a triangular barrier, this expression reduces to

$$T_{\text{tun}}(E) = \exp \left[-\frac{4\sqrt{2m^*}}{3\hbar q|F|} (q\Phi_B - E)^{3/2} \right]. \quad (11)$$

The total Schottky current consists of thermionic and tunneling components,

$$I_{\text{SB}}(x) = I_{\text{thermo}}(x) + I_{\text{tunnel}}(x). \quad (12)$$

B. vdW Contacts

For a vdW contact, a finite vdW gap is present between the metal and the 2D semiconductor. In this case, carrier injection from the metal into the semiconductor is described by electron tunneling through the vdW gap followed by thermionic emission over the Schottky barrier. Thus, we express the current through the vdW contacts as

$$J_{\text{vdW}}(x) = A^* T^2 \exp \left(-\frac{q\Phi_B(x)}{k_B T} \right) T_{\text{vdW}} \times [1 - \exp(\eta_{\text{back}}(x))], \quad (13)$$

where A^* is the 3D Richardson constant and

$$\eta_{\text{back}} = \frac{E_{F,n} - E_{F,M}}{k_B T}. \quad (14)$$

The local Schottky barrier height is given by

$$\Phi_B(x) = E_C(x) - E_{F,M}, \quad (15)$$

where $E_C(x)$ is the conduction-band edge and $E_{F,M}$ is the metal Fermi level. The vdW-gap transmission probability is evaluated using the WKB approximation,

$$T_{\text{vdW}} = \exp \left(-2d_{\text{vdW}} \sqrt{\frac{2m_t \Phi_{\text{vdW}}}{\hbar^2}} \right), \quad (16)$$

where d_{vdW} and Φ_{vdW} denote the vdW-gap thickness and barrier height, respectively. The current passing through the vdW contact is incorporated into the TCAD simulation through the carrier injection rate

$$R_{\text{vdW}}(x) = \frac{J_{\text{vdW}}(x)}{q}, \quad (17)$$

which is included in the continuity equation through Eq. (4).

III. INTERFACE TRAP MODEL

In practical 2D semiconductors, carrier transport is often affected by trap-induced band-tail states. At low trap densities, the transport is dominated by band conduction and can be described using the drift-diffusion model. As the trap density increases, trap-assisted hopping transport becomes increasingly important.

To capture this behavior, the total channel current is written as

$$J(x) = -q [\mu_{\text{eff}}(x)n(x) + \mu_{\text{trap}}(x)n_{\text{trap}}(x)] \nabla \Phi(x, 0) + q D_n(x) \nabla n(x) + q D_{\text{trap}}(x) \nabla n_{\text{trap}}(x), \quad (18)$$

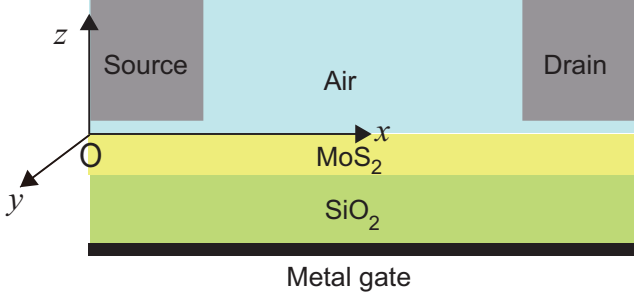


Fig. 1. Schematic illustration of the back-gated MoS₂ transistor with a vdW contact. For a metal such as Au, a vdW gap of approximately 0.3 nm is formed between the metal and semiconductor. The same gap distance was assumed in the FEM calculation of IFBL.

where n_{trap} is a trapped-carrier density. The quantities μ_{trap} denotes the mobility associated with a trap-assisted hopping transport.

To describe the interface trap-induced band-tail states, the density of states is expressed as

$$D_{\text{trap}}(E) = \begin{cases} \frac{2\pi g_s g_v m^*}{h^2}, & E \geq E_C, \\ \frac{N_{IT}}{k_B T_0} \exp\left(\frac{E - E_C}{k_B T_0}\right), & E < E_C, \end{cases} \quad (19)$$

where N_{IT} is the band-tail-state density and T_0 characterizes the disorder strength. The trapped-carrier density is

$$n_{\text{trap}}(x) = \int_{-\infty}^{E_C(x)} D_{\text{trap}}(E) f(E, E_{F,n}(x)) dE, \quad (20)$$

where $f(E, E_{F,n})$ is the Fermi distribution function. The hopping mobility is

$$\mu_{\text{trap}}(x) = \mu_{\text{hop}} \exp\left(-\frac{E_{\text{tr}}(x)}{k_B T}\right), \quad (21)$$

where μ_{hop} is the hopping-mobility parameter and $E_{\text{tr}}(x)$ is the trap activation energy [11].

IV. ANALYSIS OF IMAGE-FORCE BARRIER LOWERING

IFBL strongly depends on the local electrostatic environment near the metal/semiconductor interface. Because the electrostatic boundary conditions vary with the contact geometry, IFBL exhibits a nonuniform spatial distribution in practical 2D devices. Therefore, numerical electrostatic calculations are required for realistic device structures.

In this work, IFBL is evaluated using a three-dimensional finite-element method (FEM). Gold is assumed as the contact metal, and a vdW gap of 0.3 nm is introduced between the metal and the MoS₂ layer. A point electron is placed inside the MoS₂. Poisson's equation is then solved for two otherwise identical structures: one including the grounded metal contact and the other without the metal boundary condition. No

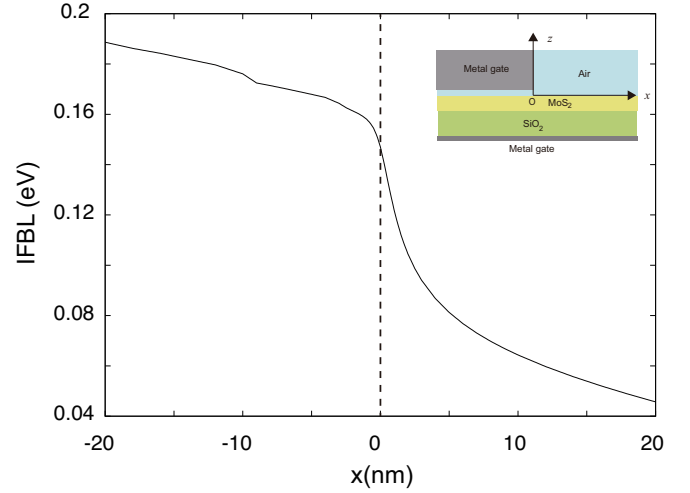


Fig. 2. Calculated image-force barrier lowering (IFBL) distribution for a vdW gap of 0.3 nm.

explicit image charge is introduced in the calculation. The electrostatic potential induced by the presence of the metal is defined as

$$\phi_{\text{ind}}(x) = \phi_{\text{metal}}(x) - \phi_{\text{ref}}(x), \quad (22)$$

where $\phi_{\text{metal}}(x)$ is the electrostatic potential evaluated at the position of the electron in the structure containing the grounded metal, and $\phi_{\text{ref}}(x)$ is the corresponding potential obtained for the reference structure without the metal boundary condition. Because the reference problem with Neumann outer boundaries is defined only up to an additive constant, ϕ_{ind} is shifted to vanish at a reference point sufficiently far from the metal contact. The local IFBL is calculated from the induced potential as

$$\Delta\Phi_{\text{IFBL}}(x) = \frac{1}{2}\phi_{\text{ind}}(x) = \frac{1}{2}[\phi_{\text{metal}}(x) - \phi_{\text{ref}}(x)]. \quad (23)$$

The factor of 1/2 accounts for the work required to induce the charge on the grounded metal as the electron is introduced.

Figure 2 shows IFBL along the MoS₂ at $V_g = 0$ V obtained from the FEM calculation. The IFBL reaches its maximum value underneath the top contact and remains relatively uniform in this region. In contrast, the largest spatial variation occurs near the contact edge, where the IFBL rapidly decreases toward the channel region. These results indicate that the barrier lowering is strongly influenced by the electrostatic environment created by the contact geometry and cannot be treated as spatially uniform.

Next, we calculate the current characteristics of the vdW-contacted back-gated two-dimensional semiconductor field-effect transistor (BG-2DFET) shown in Fig. 1 using the model described in Section II. The calculated transfer characteristics are shown in Fig. 3. In the gate-voltage range considered in this study, the drain current calculated without IFBL is higher than that obtained with IFBL.

To understand the origin of this behavior, Fig. 4 compares the potential-energy and quasi-Fermi-level profiles calculated

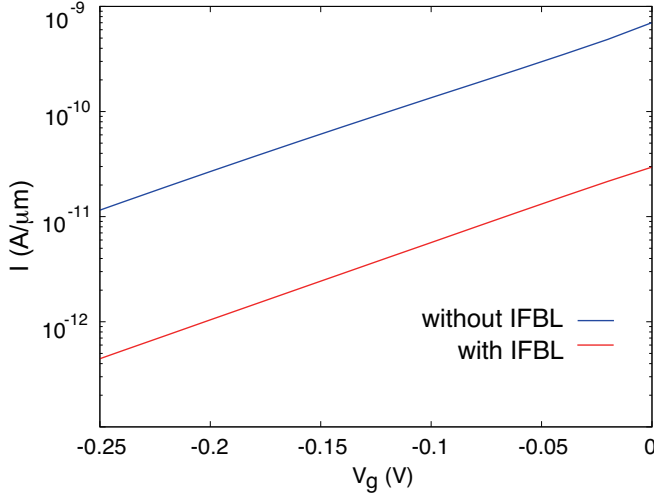


Fig. 3. Calculated drain current as a function of V_G with and without IFBL. The Schottky barrier height and vdW barrier height are $\Phi_B = 0.3$ eV and $\Phi_{\text{vdW}} = 3$ eV, respectively. The channel length is 70 nm, including 20 nm source/drain contact regions. The drain voltage, temperature, and mobility are $V_D = 0.5$ V, $T = 300$ K, and $\mu = 50$ cm²/V·s, respectively. Since tunneling transport in the channel is not included in the present drift-diffusion simulation, only the subthreshold region ($V_G < 0$ V) is shown.

with IFBL (a) and without IFBL (b). Although IFBL reduces the effective Schottky barrier height and is generally expected to enhance carrier injection, the calculated thermionic current decreases when IFBL is included. The blue line in Fig. 4(a) represents the transport potential used in the drift-diffusion calculation, which includes the effect of IFBL. Although IFBL lowers the potential energy underneath the top contact, its magnitude changes most rapidly near the contact edge. Consequently, carriers injected from the contact must overcome an additional potential barrier when entering the channel. In the present simulations, this effect outweighs the reduction of the Schottky barrier height, resulting in a lower drain current.

It should be noted, however, that the present vdW-contact model is highly simplified. In particular, the IFBL is incorporated in the manner described in Section II B, and it remains unclear whether this treatment appropriately describes realistic metal/vdW-semiconductor interfaces. A rigorous assessment of the IFBL effect would require atomistic-scale analyses of the electrostatic potential, electronic structure, and carrier injection processes at the contact interface. Therefore, the physical origin of the current reduction observed in the present simulations requires further investigation.

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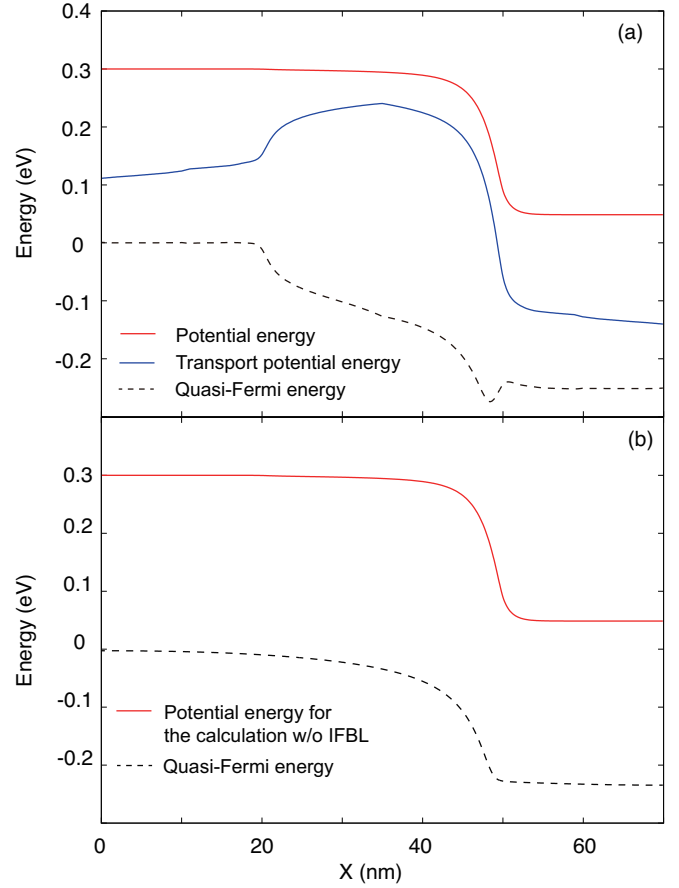


Fig. 4. (a) Potential-energy profile and quasi-Fermi level including IFBL in MoS₂. The blue line shows the transport potential used in the drift-diffusion calculation, which includes the IFBL correction. (b) Potential-energy profile and quasi-Fermi level without IFBL.

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