Ambipolar device simulation based on the drift-diffusion model in ion-gated transition metal dichalcogenide transistors

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INTRODUCTION

In ion-gated transistors, the electric double layer works as a gate dielectric layer of about 1 nm in thickness, and thus such transistors are called electric double layer transistors (EDLTs) or electrolyte gated transistors. Owing to its strong gate coupling, the operation voltage of EDLTs is dramatically reduced, and also, EDLT enables us to control the electronic phases including superconductivity. Materials for EDLTs are extremely rich including carbon nanotubes, organic semiconductors, oxide materials, two-dimensional (2D) materials such as graphene and transition metal dichalcogenides (TMDs).

In particular, TMDs have gained interest thanks to the intriguing phenomena coupled the valley and spin degrees of freedom. This ambipolar nature allows us to fabricate lateral p-n junctions. We clarified the transport voltage is significantly lower than that of the conventional FETs, and is in the voltage range similar to the bandgap energy. This offers an opportunity to determine the band gap directly from the transistor characteristics. It is also known that the p-n junctions formed in the channel emits circularly polarized light, and further, the circular polarization can be flipped by changing the direction of the injected current. This enables the generation of the circularly polarized light using the electric field. This circular dichroism is ascribed to the imbalance of K and K' points in the band structure caused by the electric field. Moreover, the strong electric field induced by the ionic gating yields superconductivity in TMDs due to the high accumulation of carrier.

To achieve more benefit of the ionic gating, the device operation mechanism of EDLTs should be understood. For theoretical studies of transistor operations, the drift-diffusion (DD) method is known as a powerful tool for device simulation to calculate the transport properties, band profile, and spatial distribution of carriers inside devices. As the down-scaling is employed to realize high performance in conventional transistors, the DD simulation is used to design ideal device structures. However, there has been no DD simulation reported on the ion-gated transistors of TMDs.

In this work, we developed a 2D layer transistor model including an ionic liquid (IL) as a gate dielectric, based on the DD method and succeeded in simulating the distribution of ions, and the dynamics of electron and holes passing through the metal contacts. We examined the characteristics of ion-gated TMD transistors whose device size is about submicron while the several microns is the common channel size reported in experiments. The simulation shows that the down-scaled ion-gated WSe$_2$ transistor holds ambipolar behavior and the formation of the p-n junctions reported in larger-scale devices. We clarified the transport...
mechanism and the fundamental physics underneath the transistor operation using the band profile and the spatial distribution of ions and carriers obtained by the calculation.

The mechanism of the ambipolar transistor has been discussed theoretically on organic and amorphous materials because it is easy to inject both electrons and holes due to the in-gap states. In single crystalline TMDs, such mid-gap states are absent. On the other hand, previous simulations on ion-gated organic transistors used a fixed capacitance induced by the ionic liquids, which cannot include the variation of the capacitance due to the modification of the ion distribution by the source-drain bias voltage and the back action from the carriers in semiconductors. The general perspective of the ambipolar transport in MOSFETs has been discussed in ref. 46.

Some specific implementations are required to adopt the DD model to the ion-gated transistors. We explain the points which differ from the DD model used for the conventional transistors in the next section. After describing the model, we show the results of device simulations on the ion-gated WSe2 transistors. The current, band profile and ion/carrier density distributions are examined for the unipolar and ambipolar operation.

**RESULTS AND DISCUSSION**

Drift-diffusion model for ion-gated transition metal dichalcogenide transistors

We start with the explanation of the DD model. We consider the 2D layer in (x, y) plane where the transport direction of the channel is set to x. The IL and oxide layer are piled up in the z direction as depicted in Fig. 1. We solve the continuity equation of each current,

\[
\frac{1}{q} \nabla J_n(x) - R(x) = 0, \quad (1)
\]

\[
\frac{1}{q} \nabla J_p(x) - R(x) = 0. \quad (2)
\]

where \( J_n(x) \) and \( J_p(x) \) denote the electron (hole) current densities. \( q \) is the elementary charge, \( n(x) \) (\( p(x) \)) is the electron (hole) density at location (x, 0) in WSe2, \( n(x) \) and \( p(x) \) are defined in units of cm\(^{-2} \). \( \mu_{n(p)} \) denotes the electron (hole) current density, and \( D_{n(p)}(x) \) is the diffusion coefficient. \( \Phi(x, 0) \) is the potential at position x. \( R(x) \) denotes the recombination rate, \( R(x) = R_{\text{dir}}(x) + R_{\text{SRH}}(x) + R_{\text{fi}}(x) \). We consider two types of the recombination rate; the direct recombination rate, \( R_{\text{dir}}(x) \), and the Shockley-Read-Hall (SRH) recombination rate, \( R_{\text{SRH}}(x) \), where

\[
R_{\text{SRH}}(x) = \frac{n(x)p(x)}{\tau(n(x) + p(x))}. \quad (6)
\]

Here, \( \beta \) is the direct recombination parameter and \( \tau \) is the recombination time of the SRH recombination, \( n_{\text{in}} \) is the intrinsic carrier density of electrons and holes. For WSe2, \( n_{\text{in}} = 2k_BT\sqrt{m_e/m_h} \exp[-\frac{\Phi_{\text{SB}}}{k_BT}] \sim 3 \times 10^{-6} \text{ cm}^{-2} \) at \( T = 220 \text{ K} \), where \( m_e \) and \( m_h \) are the effective mass of electrons (holes), \( m_0 \) is the mass of free electrons, and \( \Phi_{\text{SB}} \) is the Boltzmann constant. \( R_{\text{fi}}(x) \) indicates the generation or annihilation rate of the carriers which enter or exit from the channel at x through the thermionic or tunnel current. Thus, the boundary conditions for \( n(x) \) and \( p(x) \) are determined by the continuity equation in Eqs. (1), (2). The detailed description of \( R_{\text{fi}}(x) \) is written in the Methods section.

We also solve the Poisson equation in the (x, z) plane in the whole system (WSe2, ILs, SiO2, and the metal contact)

\[
\nabla \Phi(x, z) = -qC(x, z), \quad (7)
\]

where \( C(x, z) = \epsilon(x, z) - \epsilon(x, z) \) for \( z > 0 \), \( C(x, z) = [p(x) - n(x)]d \) for \( -d < z < 0 \), and \( C(x, z) = 0 \) for \( z < -d \). Here, \( \epsilon(x, z) \) is the relative permittivity of the material \( \alpha \) (\( \epsilon \) in WSe2, SiO2, and IL), and \( \epsilon_0 \) is the permittivity of vacuum. \( \epsilon_{\text{WSe2}} \) is direction dependent as shown in Table 1. The boundary condition is set to satisfy the continuity of the normal vector of the electric flux density at the interface between materials. The boundary condition at the metal

| Parameter            | Symbol | Value       |
|----------------------|--------|-------------|
| Electron mobility    | \( \mu_n \) | 43 cm\(^2\)/(V s)\(^a\) |
| Hole mobility        | \( \mu_p \) | 84 cm\(^2\)/(V s)\(^a\) |
| Channel length in x direction | \( L_x \) | 80 nm |
| Channel length in y direction | \( L_y \) | 100 nm |
| Thickness of WSe2 layer | \( d \) | 0.65 nm\(b\) |
| Thickness of IL      | \( t_{\text{IL}} \) | 10 nm |
| Thickness of SiO2 layer | \( t_{\text{SiO2}} \) | 10 nm |
| Band gap             | \( E_g \) | 1.6 eV\(^c\) |
| Electron effective mass | \( m_e \) | 0.33\(a\) |
| Hole effective mass   | \( m_h \) | 0.46\(a\) |
| Direct recombination rate | \( \beta \) | 1 \times 10^{-5}\((\text{m}^2/\text{s})\)^\(a\) |
| SRH rate             | \( \tau \) | 40 ns\(a\) |
| Temperature          | \( T \) | 220 K\(^f\) |
| Relative permittivity of ion | \( \epsilon_{\text{WSe2}} \), \( \epsilon_{\text{SiO2}} \) | 7.25, 5.16\(^b\) |
| Relative permittivity of WSe2 | \( \epsilon_{\text{WSe2}} \) | 3.8 |
| Height of Schottky barrier | \( \Phi_{\text{SB}} \) | 0.6 eV\(^b\) |
| Average ion concentration | \( n_i \) | 2 \times 10^{20} \text{ cm}^{-3} |
| Screening parameter of ions | \( y \) | 0.2 |

\(^a\) Extracted from the density of states and the four terminal resistance in ref. 15.
\(^b\) See ref. 62.
\(^c\) See ref. 26,27.
\(^d\) See ref. 63.
\(^e\) Estimated from the size of the recombination zone in ref. 15.
\(^f\) See ref. 15.
\(^g\) See ref. 64.
\(^h\) See ref. 65.
\(^i\) See ref. 56.
contact is set as $\Phi(x, t_s) = V_{ds} + \Phi(x, 0)$, where $t_s$ is the thickness of IL. At the other edges, we adopt the Neumann's boundary condition, $\frac{\partial \Phi(x, t_s)}{\partial x} = 0$, where $L_x$ is the length of WSe$_2$ layer in x direction, and $t_{SiO_2}$ is the thickness of the SiO$_2$. The carrier densities [$n(x)$ and $p(x)$] in the DD equation and the potential [$\Phi(x, z)$] in the Poisson equation are determined self-consistently in the numerical calculations.

To adopt the above DD model to the ion-gated transistors, there are three points to be noticed regarding the difference between the conventional and ion-gated transistors. Firstly, in Eqs. (3) and (4) the ordinary Einstein relation between the mobility and the diffusion coefficient is not appropriate for ion-gated transistors since the ions attract the high concentration of carriers above $10^{13}$ cm$^{-2}$ while the carrier concentration is usually below $10^{12}$ cm$^{-2}$ in the conventional transistors. Instead, we introduce the generalized Einstein relation (as explained in the Methods section) for the DD model at high carrier concentrations.

The second point is the treatment of the contact. It is known that metal-TMD junctions usually show the Schottky behavior in the conventional TMD transistors with some exceptions such as ones using graphene or Scandium contacts. The mechanism of the Schottky transport has been precisely studied theoretically. The conventional TMD transistors also have the problem of the Fermi-level-pinning due to the defect at the TMD-metal junctions. Thus, only n-type operations have been reported in many works for conventional MoS$_2$ FETs. However, the Fermi-level pinning seems to be weak in the ion-gated TMDs, according to the experimental results. We assume the contact made of an alloy of Ti and Au. The mechanism of the Schottky transport has been precisely studied theoretically. The conventional TMD transistors also have the problem of the Fermi-level-pinning due to the defect at the TMD-metal junctions. Thus, only n-type operations have been reported in many works for conventional MoS$_2$ FETs. However, the Fermi-level pinning seems to be weak in the ion-gated TMDs, according to the experimental results. We assume the contact made of an alloy of Ti and Au.

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Device simulation of WSe$_2$ transistors

The schematic view of ion-gated monolayer WSe$_2$ transistors considered is depicted in Fig. 1. The employed parameters for the calculation are written in Table 1. The length of WSe$_2$ in the $x$ (channel) direction is set at 100 nm and the source and drain contacts with 10 nm length are attached to the top of WSe$_2$ monolayer. We assume that electrons tunnel between metal contacts and the channel at $x = 10$ nm and $x = 90$ nm so that the real channel length is 80 nm. We set the energy difference between the work function of TMD and metal contact to 0.6 eV considering the metal contact made of the alloy of Ti and Au. In this calculation, we set the Fermi energy of the metal source to be zero. The energy level of the bottom of the conduction band is 0.6 eV at the source contact surface while the top of the valence band is $-1.0$ eV. The thickness of the IL is 10 nm and the metallic gate contact is attached to the top of the IL. The thickness of the SiO$_2$ layer at the bottom of the WSe$_2$ is 10 nm with the Neumann condition. We assume ions such as DEME-TFSI (N,N-diethyl-N-methyl-N- (2-methoxyethyl) ammonium bis (trifluoromethylsulfonyl)-imide) whose size is approximately 1 nm so that we fix the maximum ion concentration on the ion layer at the electric double layer to $n_{max} = 1 \times 10^{11}$ cm$^{-2}$. The average ionic concentration is set to $n_i = 2 \times 10^{29}$ cm$^{-3}$. Though the employed $n_i$ is lower than the real concentration due to the restriction in the numerical calculation (abrupt change of the carrier and ion concentrations), the approximate maximum of the IL capacitance is $40 \mu$F/cm$^2$, which is large enough to bend the potential and make the Schottky barrier sufficiently thin so that the source and drain contacts show the Ohmic behavior. We use the constant mobility extracted from the experiment in ref. We neglect the $V_{ds}$ dependence of mobility since the potential is relatively flat inside the channel region beside the metal-TMD surface, as described later in the next section. Furthermore, we assume that the concentration of defects inside WSe$_2$ is negligible so that mobility is not affected by carrier concentration tuned by the gate voltage.

We start from examining the transport characteristics of ion-gated WSe$_2$ transistors using the theoretical model. As shown in Fig. 2a, b, the drain-source current, $I_{ds}$, is calculated as a function of the voltage determined from the potential difference between the source contact and the center of the ionic liquid, $V_{ref} = \Phi(10, 5) - \Phi(10, 0)$ [see inset of Fig. 2b]. We should mention that $V_{ref}$ is adopted in Fig. 2a, b instead of the gate voltage between the source contact and the metal gate, $V_{gs}$ to subtract the potential drop occurs at the surface of the gate contact for the considered system. Note that IL can be considered as two capacitors in series; one is the electric double layer capacitor (EDLC) of the gate electrode and the ionic liquid, and the other is the EDLC of WSe$_2$ and the ionic liquid. The surface area of the metal gate attached to the IL is usually much more substantial in experiments. Since the number of net ions at both capacitors should be the same, the ion concentration at the substantial metal gate is much smaller than the one at the WSe$_2$ surface. Thus, potential drops at the metal gate is negligible. However, in our calculation we set the surface area of the metal gate 100 nm/80 nm larger than the one of the WSe$_2$ due to the constraints of the numerical calculation. Thus, approximately half of the potential drops at the metal gate. So we define $V_{ref}$ to compare the results with experiments. The bias voltage between the drain and source electrodes is set at $V_{ds} = 0.2$ V. Note that the current flows from the drain contact to the source contact when $V_{ds}$ is positive. The center of the off-gate voltage slides to the minus ($-0.2$ V) from the zero point since the energy difference between the metal contact and WSe$_2$ is 0.6 V which is 0.2 V above the center of the band gap. As shown in Fig. 2b, using the linear-scale plot, we estimate the threshold voltage from the intersection point of the line $V_{th} = 0$ and the dotted linear line of the current. Here, the dotted line is determined from the least-square method using the data from $1.2 < V_{ref} < 1.5$ V for the electron current, and $-1.5 < V_{ref} < -1.3$ V for the hole current. The determined threshold voltage is $V_{th,e} = 0.94$ V for the electron current, and $V_{th,h} = -1.17$ V for the hole current, respectively. The threshold voltages for electrons and holes have been used to measure the bandgap of the semiconductor as reported in ref. 38. In our numerical calculation, the energy difference between the threshold voltages of electron and hole currents is $e(V_{th,e} - V_{th,h}) = 2.11$ eV, which is 0.51 eV larger than the real band gap, $E_g$. Figure 2c shows the distribution of the net carrier concentration inside the channel. The net carrier is only electrons when $V_{ref} > 0$, while holes become carriers for $V_{ref} < 0$. Note that minor carrier...
is negligibly small and can not be determined by the numerical calculation. The carrier density of electrons or holes is almost constant besides the region around the contact.

Top panels in Fig. 3 show two-dimensional plots of the net ion density $i'(x, z) - i'(x, z)$ for $V_{gs} = -2 V$ (a: $V_{ref} = -1.46 V$, $V_{gs} = 0.2 V$). The dotted linear lines are determined by the least-square method using data from $1.3 V < V_{ref} < 1.5 V$ for the electron current and $-1.5 V < V_{ref} < -1.3 V$ for the hole current. The interaction points of $i_{ds} = 0$ and the linear lines indicate the threshold voltages for the electron and hole currents; $V_{th-e} = 0.94 V$, and $V_{th-h} = -1.17 V$ respectively. Net carrier concentration for $V_{ref} = -2 V (V_{ref} = -1.46 V)$ [dot-dashed line], $V_{gs} = 0.2 V (V_{ref} = 0.19 V)$ [solid line], and $V_{gs} = 2 V (V_{ref} = 1.38 V)$ [dotted line].

Next, we calculate the $I_{ds}-V_{ds}$ characteristics at $V_{gs} = 1.5 V$ where the carrier type is n-type. We plot the electron (dotted line), hole current (dot-dashed line), and the total current (solid line) as shown in Fig. 4. The $I_{ds}-V_{ds}$ characteristics can be classified to the three regions: the linear ($0 \lesssim V_{ds} \lesssim 1.2 V$), the saturation ($1.2 V \lesssim V_{ds} \lesssim 2.8 V$), and the ambipolar region ($V_{ds} \gtrsim 2.8 V$). In the linear region, the current increases with $V_{ds}$ approximately linearly around $V_{ds} = 0 V$, followed by the saturation region starting at $V_{ds} \gtrsim 1.2 V$. Above $V_{ds} \gtrsim 2.8 V$, $I_{ds}$ takes off again, indicating the onset of hole current injected from the drain electrode (ambipolar transport). This feature is similar to the experimental output curve of WSe2 device for larger devices. The increase of electron current in the ambipolar region is due to the recombination of electrons and holes inside the channel.

Figure 5 shows the 2D plot of the net ion density of the IL (top), and band profile of the WSe2 channel and the metal contacts (bottom) for the linear region (a: $V_{ds} = 0.5 V$), saturation region (b: $V_{ds} = 2.5 V$) and ambipolar region (c: $V_{ds} = 4 V$). The figures from d to f are the enlarged views of the potential profile around the contacts. The open arrows denote the tunnel transport while the solid arrows denote the thermionic transport where carriers go beyond the barriers.

In the linear region (Fig. 5a), the cations are dominant at the interface attached to WSe2. Therefore, the current is dominated by electrons since the band gap allows only electrons to tunnel through the metal-WSe2 junctions as depicted in Fig. 5d. By increasing the bias voltage $V_{ds}$, the electrons tunneling from the channel to the drain contact gains. The inclination of the current in the linear region is estimated to be $7.5 \times 10^{-4} \Omega^{-1}$. Thus, the estimated contact resistance is $R_{contact} \approx 10 k\Omega$ while the channel resistance is $R_{ch} = 1/\mu_{eff} \approx 4 k\Omega$ ($\mu_{eff} \approx 4 \times 10^{13} \text{cm}^{2}\text{V}^{-1}\text{s}^{-1}$) so that the contact resistance is comparable to the channel resistance, which results in the linear behavior.

In the saturation region, cations are dominant at the interface attached to WSe2 while anions assemble at the drain contact as shown in the top panel of Fig. 5b. The potential energy at the drain contact switches from upward to downward (the bottom
The ambipolar behavior does not occur for the conventional metal-oxide-semiconductor (MOS) transistors with the same $V_{ds}$. In the Section III of the Supplementary information, we show the current and band profile of the WSe$_2$ MOS transistor, whose oxide layer has the same permittivity with IL (Supplementary Fig. 2a). To fix the carrier concentration to the same order to the ion-gated transistors, we set the gate voltage to $V_{gs} = 10$ V so that $n \sim 5 \times 10^{13}$ cm$^{-2}$ at the equilibrium condition. The current increases monotonously with $V_{ds}$, and the transistor is always n-type as shown in Supplementary Fig. 2b. Supplementary Fig. 3 is the band profile for the MOS transistor. The potential energy decreases linearly at the channel region by applying $V_{gs}$, and the Schottky barrier at the drain area becomes perfect contact for electrons to pass through from WSe$_2$ to the metal. The Fermi energy of the metal contact is located inside the band gap so that the holes cannot pass through the barrier. Thus, the drain contact keeps acting as n-type contact and the current holds unipolar up to $V_{ds} = 4$ V.

Figure 6 displays the spatial distributions of the net carriers, electrons, and holes at the channel area for the linear region (a: $V_{ds} = 0.5$ V), saturation region (b: $V_{ds} = 2.5$ V), and ambipolar region (c: $V_{ds} = 4$ V). In the linear region, the electron density slightly varies around $n \sim 4 \times 10^{13}$ cm$^{-2}$. In the saturation region, on the other hand, the electron densities are not constant anymore, and a depletion point appears at the drain contact. There are a few numbers of holes as shown in the inset of Fig. 6b ($p \sim 10^{9}$ cm$^{-2}$) which is injected from the drain contact by the thermionic transport although the hole tunneling is prohibited in the saturation region. In the ambipolar region, electrons and holes are spread throughout the whole channel area so that small difference between the electron and hole concentrations makes the p-n junction. Therefore, the electrons and holes can recombine in the whole area of the channel as shown in the Supplementary Fig. 1 of the Supplementary information (Section II). There is no depletion region when the applied voltage is higher than the built-in potential. Then, the potential drop at the p-n junction is determined by the recombination zone. The size for the recombination zone is estimated to be $1/\sqrt{\beta/D_n \max[p(x)]}$ $\sim 1 \mu$m in our case. Thus, the channel size we consider is much smaller than the recombination region. It leads to no potential change at the cross-section between n and p regions.

The application of the ion-gated TMD transistors can be very broad, stemming from light emitting devices.$^{3,57}$
superconductivity\textsuperscript{58}, to thermoelectric properties\textsuperscript{59}. Here, we pick up transistors that emit circularly polarized light owing to the peculiar electronic structure of TMDs. Since there has been no simulation model constructed in this area, the essential physical factor in determining the performance of the light-emitting device is yet not known. This simulation method is advantageous to explore the crucial factors and design the ideal device structure. We can examine the characteristics of light emission by calculating the recombination rate, as demonstrated in Section II of Supplementary Information. In the simulation, the parameters presented in Table 1 can be tuned to explore the crucial factors. These factors can also be realized in experiments by changing the materials and device structures.

In conclusion, we have developed the DD model for the ion-gated TMD transistors and explained the characteristic transport behavior of the ion-gated WSe\textsubscript{2} transistors. We adopt the DD model coupled to the Poisson equation for calculating the band profile, carrier densities, and current. In the Poisson equation, the model including the screening effect of charge is employed to derive the potential profile of the IL. In the DD model, the generalized Einstein relation is considered for high carrier densities and the model of the practical Schottky contact is

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**Fig. 5** Ion density and band profile as a function of \(V_{ds}\). a–c (Top) Net ion density \(i^{−}(x, z) − i^{+}(x, z)\) on the ionic liquid for a \(V_{ds} = 0.5\) V, b \(V_{ds} = 2.5\) V, and c \(V_{ds} = 4\) V. The gate voltage is fixed to \(V_{gs} = 1.5\) V. (Bottom) Band profile of WSe\textsubscript{2} and the metal. The Fermi-energy of the source contact is set to \(\phi_{metal} = 0\). The dotted lines indicate the bottom of the conduction band, \(E_c\) (blue), and top of the valence band, \(E_v\) (red). The solid lines are the quasi-Fermi energy for electron \(\phi_e(x)\) (blue) and hole \(\phi_p(x)\) (red). d–f The extension view of the potential profile around the contacts (\(x = 7–13\) nm and \(x = 87–93\) nm) for a \(V_{ds} = 0.5\) V, b \(V_{ds} = 2.5\) V, and f \(V_{ds} = 4\) V. Black lines are the Fermi-level at the metal contacts. The arrows show the transport direction of electrons (blue) and holes (red). The open arrows indicate the tunnel transport and the solid arrows denote the thermionic transport. The thicker arrows indicate the dominant paths of the current.

**Fig. 6** Electron concentration, \(n(x)\) (dashed line), hole concentration, \(p(x)\) (dot-dashed line), and net carrier concentration, \(n(x) − p(x)\) (solid line) inside the channel. The three panels are for a \(V_{ds} = 0.5\) V, b \(V_{ds} = 2.5\) V, c \(V_{ds} = 4\) V, respectively. For b, the hole concentration is plotted instead of \(p(x)\).
employed for considering the Schottky and Ohmic behavior of the transistors. One of the peculiar features of ion-gated transistors of 2D materials is the ambipolar behavior with the application of the gate voltage comparable to the band gap energy. The simulation explains the fundamental physics underneath ambipolar transport and the formation of p–n junctions in the channel. The present result indicates that the DD model coupled with the Poisson equation is a fascinating tool to study ion-gated transistors. By including the spin, valley, and optical degree of freedom to the DD model, we can examine the functionality and to design the device structure of ion-gated transistors.

**METHODS**

We introduce the concrete explanation of the models. In the DD equation, Eqs. (3) and (4), \(D_{i(g)}(x)\) is not described using the ordinary Einstein relation since the Boltzmann distribution is not satisfied in the considered system due to the high carrier concentration above \(10^{13}\) \(\text{cm}^{-2}\). Then, we adopt the generalized Einstein relation for the DD model\(^47\). The generalized Einstein relation which obeys the Fermi distribution is expressed as

\[
D_{i(g)}(x) = g_{i(g)}(x) \frac{k_B T}{q} \mu_{i(g)},
\]

where

\[
g_{i}(x) = \frac{1}{k_B T} n_i(x) \left( \frac{\partial n_i(x)}{\partial \varphi_i(x)} \right)^{-1}, \tag{9}
\]

\[
g_{p}(x) = \frac{1}{k_B T} p_i(x) \left( \frac{\partial p_i(x)}{\partial \varphi_i(x)} \right)^{-1}. \tag{10}
\]

Here, \(\varphi_{i(g)}\) is the quasi Fermi potential of electrons (holes). \(k_B\) is the Boltzmann constant, and \(T\) is the temperature. Note that \(g_{\text{RGG}} = 1\) for the ordinary Einstein relation.

For realizing the practical Schottky contact, we consider the thermionic current and tunnel current passing through the metal–TMD junctions. For the thermionic current density of electrons at the source (drain) contact is written as

\[
J_{\text{therm}}(x) = \pm A_{2D} \gamma T^{3/2} \left[ F_{1/2} \left( \frac{E_i(x) - \varphi_i(x)}{k_B T} \right) - F_{1/2} \left( \frac{E_i(x) - \varphi_{\text{metal}}(x)}{k_B T} \right) \right], \tag{11}
\]

while the thermionic current density of holes is

\[
J_{\text{therm}}(x) = \pm A_{2D} \gamma T^{3/2} \left[ F_{1/2} \left( \frac{E_i(x) - \varphi_i(x)}{k_B T} \right) - F_{1/2} \left( \frac{E_i(x) - \varphi_{\text{metal}}(x)}{k_B T} \right) \right]. \tag{12}
\]

Here, \(F_{1/2}\) is the Fermi integral

\[
F_{1/2}(\eta) = \frac{1}{1 + \exp \left( \frac{\eta}{T} \right)} \tag{13}
\]

where \(\Gamma(x)\) is the gamma function. \(A_{2D}\) is the Richardson constant for the 2D materials\(^49\),

\[
A_{2D} = 2 \times 10^4 \left( \frac{8nk_B^2m_0^2m_e}{h^2} \right)^{1/2} / [\text{cm}^{-2}/\text{K}^2]. \tag{14}
\]

\(E_i(x)\) and \(E_j(x)\) denote the energy at the bottom of the conduction band and the top of the valence band, respectively. \(\varphi_{\text{metal}}(x)\) is the Fermi energy of the source (drain) metal contact. Two is the factor stemmed from the valley degree of freedom of the monolayer TMD. We should mention that the thermionic current is considered only at the junction between the source (or drain) contact and channel, \(x_c(x)\). The tunnel current densities at \(x\) from source (drain) contact for electrons and holes are written as

\[
J_{\text{tunnel}}(x) = \frac{A_{2D}}{k_B} \gamma T^{1/2} \int_{E_i(x_c)}^{E_j(x_c)} \left( F_{1/2} \left( \frac{\varphi_i(x)}{k_B T} \right) - F_{1/2} \left( \frac{\varphi_{\text{metal}}(x)}{k_B T} \right) \right) dx \tag{15}
\]

and

\[
J_{\text{tunnel}}(x) = \frac{A_{2D}}{k_B} \gamma T^{1/2} \int_{E_i(x_c)}^{E_j(x_c)} \left( F_{1/2} \left( \frac{\varphi_i(x)}{k_B T} \right) - F_{1/2} \left( \frac{\varphi_{\text{metal}}(x)}{k_B T} \right) \right) dx.
\]

The datasets generated during and analyzed during the current study are available from the corresponding author on reasonable request.

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A.U., Y.Z. and Y.I. conceived the work. A.U. proposed the simulation model and performed the simulation. All authors analyzed the results and wrote the paper.

COMPETING INTERESTS
The authors declare no competing interest.

ADDITIONAL INFORMATION
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