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Analyzing the Contact-Doping Effect in In₂O₃ FETs: Unveiling the Mechanisms Behind the Threshold-Voltage Roll-Off in Oxide Semiconductor Transistors

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Abstract—In this work, the contact-doping effect (CDE) and its impact on the threshold voltage (V_T) roll-off in indium oxide (In2O3) field-effect transistors (FETs) are systematically studied. By analyzing the long channel length (L_{ch}) and short L_{ch} devices separately using a modified transfer length method (TLM), ΔL can be extracted to quantify the CDE. The correlation between ΔL and the \dot{L}_{ch} at which V_{T} roll-off occurs suggests that CDE may be a key factor contributing to the V_T roll-off in In₂O₃ transistors. Next, the underlying mechanisms of CDE are investigated. It is found that oxygen scavenging reactions (OSRs) during the deposition of source/drain (S/D) metals on the In₂O₃ channel is one of the reasons behind CDE. S/D metals can scavenge oxygen atoms from In₂O₃, creating oxygen vacancies and increasing the carrier density near the S/D regions. Additionally, the Schottky barrier height (Φ_{SB}) of metal/ $\ln_2 O_3$ contacts might also influence the CDE: a positive Φ_{SB} depletes carriers, while a negative Φ_{SB} accumulates them in the In₂O₃ channel under the S/D. This study provides a new approach to investigating CDE and highlights its critical role in understanding the V_T roll-off in oxide semiconductor (OS) transistors.

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I. INTRODUCTION

NDIUM oxide (In₂O₃) based oxide semiconductor (OS) field-effect transistors (FETs) have gained increasing research attention in recent years due to their promising application for monolithic 3-D integration (M3DI) [1], [2], [3], [4], [5], [6], [7], [8], [9], [10], [11], [12], [13], [14], [15]. The concept of M3DI is to directly grow and fabricate semiconductor devices on top of an already processed front-end-of-line (FEOL) layer, such as silicon logic devices or chips [1], [16]. This approach enhances chip performance in two ways: *more Moore* and *more than Moore*. First, M3DI increases the device density per area by stacking additional transistors above the FEOL layer (*More Moore*) [7], [14]. Second, it enables heterogeneous integration of various semiconductor devices—such as radio frequency (RF) [17], [18], memory [15], and power devices [19]—to enhance chip functionality (*More than Moore*).

A key challenge in achieving M3DI is the strict back-end-of-line (BEOL) thermal budget, which typically requires processing temperatures below 400 °C [1]. Fortunately, OSs can be deposited and further processed at temperatures below this limit, making them excellent candidates for M3DI [5]. Among various OS FETs, atomic-layer-deposited (ALD) In_2O_3 FETs offer several advantages, including excellent conformality and uniformity on 3-D structures [5], high electron mobility of 152 cm²/(V·s) [20], ultrahigh ON-current (\sim 20 mA/ μ m) in gate-all-around structure [21], good reliability [13], and ultralow contact resistance (R_C) of 23.4 $\Omega \cdot \mu$ m, approaching the quantum limit of metal/semiconductor contacts [8], [22].

The channel length (L_{ch}) dependent threshold voltage (V_T) —specifically, the V_T roll-off phenomenon as the L_{ch}

decreases—has been widely reported in In₂O₃ and doped-In₂O₃ [e.g., InSnO, InZnO (IZO), InGaO (IGO), and InGaZnO (IGZO)] FETs [4], [6], [9], [12], [18], [22], [23], [24], [25], [26], [27]. While many studies have investigated methods to mitigate $V_{\rm T}$ roll-off, relatively few have explored the underlying mechanisms responsible for the L_{ch} -dependent V_{T} shifts in In₂O₃-based FETs [23]. A common assumption is that this roll-off stems from the short-channel effect (SCE), which occurs when electrostatic control of gate to channel weakens as the source/drain (S/D) spacing or L_{ch} shrinks. However, most In₂O₃-based FETs are thin-film transistors (TFTs) with channel thickness far below 10 nm [3], [4], [5], [6], [7], [8], [9], [10], [11], [12], [18], [26]. In such ultrathin channels, strong gate control should effectively suppress the traditional SCE in the investigated $L_{\rm ch}$ range (\geq 40 nm). This suggests that the observed V_T roll-off in In₂O₃-based TFTs is driven by mechanisms beyond conventional SCE.

In this work, we propose that the contact-doping effect (CDE) is responsible for the $V_{\rm T}$ roll-off in $\rm In_2O_3$ FETs. Using a modified transfer length method (TLM), we systematically investigate and verify the relationship between CDE and $V_{\rm T}$ roll-off. Additionally, by varying S/D metal materials, we explore the physical mechanisms underlying CDE. This research offers new insights into CDE and its influence on $V_{\rm T}$ roll-off, emphasizing its significance in the design and optimization of aggressively scaled OS transistors.

II. EXPERIMENTS AND SIMULATIONS

Fig. 1(a) illustrates the schematic of the back-gate (BG) In₂O₃ transistors analyzed in this study, and Fig. 1(b) outlines the fabrication process. The process began with the deposition of 6 nm Al₂O₃ adhesion layer via ALD at 175 °C on SiO₂/Si substrate, followed by 60 nm Ni BG deposited through electron-beam evaporation. Next, 4 nm HfO2 gate dielectric was deposited by ALD at 200 °C. In₂O₃ with channel thickness (T_{ch}) ranging from 1.2 to 2.0 nm was used as transistor channel and was grown by ALD at 225 °C. Various metals were then deposited by electron-beam evaporation to serve as the S/D electrodes, as listed in Fig. 1(c). Different S/D materials were employed to investigate the CDE in In₂O₃ transistors. Finally, channel isolation and the definition of transistor channel width (W_{ch}) of 1 μ m were achieved through inductively coupled plasma (ICP) etching using Ar/BCl₃ plasma. For the ALD processes above, Al(CH₃)₃ (TMA), [(CH₃)₂N]₄Hf (TDMAHf), (CH₃)₃In (TMIn), and H₂O were used as Al, Hf, In, and O precursors, respectively. Fig. 1(d) shows a cross-sectional scanning transmission electron microscopy (STEM) image with energy-dispersive X-ray spectroscopy (EDS) elemental mapping of an In₂O₃ FET with Ni as the S/D material, while Fig. 1(e) presents the corresponding image for a device with Pt as S/D.

Electrical characterizations were conducted at room temperature in a Cascade probe station under an N_2 ambient using the Keysight B1500A system. The V_T of the devices was determined via the linear extrapolation method based on their transfer characteristics.

To investigate the oxygen interstitial formation energy for different metals, *ab initio* calculations were performed using the QuantumATK software with the GGA-PBE functional and

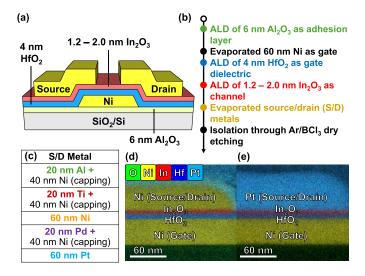


Fig. 1. (a) Schematic device structure of BG In_2O_3 transistors. (b) Fabrication process flow of BG In_2O_3 FETs. (c) List of S/D metals used in this work. Different S/D metals were utilized to study the CDE in In_2O_3 devices. Cross-sectional STEM image with EDS elemental mappings of In_2O_3 FETs with (d) Ni as S/D and (e) Pt as S/D.

PseudoDojo basis sets. Oxygen atoms were placed at interstitial sites, identified based on the lowest energy configuration.

III. RESULTS AND DISCUSSION

A. Quantification of the CDE

Fig. 2 presents the transfer characteristics of In_2O_3 FETs with different L_{ch} , Ni as the S/D metal, and $T_{ch} = 1.2$, 1.6, and 2.0 nm. Noticeable V_T roll-off is observed as the L_{ch} decreases from 1000 to 40 nm across all T_{ch} conditions. To elaborate, for $T_{ch} = 1.2$ and 1.6 nm, the I_D – V_{GS} curves exhibit a negative shift when L_{ch} falls below 600 nm [Fig. 2(a) and (b)]. For $T_{ch} = 2.0$ nm, a similar leftward shift is observed when L_{ch} is reduced to below 200 nm [Fig. 2(c)]. The V_T roll-off observed in Fig. 2 is unlikely to be caused by the traditional SCE. SCE can be quantified by the natural length theory of MOSFETs [28], [29]. The natural length (λ) of silicon-oninsulator (SOI) MOSFETs—whose structure is similar to BG In_2O_3 FETs—is given by

$$\lambda = \sqrt{\frac{\varepsilon_{\rm ch}}{\varepsilon_{\rm ox}} \cdot T_{\rm ch} \cdot T_{\rm ox}} \tag{1}$$

where ε_{ch} is the dielectric constant of the channel material (In₂O₃ with $\varepsilon_{ch} = 8.9$ [3]), ε_{ox} is the dielectric constant of the gate oxide (HfO₂ with $\varepsilon_{\rm ox} \sim$ 8.6, calculated based on the measured gate oxide capacitance of 1.9×10^{-6} F/cm²), $T_{\rm ch}$ is the channel thickness, and T_{ox} is the gate oxide thickness $(T_{\rm ox} = 4.0 \text{ nm})$. For our In₂O₃ devices with $T_{\rm ch} = 1.2$ –2.0 nm, λ values are calculated to be 2–3 nm using (1), as shown in Fig. 3(a). Given that SCE should only become significant when $L_{\rm ch} \leq 5 \times \lambda = 10\text{--}15$ nm [29], the In₂O₃ transistors in this study should remain unaffected by the SCE since the gate control over the channel center is still stronger than the control from S/D. However, the calculated 5 \times λ values contradict our experimental observations of V_T roll-off happening at L_{ch} below 600 nm (Fig. 2). This discrepancy suggests that the roll-off is not caused by SCE but rather by other reasons, such as CDE.

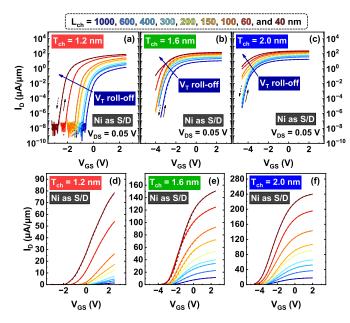


Fig. 2. Transfer characteristics of $\ln_2 O_3$ transistors with Ni as S/D metal, channel length $(L_{\rm ch})=1~\mu{\rm m}-40$ nm, and channel thickness $(T_{\rm ch})$ of 1.2 nm [(a): $I_{\rm D}$ in log scale; (d): $I_{\rm D}$ in linear scale], 1.6 nm [(b): $I_{\rm D}$ in log scale; (e): $I_{\rm D}$ in linear scale], and 2.0 nm [(c): $I_{\rm D}$ in log scale; (f): $I_{\rm D}$ in linear scale]. Solid lines indicate $V_{\rm GS}$ sweeping forward, while dashed lines represent $V_{\rm GS}$ sweeping backward.

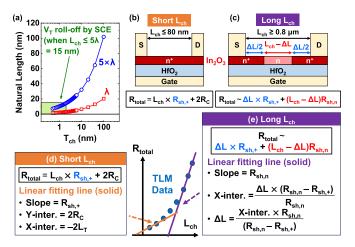
It is suspected that the carrier density (i.e., electron density) within the In₂O₃ channel is non-uniform, with a higher carrier concentration near the S/D contacts compared to the channel center [Fig. 3(c)]. This phenomenon is referred to as CDE, as if the S/D contacts effectively increase the carrier density of the In₂O₃ channel under them. The non-uniform carrier distribution caused by CDE is illustrated in Fig. 3(b) and (c). Fig. 3(c) shows a schematic carrier density profile for In₂O₃ transistors with long $L_{\rm ch}$ ($\geq 0.8~\mu {\rm m}$), featuring n^+ (high electron density) regions near the S/D and an n (medium electron density) region at the channel center. ΔL is defined as the length of the n^+ regions extending into the channel, with $\Delta L/2$ contributed by the source and $\Delta L/2$ by the drain. When $L_{\rm ch}$ is sufficiently short (≤ 80 nm), the n^+ regions from the S/D merge, as shown in Fig. 3(b). To extract the ΔL and quantify the CDE, a modified TLM is developed based on Fig. 3(b) and (c). From the long $L_{\rm ch}$ ($\geq 0.8~\mu {\rm m}$) devices, the total resistance (R_{total}) of the transistors can be written as

$$R_{\text{total}} \sim \Delta L \times R_{\text{sh},+} + (L_{\text{ch}} - \Delta L) R_{\text{sh},n}$$
 (2)

where $R_{\rm sh,+}$ is the sheet resistance of the n^+ region and $R_{\rm sh,n}$ is the sheet resistance of the n region. Using (2), $R_{\rm sh,n}$ can be extracted from the slope of the linear fitting lines in the long $L_{\rm ch}$ regime TLM analysis [Fig. 3(e)]. As for the short $L_{\rm ch}$ (\leq 80 nm) devices, the $R_{\rm total}$ is given by

$$R_{\text{total}} = L_{\text{ch}} \times R_{\text{sh},+} + 2R_C. \tag{3}$$

Utilizing (3), $R_{\text{sh},+}$ can be determined from the slopes and R_C can be calculated from the *Y*-intercept of the linear fitting lines in the short L_{ch} regime [Fig. 3(d)]. By combining the $R_{\text{sh},n}$ and $R_{\text{sh},+}$, ΔL can be calculated using the following



(a) Calculated natural length (λ) as a function of T_{ch} . When $L_{\rm ch}$ is smaller than 5 \times λ , $V_{\rm T}$ roll-off due to SCE is expected. For T_{ch} below 10 nm, the calculated λ remains under 6.5 nm, with 5 \times $\lambda \leq 33$ nm. (b) and (c) Illustrate schematic cross sections of In_2O_3 transistors, showing carrier density profiles along the Lch direction for short L_{ch} (\leq 80 nm) and long L_{ch} (\geq 0.8 μ m) devices, respectively. The n^+ region represents a high carrier density area, while the n region corresponds to a medium carrier density area. ΔL denotes the length of the n^+ regions extending into the channel. R_{total} is the total channel resistance, with $R_{sh,+}$ and $R_{sh,n}$ representing the sheet resistances of the n^+ and n regions, respectively. If the carrier density in the $\ln_2 O_3$ channel is nonuniform, the TLM analysis of Rtotal-Lch data can be divided into two parts: (d) short L_{ch} segment, corresponding to the case of (b); (e) long L_{ch} segment, corresponding to the case of (c). Y-inter. and X-inter. represent the Y- and X-intercepts of the linear fitting lines, respectively. R_C is the contact resistance, and L_T is the transfer length.

equation derived from (2):

$$\Delta L = \frac{X \text{-inter.} \times R_{\text{sh},n}}{\left(R_{\text{sh},n} - R_{\text{sh},+}\right)} \tag{4}$$

where X-inter. represents the X-intercept of the linear fitting lines in the long $L_{\rm ch}$ regime TLM analysis [Fig. 3(e)]. It should be noted that in the analysis of Fig. 3(b)–(e), the transition between n^+ and n regions is approximated as a step change to simplify the calculations and TLM analysis. A gradual transition from n^+ to n regions could be present, which may need to be considered for a more precise estimation of the CDE.

Fig. 4 presents the TLM analysis of total resistance (R_{total}) as a function of L_{ch} for In_2O_3 transistors with various T_{ch} . To accurately quantify the CDE, each set of R_{total} - L_{ch} data is analyzed at the same V_{GS} rather than the same V_{GS} - V_{T} . While adjusting R_{total} - L_{ch} data based on V_{GS} - V_{T} for each L_{ch} is a common practice to improve TLM linear fitting, particularly when $V_{\rm T}$ depends on $L_{\rm ch}$ [8], [25], [30], such normalization would exclude the information about CDE, as CDE itself is the potential cause of the V_T roll-off in In_2O_3 devices. For each $T_{\rm ch}$, the $R_{\rm total}$ – $L_{\rm ch}$ data at a given $V_{\rm GS}$ is divided into two segments: short L_{ch} (40-80 nm) [Fig. 4(a), (c), and (e)] and long L_{ch} (0.8–1.0 μ m) [Fig. 4(b), (d), and (f)], which are then analyzed using linear regression. According to the proposed TLM framework [Fig. 3(d) and (e)], $R_{sh,+}$ and $R_{sh,n}$ are extracted from the short- and long- L_{ch} regimes, respectively, as shown in Fig. 5(a)-(c). The extracted $R_{sh,+}$ values are

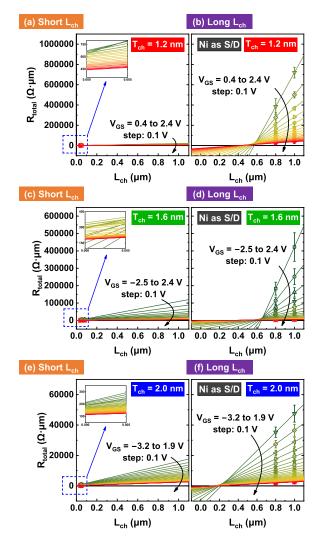


Fig. 4. TLM analysis of total resistance (R_{total}) versus L_{ch} for $\ln_2 O_3$ FETs with different T_{ch} values: (a) and (b) 1.2 nm, (c) and (d) 1.6 nm, and (e) and (f) 2.0 nm. For each T_{ch} , the $R_{\text{total}}-L_{\text{ch}}$ data is divided into two regions: short L_{ch} (40–80 nm) in (a), (c), and (e); long L_{ch} (0.8–1 μ m) in (b), (d), and (f). Symbols represent experimental data, averaged over at least five devices. Solid lines indicate the linear fitting of the data. For the short L_{ch} regime [(a), (c), and (e)], $R_{\text{sh},\text{h}}$ and R_{C} are extracted using the equations in Fig. 3(d) For the long L_{ch} regime [(b), (d), and (f)], $R_{\text{sh},\text{h}}$ is extracted using the equation in Fig. 3(e).

consistently lower than $R_{\text{sh},n}$ across all T_{ch} , confirming the presence of a non-uniform carrier density in the In_2O_3 channel.

Fig. 5(d) shows the extracted R_C as a function of $V_{\rm GS}$, revealing that the R_C decreases as the $T_{\rm ch}$ increases. This behavior is linked to the transition from a positive to a negative Schottky barrier height ($\Phi_{\rm SB}$) at the metal/In₂O₃ contact [25], [31], as illustrated in Fig. 5(e). The quantum confinement effect (QCE) modifies the band structure of In₂O₃ as the $T_{\rm ch}$ becomes thinner [3], [25]. For instance, when $T_{\rm ch}$ is reduced from 1.6 to 1.2 nm, the QCE shifts the conduction band minimum ($E_{\rm C}$) upward, moving it above the charge neutrality level (CNL) of In₂O₃. Due to strong Fermi-level pinning at the metal/In₂O₃ interface, the metal Fermi level ($E_{\rm FM}$) remains close to the CNL of In₂O₃ [25]. Consequently, the alignment between $E_{\rm C}$ and CNL (which closely matches $E_{\rm FM}$) dictates the value of $\Phi_{\rm SB}$. If $E_{\rm C}$ is above CNL (as in the case of $T_{\rm ch}$

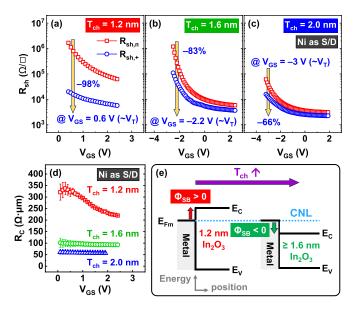


Fig. 5. Extracted $R_{\mathrm{sh},n}$ and $R_{\mathrm{sh},+}$ as a function of V_{GS} for $\ln_2\mathrm{O_3}$ FETs with T_{ch} of (a) 1.2 nm, (b) 1.6 nm, and (c) 2.0 nm. The $R_{\mathrm{sh},n}$ and $R_{\mathrm{sh},+}$ near $V_{\mathrm{GS}}{\sim}V_{\mathrm{T}}$ (V_{T} from the devices with $L_{\mathrm{ch}}=1~\mu\mathrm{m}$) are highlighted in orange arrows to emphasize their differences. (d) Extracted R_{C} as a function of V_{GS} for $\ln_2\mathrm{O_3}$ transistors with T_{ch} ranging from 1.2 to 2.0 nm. R_{C} are extracted based on the short L_{ch} TLM analysis. (e) Schematic band diagrams of metal/ $\ln_2\mathrm{O_3}$ contacts for different $\ln_2\mathrm{O_3}$ thicknesses. E_{C} : conduction band minimum, CNL: CNL of $\ln_2\mathrm{O_3}$, and E_{FM} : metal Fermi level.

1.2 nm), a positive $\Phi_{\rm SB}$ forms at the metal/In₂O₃ contact. Conversely, when $E_{\rm C}$ falls below CNL (as seen for $T_{\rm ch} \geq$ 1.6 nm), $\Phi_{\rm SB}$ becomes negative. This transition in $\Phi_{\rm SB}$ with increasing $T_{\rm ch}$ from 1.2 nm to above 1.6 nm has been studied and corroborated in our earlier work [25].

Fig. 6(a) presents the extracted ΔL as a function of V_{GS} , calculated using (4). The ΔL values at $V_{\rm GS} \sim V_{\rm T}$, ranging from 0.30 to $0.73 \mu m$, are highlighted for reference. Fig. 6(b) shows the relationship between $V_{\rm T}$ and $L_{\rm ch}$ for different $T_{\rm ch}$. As previously discussed in Fig. 2, all devices exhibit significant $V_{\rm T}$ roll-off, even when $L_{\rm ch}$ remains larger than $5 \times \lambda$. Notably, the $L_{\rm ch}$ at which $V_{\rm T}$ roll-off begins aligns well with the extracted ΔL values at $V_{\rm GS} \sim V_{\rm T}$ [Fig. 6(a) and (b)], substantiating the impact of the CDE on V_T roll-off. The relatively large ΔL values further explain why $V_{\rm T}$ roll-off occurs even when $L_{\rm ch}$ is much greater than the natural length (5 \times λ = 10–15 nm) of the transistors. When $L_{\rm ch} > \Delta L$, reducing $L_{\rm ch}$ has minimal impact on $V_{\rm T}$, as the carrier density at the channel center stays unaffected by the n^+ regions extending from the S/D contacts [like Fig. 3(c)]. However, when $L_{\rm ch} \leq \Delta L$, the n^+ regions from the S/D begin to merge, increasing the carrier density at the channel center [like Fig. 3(b)]. This results in a negative shift of V_T and a pronounced V_T roll-off as L_{ch} decreases.

B. Mechanisms Behind the CDE

The high carrier density n^+ regions beneath the S/D electrodes, referred to as the CDE, have been identified as a key factor contributing to the $V_{\rm T}$ roll-off of ${\rm In_2O_3}$ FETs in the previous section. The remaining questions are: what causes this CDE in ${\rm In_2O_3}$ transistors, and why do S/D metals increase the carrier density in the underlying ${\rm In_2O_3}$? In this work,

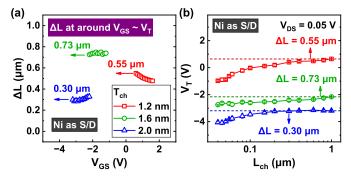


Fig. 6. (a) Extracted ΔL as a function of $V_{\rm GS}$ for $\ln_2 O_3$ FETs with $T_{\rm ch}$ ranging from 1.2 to 2.0 nm. The ΔL values at $V_{\rm GS} \sim V_{\rm T}$ are highlighted for reference. (b) Linearly extrapolated $V_{\rm T}$ as a function of $L_{\rm ch}$. Each data point represents the average of at least five devices. All $T_{\rm ch} \ln_2 O_3$ FETs exhibit a clear $V_{\rm T}$ roll-off phenomenon, even when $L_{\rm ch}$ is still significantly larger than $5 \times \lambda$, suggesting that the CDE might influence the $V_{\rm T}$ behavior. The ΔL values at $V_{\rm GS} \sim V_{\rm T}$ are marked in the figure and show good consistency with the $L_{\rm ch}$ at which the $V_{\rm T}$ roll-off begins.

we propose two mechanisms that may contribute to the contact doping in In₂O₃ FETs. The first one is oxygen-scavenging reactions (OSR) at the metal/In₂O₃ S/D contacts (Fig. 7), and the second one is the change in the sign of the Φ_{SB} at metal/In₂O₃ interface (Fig. 8). These mechanisms provide insight into why CDE, quantified by ΔL , depends on the $T_{\rm ch}$ of In₂O₃, as shown in Fig. 6(a). When Ni is deposited as the S/D metal, it may react with In₂O₃, scavenging oxygen atoms from the channel. This scavenging process generates oxygen vacancies (V_0^+) in the In_2O_3 channel [Fig. 7(a)]. Since V_0^+ acts as a shallow donor and directly correlates with the carrier density in doped In₂O₃ (such as IGZO and ITO) and pure In_2O_3 [4], [6], [9], [32], the introduction of V_0^+ via OSR increases electron density, forming n^+ regions near the S/D contacts. The length of the n^+ region induced by OSR is denoted as ΔL_{SC} , as illustrated in Fig. 7(b). For the same type of S/D metal, assuming a consistent amount of oxygen is scavenged from the In_2O_3 channel, the product $\Delta L_{SC} \times T_{ch}$ which is proportional to the total number of oxygen atoms involved in the scavenging reactions—should remain similar. Consequently, in thinner $T_{\rm ch}$ devices, $\Delta L_{\rm SC}$ must be longer than in thicker T_{ch} transistors to provide sufficient oxygen atoms for the scavenging reaction.

The Φ_{SB} at the metal/ In_2O_3 interface also influences the carrier density beneath the S/D contacts, as illustrated in Fig. 8. When $\Phi_{SB} > 0$, electrons near the contact are depleted due to the upward band bending at $V_{GS} = V_{T}$, forming a depletion region with width = W_{dep} [Fig. 8(a)]. This depletion effect counteracts the OSR-induced carrier increase, potentially leading to n^- rather than n^+ regions in In_2O_3 . Conversely, when Φ_{SB} < 0, the metal/In₂O₃ interface accumulates electrons due to downward band bending [22], creating an accumulation region with width = $W_{\rm acc}$ [Fig. 8(b)]. Defining $\Delta L_{\rm SBH}$ as the length of the n^+ region induced by the Φ_{SB} from S/D, a positive Φ_{SB} at $T_{ch} = 1.2$ nm results in $\Delta L_{SBH} < 0$, reducing the n^+ region length generated from OSR. Meanwhile, a negative $\Phi_{\rm SB}$ at $T_{\rm ch} \geq 1.6$ nm leads to $\Delta L_{\rm SBH} > 0$, expanding the n^+ region. The overall dependencies of ΔL , ΔL_{SC} , and ΔL_{SBH} on T_{ch} are summarized in Fig. 9, where ΔL is determined by

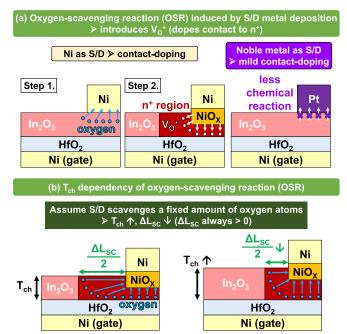


Fig. 7. (a) Schematic illustration of the oxygen-scavenging reaction (OSR) induced by the S/D metal. When a metal such as Ni is deposited on $\rm In_2O_3$, it may react with $\rm In_2O_3$ and scavenge oxygen atoms from the channel. Oxygen vacancies (V_O^+) are generated during the OSR process. In contrast, using noble metals like Pt as S/D can suppress the OSR. (b) Schematic representation of the $T_{\rm Ch}$ -dependent OSR effect, where $\Delta L_{\rm SC}/2$ denotes the length of the n^+ region formed due to the OSR from the source or drain metal. The total length of n^+ region from S/D is $\Delta L_{\rm SC}$.

the sum of $\Delta L_{\rm SC}$ and $\Delta L_{\rm SBH}$ ($\Delta L = \Delta L_{\rm SC} + \Delta L_{\rm SBH}$). Fig. 9 explains the ΔL - $T_{\rm ch}$ relationship observed in Fig. 6. Note that the impact of $\Phi_{\rm SB}$ on ΔL is constrained by the small values of $W_{\rm dep}$ and $W_{\rm acc}$, leading to a relatively minor $|\Delta L_{\rm SBH}|$. As a result, the $\Phi_{\rm SB}$ effect on ΔL and $V_{\rm T}$ may be overshadowed unless OSR at the S/D contact is mitigated—an aspect that will be further explored in Figs. 10 and 11.

Since OSR plays a critical role in the CDE, there are two effective strategies to reduce the OSR and improve the $V_{\rm T}$ roll-off caused by the CDE in In₂O₃ FETs. These strategies also reinforce the idea that OSR is a key contributor to CDE and V_T roll-off. The first approach is using O_2 annealing or O_2 plasma treatments to reduce the V_O^+ generated by the OSR, a method that has been well-studied in our previous works [4], [24]. The second approach involves replacing the S/D metals with noble metals, such as Pt, which should experience less OSR with In₂O₃ [as illustrated in Fig. 7(a)]. Therefore, noble metals are expected to alleviate the V_T roll-off issue and reduce the CDE. Fig. 10 presents the transfer characteristics of In₂O₃ FETs with different $L_{\rm ch}$, $T_{\rm ch}=1.2$, 1.6, and 2.0 nm, and Pt as the S/D metal. Fig. 11 shows the V_T - L_{ch} dependencies extracted from the I_D – V_{GS} curves in Fig. 10. When compared to devices with Ni as S/D [Fig. 2 for transfer curves and Fig. 6(b) for V_T – L_{ch} dependency], In_2O_3 FETs with Pt as the S/D metal clearly exhibits improved $V_{
m T}$ roll-off as the $L_{
m ch}$ decreases. This supports the hypothesis that OSR at the S/D interfaces contributes significantly to the V_T roll-off and CDE in In_2O_3 transistors.

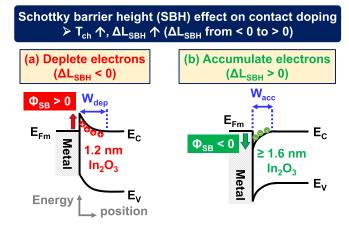


Fig. 8. Schematic band diagrams of metal/ln₂O₃ contacts for (a) $T_{\rm ch}=1.2$ nm (with $\Phi_{\rm SB}>0$) and (b) $T_{\rm ch}\geq 1.6$ nm (with $\Phi_{\rm SB}<0$) at $V_{\rm GS}=V_{\rm T}$. The length of the n^+ regions induced by the $\Phi_{\rm SB}$ at the metal/ln₂O₃ contacts is denoted as $\Delta L_{\rm SBH}$. A positive $\Phi_{\rm SB}$ depletes electrons at the interface, creating a depletion region with a width $W_{\rm dep}$, which counteracts the carrier increase caused by OSR at the S/D contacts ($\Delta L_{\rm SBH}<0$). In contrast, a negative $\Phi_{\rm SB}$ leads to electron accumulation, contributing to an accumulation width $W_{\rm acc}$, which further intensifies the CDE in the $\ln_2{\rm O_3}$ channel ($\Delta L_{\rm SBH}>0$). Since $\ln_2{\rm O_3}$ is an n-type semiconductor, $W_{\rm acc}$ is inherently smaller than $W_{\rm dep}$.

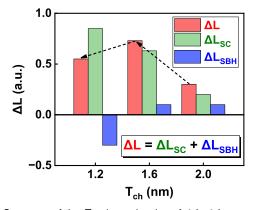


Fig. 9. Summary of the $T_{\rm ch}$ dependencies of ΔL , $\Delta L_{\rm SC}$, and $\Delta L_{\rm SBH}$, where $\Delta L = \Delta L_{\rm SC} + \Delta L_{\rm SBH}$. The values of $\Delta L_{\rm SC}$ and $\Delta L_{\rm SBH}$ are estimated for qualitative understanding of their $T_{\rm ch}$ dependencies and may involve some degree of inaccuracy.

Interestingly, In_2O_3 devices with Pt as S/D and T_{ch} = 1.2 nm exhibit an unusual V_T roll-up as the L_{ch} scales down (Fig. 11), which contrasts sharply with the typical V_T rolloff seen in the devices with Ni as S/D and $T_{\rm ch}=1.2~{\rm nm}$ [Fig. 6(b)]. Normally, OSR dominates the influence of Φ_{SR} on the CDE in In₂O₃ transistors. However, with Pt as the S/D metal, where OSR is largely suppressed, Φ_{SB} becomes the dominant factor affecting the V_T - L_{ch} relationship. For T_{ch} = 1.2 nm devices, where $\Phi_{SB} > 0$, the upward band bending profile forms a depletion region and depletes electrons from the Pt/In₂O₃ contact [Fig. 8(a)]. As the L_{ch} decreases, the depletion regions near the S/D start to influence the electron density at the In₂O₃ channel center, resulting in the observed $V_{\rm T}$ roll-up in Fig. 11. For $T_{\rm ch} \geq 1.6$ nm devices, the negative $\Phi_{\rm SB}$ with downward band bending has less effect on the $V_{\rm T}$ - $L_{\rm ch}$ dependency (Fig. 11) because the accumulation region width $[W_{acc}, as shown in Fig. 8(b)]$ is not long enough to affect the channel center when $L_{\rm ch} \geq 40$ nm.

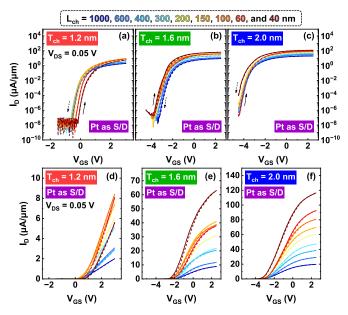


Fig. 10. Transfer characteristics of $\ln_2 O_3$ transistors with Pt as the S/D metal, featuring $L_{\rm ch}$ ranging from 1 $\mu{\rm m}$ to 40 nm and $T_{\rm ch}$ of 1.2 nm [(a): $I_{\rm D}$ in log scale; (d): $I_{\rm D}$ in linear scale], 1.6 nm [(b): $I_{\rm D}$ in log scale; (e): $I_{\rm D}$ in linear scale], and 2.0 nm [(c): $I_{\rm D}$ in log scale; (f): $I_{\rm D}$ in linear scale]. Solid lines represent forward $V_{\rm GS}$ sweeps, while dashed lines indicate backward sweeps. Compared to $\ln_2 O_3$ FETs with Ni as the S/D metal (Fig. 2), devices using Pt exhibit a milder $V_{\rm T}$ roll-off.

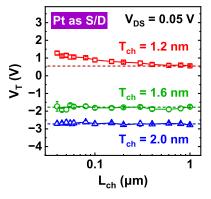


Fig. 11. Linearly extrapolated V_T as a function of $L_{\rm ch}$ of $\ln_2 O_3$ FETs with Pt as S/D and various $T_{\rm ch}$. Each data point represents the average of at least five devices.

In addition to Pt and Ni, other metals, such as Al, Ti, and Pd, are also used as the S/D electrodes in In₂O₃ transistors to investigate their impact on the V_T roll-off. Fig. 12(a) summarizes the V_T - L_{ch} dependencies for In_2O_3 FETs with these different S/D metals. Except for the devices using Pt as the S/D, all the other transistors exhibit significant V_T rolloff as the L_{ch} decreases. To understand these observations, the oxygen interstitial formation energies for various metals are simulated by ab initio calculations using QuantumATK, as shown in Fig. 12(b). The oxygen interstitial formation energy indicates how easily a material reacts with oxygen atoms: a lower formation energy suggests that the material is more likely to react with oxygen. Therefore, at the metal/In₂O₃ interface, if the metal has a smaller oxygen interstitial formation energy than In, the oxygen atoms in In-O bonds will preferentially react with the metal, rather than staying in the

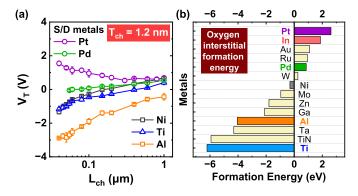


Fig. 12. (a) Linearly extrapolated V_T as a function of $L_{\rm ch}$ for $\ln_2 O_3$ FETs with various metals as S/D and $T_{\rm ch}=1.2$ nm. Each data point represents the average of at least five devices. A broad range of metals were examined to assess their impact on the V_T roll-off in $\ln_2 O_3$ transistors. (b) Simulated formation energies of oxygen interstitials in various metals. The energies were simulated by *ab initio* calculations using QuantumATK. Metals with smaller formation energies are more likely to react with oxygen.

In₂O₃, which leads to OSR. In Fig. 12(b), Pt is the only metal with a larger oxygen interstitial formation energy than In, meaning it does not scavenge oxygen from In₂O₃, and thus does not contribute to CDE and V_T roll-off. In contrast, metals like Pd, Ni, Al, and Ti have lower formation energies versus In, which facilitates the OSR at the metal/In₂O₃ interface. The fact that many metals tend to have OSR with In-O bonds also explains why the V_T roll-off phenomenon is commonly observed not only in In₂O₃ FETs [4], [22], [23], [24], [25] but also in other doped In₂O₃ transistors like InSnO (ITO) [6], [26], IZO [18], IGO [12], and IGZO devices [9], [27], [31]. Notably, all these studies have used S/D metals (such as Ni, TiN, and Mo) with low oxygen interstitial formation energies.

IV. CONCLUSION

In summary, this work systematically investigates the CDE and its impact on the V_T roll-off issue in In_2O_3 FETs. The CDE describes the increase in carrier density near the S/D electrodes, forming n⁺ regions, which leads to a non-uniform carrier concentration profile along the In₂O₃ channel. By analyzing long L_{ch} and short L_{ch} devices separately, we extract $R_{\text{sh},n}$, $R_{\text{sh},+}$, and ΔL to quantify the CDE. The strong correlation between ΔL and the $L_{\rm ch}$ where $V_{\rm T}$ roll-off begins suggests that the $V_{\rm T}$ roll-off in $\rm In_2O_3$ transistors is caused not by the traditional SCE but by the CDE. Next, the underlying mechanisms of the CDE are explored. It is found that the OSR that occurs when depositing the S/D metals on the In₂O₃ channel is one of the reasons contributing to the CDE. The S/D metals may scavenge oxygen atoms from In₂O₃, generating oxygen vacancies and increasing the carrier density near the S/D. This OSR mechanism is verified through experiments with different S/D metals and simulations of oxygen interstitial formation energy. Additionally, the Schottky barrier height (Φ_{SB}) at the metal/ In_2O_3 contacts also has minor influences on the CDE. Positive Φ_{SB} (when $T_{ch} = 1.2$ nm) depletes carriers, while negative Φ_{SB} (when $T_{ch} \ge 1.6$ nm) accumulates carriers at the In₂O₃ channel beneath the S/D electrodes. This research offers new insights into the CDE and its crucial role in the $V_{\rm T}$ roll-off behavior of OS transistors. It lays the foundation for future studies aimed at mitigating CDE and improving the performance of $\rm In_2O_3$ and other $\rm In_2O_3$ -based transistors.

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