Positive to Negative Schottky Barrier Transition in Metal/Oxide Semiconductor Contacts by Tuning Indium Concentration in IGZO

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Abstract

In this work, we report the tunability of electrical performance and metal-to-semiconductor contact properties in atomic-layer-deposited (ALD) InGaZnO (IGZO) field-effect transistors (FETs) by precisely manipulating the In:Ga:Zn ratios. Our fabricated IGZO FETs exhibit well-behaved saturation in the short channel length (L_{ch}) of 80 nm and a high on-current of 850 µA/µm. Through temperature-dependent characterizations, we observed the transition from a negative to a positive Schottky barrier (Φ_{SB}) by adjusting the indium (In) concentrations. This transition is explained by the changes in the charge neutrality level (CNL) and Fermi level (E_F) at the contact interface. The impact of surface accumulation/depletion at the metal/semiconductor interface provides the new insight into the realm of contact engineering.

Introduction

As transistors continue to scale down, the significance of addressing electrical contact resistance (R_c) at metal–semiconductor interface intensifies. This issue poses a growing challenge for the semiconductor industry, acting as a barrier to achieving ultimate scaling and optimal device performance [1]-[3]. The impact is substantial and is influenced by various factors, such as band alignment, semiconductor interface states, and Fermi-level pinning [4]. Traditionally, metal/semiconductor has a positive Φ_{SB} at the interface, requiring carriers to expend additional energy to overcome this barrier [5]. Consequently, this leads to significant R_c and limits the scaled transistor performance, especially as carriers' thermal activation diminishes at lower temperatures. Notably, simulations underscore the requirement of a negative Φ_{SB} for a transistor to exhibit behavior akin to a ballistic MOSFET [6]. In this context, our result highlights the transition of Φ_{SB} in IGZO films from a positive to near zero by increasing indium concentration and eventually becomes a negative Φ_{SB} in pure In_2O_3. This transition can be explained through CNL changes on the channel surface induced by modulating Ga and Zn doping ratios in IGZO.

Experiments

Fig. 1 shows the schematic device structure and fabrication flow of bottom-gate IGZO FETs. The gate dielectric is 5 nm Al_2O_3 grown by plasma enhanced (PE)-ALD at 200 ºC. The IGZO channel was deposited by ALD at 225 ºC using $In(CH_3)_3$, $(C_2H_5)_2Zn$, and $Ga_2(NMe_2)_6$ as precursors. The thickness of the IGZO layer is precisely controlled by adjusting the number of super-cycles, which contains the sequential deposition of ZnO, Ga_2O_3, and n cycles of In_2O_3 (n = 2 to 7). This paper describes the In:Ga:Zn ratio (n:1:1) by the number of In, Ga, and Zn ALD cycles within a super-cycle. A smaller n corresponds to higher Ga and Zn doping levels. Fig. 2 shows scanning transmission electron microscopy (STEM) and energy dispersive x-ray spectroscopy (EDS) element mapping images of an IGZO FET with a channel thickness (T_{ch}) of 4.8 nm, confirming the device structure. The electrical characterization was measured with the Keysight B1500 system. The temperature-dependent characterization was performed in a Lakeshore CRX-VF cryogenic probe station.

Results and Discussion

The transfer and output characteristics of a short channel (L_{ch} = 50 nm) IGZO 1:0:0 (i.e., pure In_2O_3) FET with T_{ch} of 1.2 nm are shown in Fig. 3 at both 295 K and 10 K [7]. The on-current increases at low temperatures under the same V_{DS} and V_{GS} despite the positively shifted threshold voltage (V_T), indicating unique and excellent contact between In_2O_3 and Ni even at cryogenic temperatures. This is because the improved transport properties in In_2O_3 at low temperatures and negative Φ_{SB} in pure In_2O_3 [7]. Figs. 4 and 5 present the short channel (L_{ch} = 80 nm) transfer and output characteristics of lightly doped (7:1:1) and highly doped (2:1:1) IGZO FETs, respectively. Introducing Ga and Zn doping slightly decreases the on-current and shifts the V_T positively. Well-behaved current saturation is observed in the short channel 7:1:1 and 2:1:1 FETs with on-current of 850 µA/µm and 450 µA/µm, respectively. In contrast to pure In_2O_3, a reduced on-current is evident at 10 K under constant V_{DS} due to the surface depletion induced by the change of E_{CNL} and E_F. Fig. 6 shows the transfer characteristics and extracted μ_{FE} and g_m of the long channel (L_{ch} = 1 µm) IGZO FETs with varying In ratios. Increasing the Ga and Zn doping ratio results in a higher V_T with lower μ_{FE} and g_m.

The distinct trends observed in the low-temperature results of In_2O_3 and different ratios of IGZO can be attributed to variances in their Φ_{SB} heights, assumed to arise from Ga and Zn doping. Fig. 7(a) illustrates the trap density distribution in pure In_2O_3 and IGZO. In In_2O_3, the E_{CNL} is above the E_F and deeply inside the conduction band, generating donor-like trap charges at the interface [7]-[8]. These positive interface donor traps instigate accumulated negative electron charges at the In_2O_3 surface, resulting in a negative Schottky contact barrier in Fig. 7(b). In contrast, as In_2O_3 undergoes doping with Ga and Zn, the CNL gradually shifts under the E_F into the bandgap, forming acceptor-like traps at the interface. This transition changes the surface state from accumulation to depletion, raising the Φ_{SB} height from a negative Φ_{SB} to a positive Φ_{SB}. It is corroborated by the observed increase in R_c in Fig. 8, attributed to this heightened barrier height (Φ_B).

The Φ_{SB} heights for the various compositions of IGZO were experimentally determined by measuring the temperature-dependent (T = 295 K to 33 K) transfer characteristics of IGZO FETs with L_{ch} of 1 µm, as shown in Fig. 9. The most important and direct experimental evidence to support our conclusion is following. Arrhenius plots extracted from the transfer characteristics of both In_2O_3 and IGZO FETs with different Ga and Zn ratios (low and high) are presented in Fig. 10. A notable variation is observed in the V_{GS}-dependent slope (proportional to -Φ_B) trends. In pure In_2O_3, the slope rapidly transitions from negative to positive under more positive gate biases. Similarly, in IGZO 7:1:1, it ultimately shifts to a barely positive slope at a much slower pace, and in IGZO 3:1:1, it consistently remains negative. This observation highlights the impact of Ga and Zn doping in IGZO on the Schottky barrier behavior, providing the direct experimental evidence on the role of these dopants in altering the channel interfaces and Schottky barriers. The gate-dependent Φ_B calculated from these slopes are summarized in Fig. 11(a). Specifically, In_2O_3 exhibits a negative Φ_B under flat band condition, and this negative Φ_B is consistently observed in IGZO FETs with lower Ga and Zn ratios (7:1:1 and 5:1:1). Further comparison of quantified Φ_{SB} under flat band conditions for differently doped IGZO in Fig. 11(b) reveals a clear increasing trend from negative Φ_{SB} to positive Φ_{SB} with higher Ga and Zn ratios.

Conclusion

This paper investigates the electrical performance and metal-to-semiconductor contacts of ALD IGZO films with different In:Ga:Zn composition under different temperatures (295 K to 10 K). By controlling doping ratios in the In_2O_3 film with Ga and Zn, the CNL and E_F undergo a gradual shift from deeply inside the conduction band to inside the bandgap, consequently inducing a transition in the surface state from accumulation to depletion. Moreover, by studying the gate-dependent Φ_B, the transition from negative to positive Φ_{SB} is clearly experimentally observed, consistent with the CNL model and band-alignment theory. This work provides a new and deep insight on the contact engineering of oxide semiconductor devices.

Acknowledge: The work is supported by NSF and SRC GRC Program.

References: [1] PC. Shen et al., Nature, 593, 211–217, 2021. [2] A. Razavieh et al., IEEE Transactions on Nanotechnology, 18, pp. 999-1004, 2019. [3] S. G. Louie et al., Phys. Rev. B 13, 2461–2469, 1976. [4] F. Léonard et al., Phys. Rev. Lett. 84, 4693, 2000. [5] R. T. Tung, Appl. Phys. Rev. 1, 011304, 2014. [6] J. Guo, IEEE TED, 49, 11, 1897-1902, Nov. 2002. [7] C. Niu et al., 2023 IEEE IEDM, 37-2, 2023. [8] M. Si et al., Nano Letters, 21, 1, 500-506, 2021.

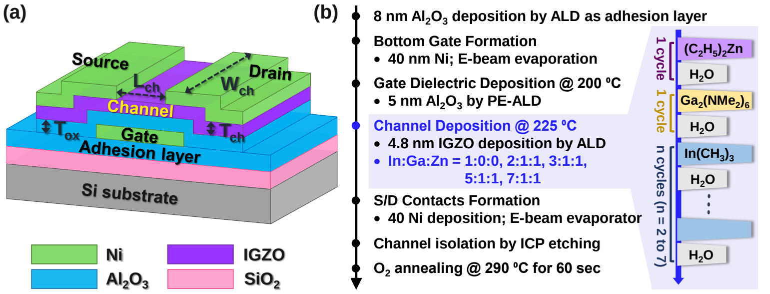

Fig. 1. (a) 3D schematic of a bottom gate IGZO FET. (b) Key fabrication steps of the IGZO FETs and illustration of doping technique for IGZO during the ALD process.

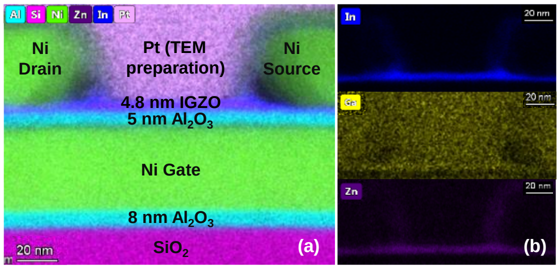

Fig. 2. (a) Cross-sectional STEM image of an IGZO FET and (b) EDX elemental mapping of In, Ga, and Zn elements. The Ga EDX image is blurred due to Ga atom contamination during FIB.

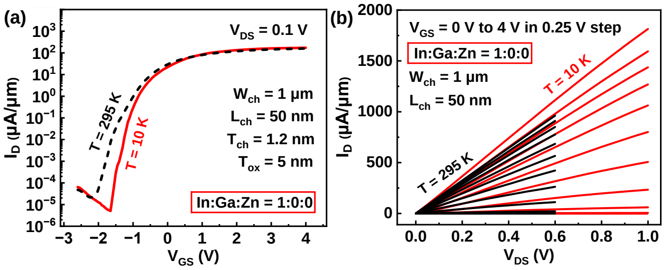

Fig. 3. (a) Transfer and (b) Output characteristics of a pure In_2O_3 FET with L_{ch} of 40 nm at 295 K (black) and 10 K (red). [7]

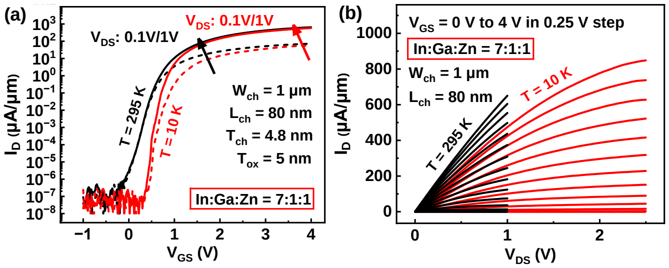

Fig. 4. (a) Transfer and (b) Output characteristics of an IGZO FET (In:Ga:Zn = 7:1:1) with L_{ch} of 80 nm at 295 K (black) and 10 K (red).

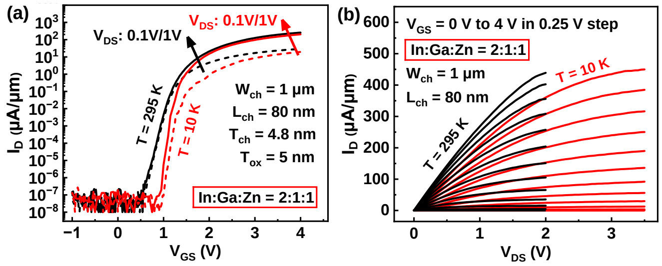

Fig. 5. (a) Transfer and (b) Output characteristics of IGZO FET (In:Ga:Zn = 2:1:1) with L_{ch} of 40 nm at 295 K (black) and 10 K (red).

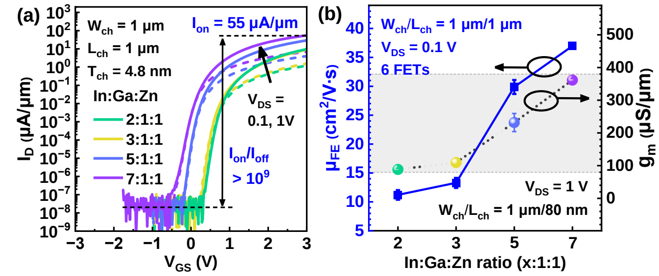

Fig. 6. (a) Transfer characteristics of IGZO FETs with L_{ch} of 1 μm (In:Ga:Zn = 2:1:1 to 7:1:1). (b) Extracted μ_{FE} and g_m of long-channel IGZO FETs with different In:Ga:Zn ratios. Pure In_2O_3 FET μ_{FE} can reach 100 cm²/Vs.

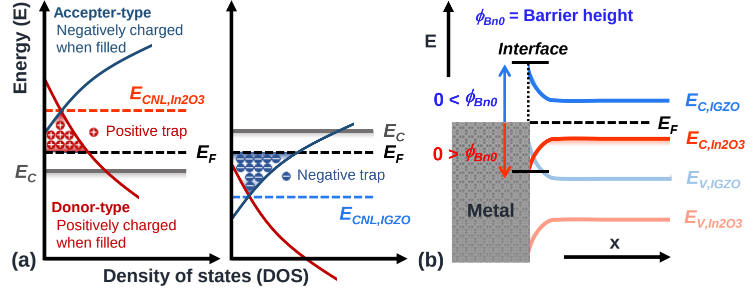

Fig. 7. (a) Comparison of the trap density schematic at the interfaces of In_2O_3 and IGZO. The charge neutrality level E_{CNL} located deep inside the conduction band and it moves toward the bandgap as doping by Ga and Zn. (b) Band alignment diagram of metal (Ni) and semiconductor (In_2O_3 and IGZO) junction. When pure In_2O_3 is doped with Ga and Zn, the Φ_B changes from negative to positive.

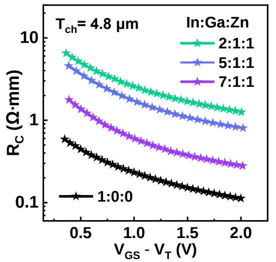

Fig. 8. Contact resistance extracted by the transfer length method (TLM) at different doping ratios.

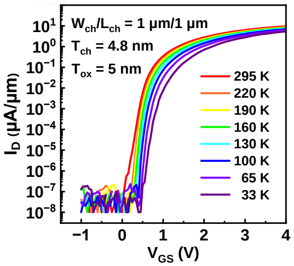

Fig. 9. Temperature-dependent transfer characteristics of an IGZO (In:Ga:Zn = 7:1:1) FET with a L_{ch} of 1 μm.

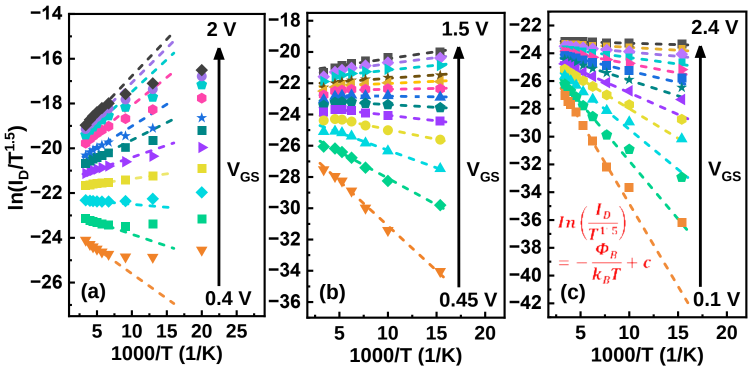

Fig. 10. The Arrhenius plots at different gate voltages are extracted from temperature-dependent transfer characteristic curves. The data is linearly fitted at high temperatures (T ≥ 175K) (a) 1:0:0, (b) 7:1:1, and (c) 3:1:1 from IGZO FETs.

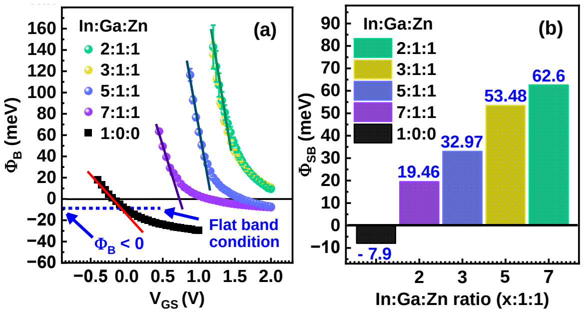

Fig. 11. (a) Barrier height (Φ_B) extraction for pure In_2O_3 (In:Ga:Zn = 1:0:0) and IGZO FETs with different doping ratios (In:Ga:Zn = 2:1:1 to 7:1:1), showing a negative contact barrier height at In_2O_3 and positive ones at IGZO. (b) Extracted Schottky barrier (Φ_{SB}) height at the flat-band voltage.