Defect Engineering in *n*-Type Oxide Semiconductor TFTs

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Disordered structural network and high-density intrinsic defects in amorphous oxide semiconductor materials, largely affect electrical performances (*e.g.* mobility, stability) of the TFTs and limit their applications in next-generation electronic device platforms, *e.g.* active-matrix liquid crystal display.

In our recent works, we comprehensively analyze the intrinsic defects inside these *n*-type oxide semiconductors and therefore understand the material physics to optimize the device performances *via* defect engineering. [1] [2] [3] [4]

In InGaZnO, besides the interface and bulk tail states, several native point defects need to be considered, as depicted in Figure 1. Regarding the neutral (Vo^0), 2+ (Vo^{2+}) charge states related to oxygen vacancy, Vo^0 defect is known to act as deep donor, with energy level above the E_V. Electron capture takes place for the Vo^{2+}, *i.e.* acting as an acceptor. In InGaZnO, zinc vacancy also easily forms as deep acceptor. [3]

In ZnO, the dominant native defects are oxygen and zinc vacancies. The zinc vacancy Zn(vac) is deep acceptor and largely degrades the subthreshold slope *SS*, whereas oxygen vacancies O(vac) behave as deep donors and are mostly neutral and electrically inactive. In the *n*-type ZnO, zinc interstitial Zn(int) is strongly suggested as one dominant native shallow donor, and can easily get positively charged, resulting in negative shift of transfer curves in the pristine ZnO TFT. [1]

In In_2O_3, the origin of the native donor is indium interstitial In(int), but also with the absolute coexistence of the oxygen vacancy for carrier generation. The In(int) as one dominant defect, can generate a shallow donor level close to the CBM. Free conduction electrons in In_2O_3 can be supplied by the In(int), consequently the In(int) is ionized to be positive univalent. On the contrary, the indium vacancies In(vac) form shallow acceptor levels above the VBM. [1]

While implementing the dopants incorporation and the bilayer stack, [3] [4] the defects density inside these *n*-type oxide semiconductors can be reduced and a barrier height is formed between the hydrogenated and pristine layers, improving the device performances like the current on/off ratio, the field-effect mobility, *SS* and stability. However, with the continuous H plasma treatment, the H dopants can behave as the positive or negative charge states, leading to various shifting trend in the transfer curves and also device degradation. [1]

Defect self-compensation $(In)^+ + (O)^- \rightarrow$ In-O is also revealed to contribute to the high mobility of the bilayer-stacked InGaZnO/In_2O_3 TFT, [2] which was deposited *via* a room-temperature RF sputtering technique. As schematically illustrated below, the abundant oxygen interstitials (O_i) in InGaZnO interact with the indium atoms or cluster (In-In) with dangling bonds in In_2O_3, replacing the In-In bond by two In-O bonds as the final state.

References

[1] H. Wang, J. He, Y. Xu, N. André, Y. Zeng, D. Flandre, L. Liao and G. Li*, Impact of hydrogen dopants incorporation on InGaZnO, ZnO and In_2O_3 thin film transistors, *Physical Chemistry Chemical Physics*, 22(3), 2020.

[2] J. He, G. Li*, Y. Lv, C. Wang, C. Liu, J. Li, D. Flandre, H. Chen, T. Guo and L. Liao*, Defect self-compensation for high-mobility bilayer InGaZnO/In_2O_3 thin film transistor, *Advanced Electronic Materials*, 5(6), 1900125, 2019.

[3] G. Li, A. Abliz, L. Xu, N. André, X. Liu, Y. Zeng*, D. Flandre, and L. Liao*, Understanding hydrogen and nitrogen doping on active defects in amorphous In-Ga-Zn-O thin film transistors, *Applied Physics Letters*, 112, 253504, 2018.

[4] A. Abliz, J. Wang, L. Xu, D. Wan, L. Liao*, C. Ye, C. Liu*, C. Jiang, H. Chen, and T. Guo, Boost up the electrical performance of InGaZnO thin film transistors with inserting an ultrathin InGaZnO:H layer, *Applied Physics Letters*, 108, 213501, 2016.

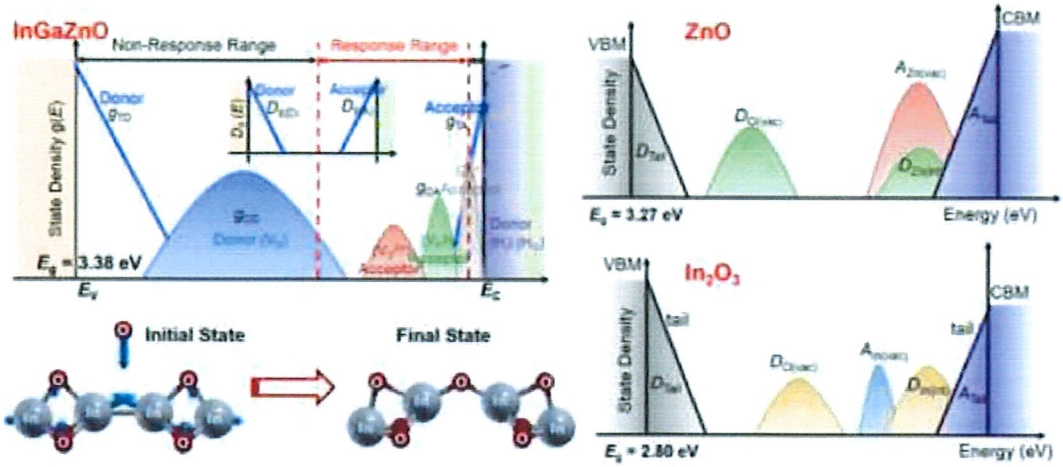

Figure 1. Schematic illustration of intrinsic defects inside the amorphous InGaZnO (with H dopants incorporation), the pristine ZnO and In_2O_3 material systems, with initial and final states of the intervention between oxygen interstitial O_i and metal cluster In-In