Thickness-Dependent Bandgap Modulation in Ga-Doped In_2O_3: A First-Principles study

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Introduction: In_2O_3-based oxide semiconductors have emerged as promising channel materials for monolithic 3D (M3D) integration due to their high mobility, wide bandgap, and compatibility with low-temperature processes [1]. As device scaling pushes channel thicknesses below 5 nm, understanding how structural confinement and doping affect the electronic structure becomes critical for enabling back-end-of-line (BEOL) device stacking. Ga-doping is commonly employed to stabilize In_2O_3 and tune its carrier concentration [2], but its role in confined geometries remains unclear. In this work, we explore how Ga substitution alters the band structure and transport-related parameters in ultrathin In_2O_3 slabs, with direct relevance to oxide-based M3D transistor design.

Results and Discussion: The quantum confinement effect on In_2O_3 and Ga-doped In_2O_3 (IGO) thin films were theoretically studied by DFT as implemented in Quantum ATK simulation package. Optimized norm-conserving pseudopotentials and the Perdew-Burke-Ernzerhof (PBE) exchange-correlation were used. We constructed hydrogen-passivated In_2O_3 slabs with thickness varying from 1–5 nm, as shown in **Fig. 1**. A vacuum layer of 2.5 nm was added to both sides of the slabs. Ga-doping was introduced by substitution at In:Ga=3:2 (≈40% Ga). Electronic structure calculations were carried out using GGA-PBE within the Quantum-ATK framework, with full relaxation of atomic positions and surfaces. Bandgap was extracted from the band structures, and electron effective mass (m*) was determined by parabolic fitting near the conduction band minimum (CBM).

Undoped slabs exhibited the expected bandgap widening by quantum-confinement from 1.31 eV (5 nm) to 2.05 eV (1 nm) as shown in **Fig. 2**. Moreover, the IGO slabs reveal a lower bandgap across thicknesses (1.29eV to 1.17 eV) than the In_2O_3 slabs, defying the expectation of bandgap widening by forming GaOx. Projected DOS analysis showed no gap states, pointing to intrinsic band edge shifts. We attribute this to Ga replacing delocalized In 5s orbitals at the CBM with more localized Ga 4s states, [3,4] thereby reducing conduction band dispersion and lowering both the bandgap and electron effective mass. m* in Ga-doped slabs remains stable (~0.19 m_e) across thicknesses, whereas undoped In_2O_3 shows m* decreasing from 0.29 to 0.20 m_e, with increasing slab thickness.

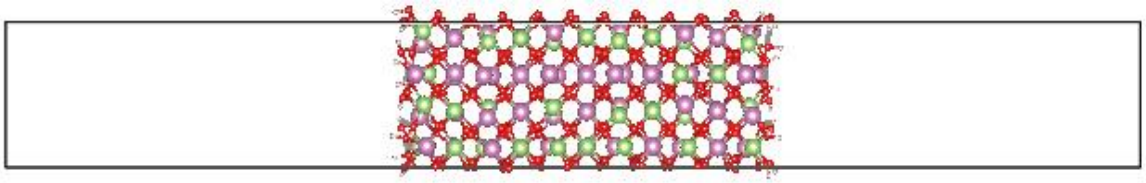

Fig.1 Atomic structure of 3nm-thick Ga-doped In_2O_3 slab

Summary: Nanosheet oxide semiconductor In_2O_3 and IGO shows bandgap widening by quantum confinement. Ga-doping in ultrathin In_2O_3 induces bandgap narrowing and stabilizes carrier effective mass by modifying conduction band orbital character. The behavior is driven by orbital hybridization rather than defect states. These findings highlight the interplay between doping and confinement, providing key insights for future oxide M3D device engineering.

References [1] Omura, Hideyuki, et al. *Journal of Applied Physics* 105.9 (2009).
[2] K. Hikake et al., *IEEE Trans. Electron Devices*, 71, 2373–2379 (2024).
[3] Alexandr I Cocemasov *et al* 2020 *J. Phys.: Condens. Matter* 32 225703
[4] Julia E Medvedeva and Chaminda L Hettiarachchi Phys. Rev. B 81, 125116

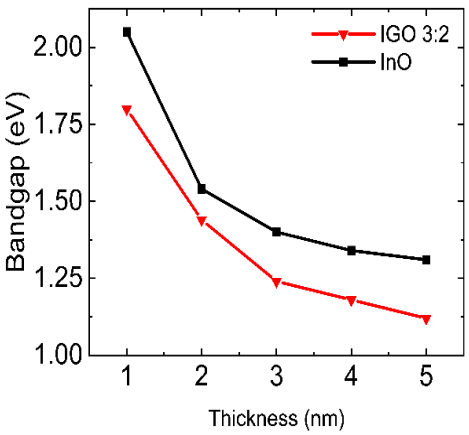

Fig.2 Bandgap versus slab thickness for In_2O_3 and IGO slabs.