Example ICDS abstract: Acceptors and hydrogen in β-Ga_2O_3

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This example shows how abstracts are formatted. Magnesium-doped gallium oxide may be utilized as a semi-insulating material for future generations of power devices. In this work, spectroscopy and hybrid functional calculations were used to investigate defect levels in Czochralski-grown β-Ga_2O_3. Substitutional Mg dopants act as deep acceptors while substitutional Ir impurities are deep donors. Hydrogen-annealed Ga_2O_3:Mg shows an IR peak at 3492 cm^{-1}, assigned to an O-H bond-stretching mode of a neutral MgH complex [1]. Despite compensation by Ir and Si, and hydrogen passivation, high densities of Mg (10^{19} cm^{-3}) can push the Fermi level to mid-gap or lower.

To assess the effects of Ir contamination and Mg incorporation, we calculated formation energy diagrams for substitutional Ir and Mg-related defects for the O-rich and Ga-rich limits. Our results identify that Ir and Mg most favorably incorporate on the octahedral Ga(II) site. Similar to previous studies [2], we find that $Mg_{Ga(II)}$ acts as a deep acceptor, with a calculated (0/–) charge-state transition level 1.06 eV above the valence-band maximum. Consistent with the work of Kananen et al. [3], we find the hole most favorably localizes on an adjacent O(I) atom, while a hole localized on the O(II) atom is 0.16 eV higher in energy. Mg on the tetrahedral Ga(I) site is less favorable by 0.5 eV for both the neutral and negative configurations, yielding a slightly deeper acceptor level of 1.27 eV. Mg interstitials (Mg_i) are shallow donors that can be favorable for Fermi levels below mid-gap. However, O-rich conditions suppress the formation of this self-compensating species.

UV/visible transmission spectra of the Mg-doped samples show an absorption threshold at 2.8 eV. This absorption threshold is not observed in the spectra of undoped Ga_2O_3, nor in Ga_2O_3:Mg produced by float-zone crystal growth [4]. Because of this, we attribute the absorption to the excitation of a valence-band (VB) electron to the $Ir^{4+/3+}$ level, rather than an excitation to/from the Mg level. There is a second threshold at 3.2 eV. This feature could be due to the transition of a VB electron to an Ir^{3+} excited state, similar to the case of Fe in GaAs [5].

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