Atomistic Simulations for Understanding the Behavior of Dopants and Impurities in Ga_2O_3 and Related Alloys

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Gallium oxide (Ga_2O_3) is rapidly developing as one of the most promising ultra-wide bandgap platforms for next-generation power electronics owing to properties like a high breakdown field, controllable (*n*-type) electrical conductivity, and commercially-available single-crystal substrates that can be grown via a number of industrially-scalable processes. Beyond exhibiting a number of polymorphs with similarly attractive properties, alloying with Al into Ga_2O_3 to form $(Al_xGa_{1-x})_2O_3$ (AGO) alloys can lead to a significant increase of the band gap to potentially access higher power device figures of merit, analogous to the AlGaN system but spanning a much larger rage of ~4.8 eV-8.6 eV. Despite the progress with Ga_2O_3 and related alloys, a number of open questions remain on the nature of fundamental defects and the role of impurities and dopants in determining the observed optical and electrical properties of these materials. This is even more of an open question in the lesser studied alloys like AGO, particularly regarding the effectiveness of donor doping and how to overcome the possibility of compensation in the limit high Al-contents. In this work we survey the current understanding of point defects in Ga_2O_3, focusing on their potential optical and electrical consequences from insights gained through first-principles-based calculations employing hybrid functionals. We discuss what is known about donor and acceptor dopants, as well as their interactions with native defects and impurities incorporated through growth and processing steps. These results provide guidance for controlling defect populations and the electrical conductivity in Ga_2O_3 and related alloys and for facilitating next-generation power electronics based on this ultra-wide bandgap semiconductor family.

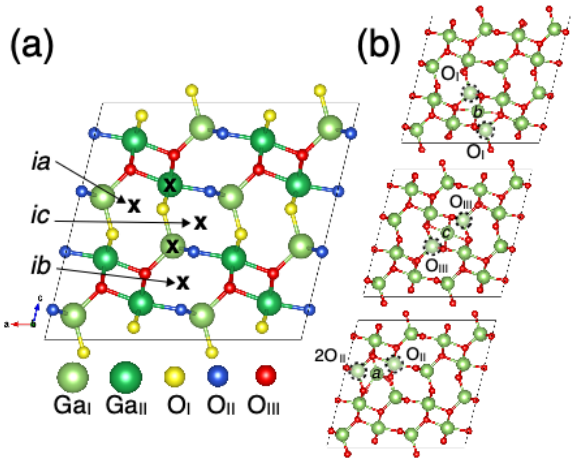

Figure 1. (a) Schematic of the ground-state β–Ga_2O_3 structure showing the various symmetry inequivalent Ga and O sites, and interstitial sites that stabilize more complex Ga vacancy configurations. (b) The three interstitial-vacancy complexes denoted as V^{ib}_{Ga}, V^{ib}_{Ga}, and V^{ib}_{Ga} from top to bottom. The vacant Ga sites adjacent to the displaced interstitial Ga in (b) are highlighted with dashed circles and also include labels for the O species with remnant dangling bonds for each vacancy configuration.

This work was partially performed under the auspices of the U.S. DOE by Lawrence Livermore National Laboratory (LLNL) under contract DE-AC52-07NA27344 and partially supported by Laboratory Directed Research and Development funding under project number 22-SI-003 and by the Critical Materials Institute, an Energy Innovation Hub funded by the U.S. DOE EERE AMMTO.