Identifying Configurations and Migration Paths of Oxygen Interstitial Defects in β-Ga_2O_3

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β-Ga_2O_3 is a wide bandgap semiconductor with potential applications in power electronics. The crystal structure of β-Ga_2O_3 is in the monoclinic C2/m space group with two Ga and three O sites. The configurations of interstitial O atoms in β-Ga_2O_3 have not been fully explored due to the low symmetry of crystals, leading to several possibilities in the potential energy landscape [1]. Recent simulations aimed to identify all possible point defect configurations in metal oxides [2]. The approach developed by Mosquera-Lois et al., introducing bond distortions and rattling as implemented in the ShakeNBreak code [3], demonstrates an efficient strategy for navigating the defect configurational landscape in high symmetry oxides, such as In_2O_3, ZnO, and a-TiO_2. In this study, we applied this approach to generate initial distorted structures, exploring all possible oxygen interstitial (O_i) defect configurations in β-Ga_2O_3 and comparing them with atomic displacements using a grid sampling method. These initial structures were optimized using Density Functional Theory (DFT) with the PBEsol functional, as implemented in the CP2K code, considering charge states q= (-2, -1, 0, +1, +2). Our findings reveal that the most stable Oi configurations for q= -1, 0, +1, +2 involve split oxygen interstitial defects (O_{si}), forming O-O dimers on the same tetrahedron (H-center), while configurations forming O-O dimers between two polyhedrons (peroxy bridge) are identified as metastable. For the -2 negative charge state (q=-2), the lowest configurations were found to be normal O_i defects without O-O dimers. Additionally, we calculated O-migration between different O_{si} sites, finding an activation energy of around 2.3 eV, which is lower than the oxygen interstitial activation enthalpy of 3.2 eV measured using secondary ion mass spectrometry depth profiling at high temperatures between 1200 and 1600 °C [4]. Our study indicates the possibility of O_i defect configurations and O-migration paths in β-Ga_2O_3.

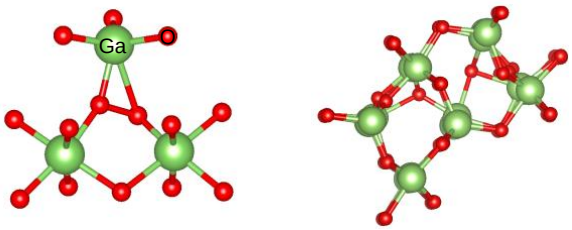

Figure 1: a) Spit oxygen interstitial (O_{si}) configuration at neutral charge state and b) normal oxygen interstitial (O_i) configuration at -2 charge state of β-Ga_2O_3

[1] Ingebrigtsen, Mads Eide, et al. "Impact of proton irradiation on conductivity and deep level defects in β-Ga2O3." APL Materials 7.2 (2019).
[2] Kononov, Alina, et al. "Identifying native point defect configurations in α-alumina." Journal of Physics: Condensed Matter 35.33 (2023).
[3] Mosquera-Lois, Irea, et al. "Identifying the ground state structures of point defects in solids." npj Computational Materials 9.1 (2023).
[4] Uhlendorf, Johanna, et al. "Oxygen diffusion in β-Ga2O3 single crystals at high temperatures." Applied Physics Letters 119.24 (2021).