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AB-INITIO CALCULATIONS OF ELECTRONIC PROPERTIES OF β-Ga_2O_3 OWN DEFECTS

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Gallium oxide is known in the scientific community for its unique electrical and optical properties. Due to its wide bandgap (~5.0 eV), it is of interest to scientists as a promising material in various fields of power electronics, optoelectronics, and photonics. [1, 2, 3].

The reflection spectrum [4] was calculated in the work for the direction of the electric vector E parallel to the b axis (E||b) (Fig. 1). It can be seen in the figure that the calculated IR reflections of the wave vector q⊥(100) and E||b are comparable with the experimental data [5], and the IR reflections of the wave vector of the other direction q⊥ (-201) and E||b are comparable with work [6]. In the work [6], pure TO phonons with Au symmetry are also observed.

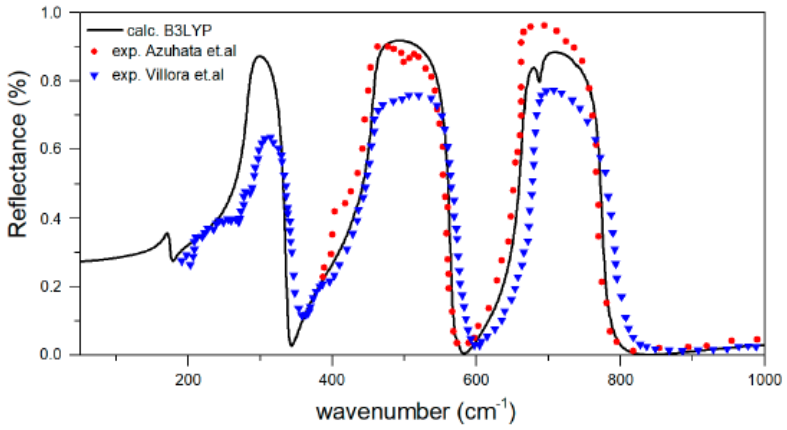

Figure 1. Estimated IR reflectance for the wave vector q⊥(100) and a specific direction of the electric vector E||b. Experimental data are presented for comparison. [5, 6]

Oxygen vacancies of gallium oxide are deep donors, since its transition levels are 1 eV below the minimum of the conduction band, and gallium vacancies are deep acceptors with empty levels that are located more than 0.7 eV above the valence band and rather lower than the donor level. [7]

Due to the fact that oxygen vacancies can easily donate their electrons to gallium vacancies, the energy of formation of oxygen vacancies decreases as the number of donors in the crystal decreases. In parallel with this process, an increase in the energy of formation of acceptors occurs, which leads to a decrease in the energy of formations of donors. Ultimately, this leads to an energy balance between the two processes and results in a constant concentration of native donors and acceptors. [7]

We assume that the observed n-type conductivity in β-Ga_2O_3 crystals can be caused by light doping of a donor impurity during crystal growth, such as hydrogen. Our calculations also show that gallium vacancies cannot be involved in p-type conductivity in β-Ga_2O_3. Because all types of gallium vacancies with different charge states are located above the valence band by more than 0.7 eV.

REFERENCES

[1] Higashiwaki M., Sasaki K., Kuramata A., Masui T., Yamakoshi S., "Gallium oxide (Ga_2O_3) metal-semiconductor field-effect transistors on single-crystal β-Ga_2O_3 (010) substrates", Appl. Phys. Lett., vol. 100, 2012

[2] Pearton S.J., Yang J., Cary P.H., Ren F., Kim J., Tadjer M.J., Mastro M.A. "A review of Ga_2O_3 materials, processing, and devices", Appl. Phys. Rev., vol. 5, 2018

[3] Zhang, J., Shi J., Qi D.-C., Chen L., Zhang K.H.L., "Recent progress on the electronic structure, defect, and doping properties of Ga_2O_3.", APL Mater., vol. 8, 2020

[4] Demichelis R., Suto H., Noël Y., Sogawa H., Naoi T., Koike C., Chihara H.;, Shimobayashi N., Ferrabone M., Dovesi R., "The infrared spectrum of ortho-enstatite from reflectance experiments and first-principle simulations", Mon. Not. R. Astron. Soc., vol. 420, 2012, pp. 147–154

[5] Víllora E.G., Morioka Y., Atou T., Sugawara T., Kikuchi M., Fukuda T., "Infrared reflectance and electrical conductivity of β-Ga_2O_3", Phys. Status Solidi Appl. Res., vol. 193, 2002, pp. 187–195

[6] Azuhata T., Shimada K., "Polar phonons in β-Ga_2O_3 studied by IR reflectance spectroscopy and first-principle calculations", Appl. Phys. Express, vol. 10, 2017

[7] Abay Usseinov , Zhanymgul Koishybayeva , Alexander Platonenko , Vladimir Pankratov , Yana Suchikova, Abdirash Akilbekov, Maxim Zdorovets, Juris Purans, Anatoli I. Popov, "Vacancy Defects in Ga_2O_3: First-Principles Calculations of Electronic Structure", Materials, vol. 14, 2021