Optical and Electronic Energy Band Properties of Nb-Doped β-Ga2O3 Crystals

Xianjian Long 1,†, Wenlong Niu 1,†, Lingyu Wan 1,*, Xian Chen 1, Huiyuan Cui 2, Qinglin Sai 2, Changtai Xia 2,*, Devki N. Talwar 3,© and Zhechuan Feng 1

1 Center on NanoEnergy Research, Laboratory of Optoelectronic Materials & Detection Technology, Guangxi Key Laboratory for the Relativistic Astrophysics, School of Physical Science & Technology, Guangxi University, Nanning 530004, China; longxianjian46@gmail.com (X.L.); niuwenlong@uniwatt.com (W.N.); cx2135012@163.com (X.C.); zcfeng@ntu.edu.tw (Z.F)
2 Key Laboratory of Materials for High Power Laser, Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Shanghai 201800, China; chy_siom@163.com (H.C.); saiqi@siom.ac.cn (Q.S.)
3 Department of Physics, University of North Florida, Jacksonville, FL 32224, USA; d.talwar@unf.edu
* Correspondence: lyw2017@gxu.edu.cn (L.W.); xia_ct@siom.ac.cn (C.X.)
† These authors contributed equally: Xianjian Long and Wenlong Niu.

Abstract: Systemic investigations are performed to comprehend the structural, optical, and electrical characteristics of four niobium (Nb) doped β-Ga2O3 crystals (β-Ga2O3:Nb) grown by the optical floating zone (OFZ) method. All of the β-Ga2O3:Nb crystals revealed monoclinic phases and good crystalline qualities. While the different Nb doped (i.e., 0.0001 mol%, 0.01 mol%, 0.1 mol% and 0.5 mol%) samples exhibited slightly changed bandgap energies \( E_g \) (≈ 4.72 eV, 4.73 eV, 4.81 eV, 4.68 eV)—the luminescence features indicated distinctive defect levels—affecting the electronic energy structure significantly. By increasing the Nb doping level from 0.0001 mol% to 0.1 mol%, the Fermi level \( E_F \) moves closer to the bottom of the conduction band. For the sample with Nb doping 0.5 mol%—no further improvement is noticed in the electronic properties. Finally, the energy band diagrams of four samples are given.

Keywords: β-Ga2O3:Nb; optical floating zone method; optical properties; electronic energy band
no systematic studies on the defect energy levels and electronic energy band structures of $\beta$-Ga$_2$O$_3$:Nb. In this paper, we report the results of a systematic study on the optical characteristics and electronic energy band structures of Nb-doped $\beta$-Ga$_2$O$_3$ crystals grown by the optical floating zone (OFZ) method. We strongly feel that the outcomes described here are of vital importance for many optoelectronic device applications.

2. Materials and Methods

By using high purity gallium oxide (Ga$_2$O$_3$) powder (99.9999%) and niobium pentoxide (Nb$_2$O$_5$) powder (99.99%) as the raw materials and a [010] oriented $\beta$-Ga$_2$O$_3$ single crystal as a seed, we grew Nb doped $\beta$-Ga$_2$O$_3$ crystals in a Quantum Design IRF01-001-00 infrared image furnace through the OFZ technique. The nominal Nb doping concentrations are about 0.0001 mol%, 0.01 mol%, 0.1 mol%, and 0.5 mol% (labeled as samples S1, S2, S3, and S4), respectively, calculated by a mixing ratio of Nb$_2$O$_5$ and Ga$_2$O$_3$ raw materials. The OFZ-grown crystals were cut into bulk samples along the (100) crystal plane by a STX-202A diamond wire cutting machine. Each sample size was $5 \times 5 \times 1$ mm$^3$ and its two (100) plane surfaces were polished for optical measurements and analysis.

To comprehend the crystal structure of the samples, we used high-resolution x-ray diffraction (HR-XRD) with a wavelength of 1.546 Å (D8 Discover, Advance Bruker, Karlsruhe, Germany). The optical transmission (OT) and photoluminescence excitation (PLE) spectra were recorded by exploiting an ultraviolet/visible/near infrared (UV/Vis/NIR) spectrometer (Zolix Omni-$\lambda$300I spectrometer). The results were used to analyze the bandgap properties. Room temperature photoluminescence (PL) measurements were performed by using a spectrometer (Zolix Omni-$\lambda$750I) with a wavelength of 213 nm (FL-213-Pico laser, Changchun New Industries, CNI., Changchun, China) to explore the luminescent features. We also employed the X-ray photoelectron spectroscopy (XPS) and an ultraviolet photoelectron spectroscopy (UPS) with a monochromatic Al K$\alpha$ X-ray source having a photon energy of 1486.7 eV (ESCALAB 250Xi+, Thermo Fisher Scientific, Waltham, MA, USA) for measuring the electronic band structures of the four samples.

3. Results and Discussion

3.1. Crystal Quality

In Figure 1, we showed the HR-XRD spectra of four samples where the scanning range was set between 10$^\circ$ and 110$^\circ$ with a step of 0.05$^\circ$. The perusal of Figure 1 revealed four strong diffraction peaks and three weak diffraction peaks assigned as the (400), (600), (800), (1200), and (200), (512), (603) crystal planes, respectively (referring to the Ga$_2$O$_3$ XRD Joint Committee on Powder Diffraction Standards (JCPDS) card 04-003-1858). The positions of four main diffraction peaks and their full width at half maxima (FWHM) are reported in Table 1. The results of HR-XRD showed that all four $\beta$-Ga$_2$O$_3$:Nb crystals with different Nb doping levels exhibited good monoclinic phases and the crystal qualities have not been lowered with the doping. Among the four samples, S4 has minimum values of FWHM for four diffraction peaks of (400), (600), (800), (1200).

The full XPS spectra of four samples are displayed in Figure 2a. To avoid surface contamination, we used an Ar ion beam to clean the sample surface for three minutes. The perusal of full spectrum (as shown in Figure 2a) revealed both Ga and O elements. Due to low Nb doping and the sensitivity limit of the XPS, it is difficult to trace the Nb element in the full spectrum. As shown in Figure 2b, there are two fitting peaks of the O 1s obtained by the peak-differential-imitating analysis. Among them, the part with lower binding energy (O(I)) was attributed to the oxidation (Ga-O-Ga) bond [15], while the part with higher binding energy (B.E.) was related to the oxygen vacancies (O(II)) in the Ga$_2$O$_3$ film [6]. The fitting results of Ga 2p 1/2 and Ga 2p 3/2 are shown in Figure 2c. The peak positions of Ga 2p 1/2 are 1118.7 eV (S1), 1118.5 eV (S2), 1118.6 eV (S3), and 1118.9 eV (S4), respectively. For Ga 2p 3/2, the peak positions are 1145.7 eV (S1), 1145.4 eV (S2), 1145.5 eV (S3), and 1145.8 eV (S4), respectively. The XPS spectral analysis results of the four samples are reported in Table 2. It was noted that the ratio of Ga and O in each sample is around
2:3 (i.e., Ga:O = 0.706484 (S1), 0.712328 (S2), 0.709421 (S3), 0.733137 (S4), respectively). The atomic ratio of Ga and O is slightly higher than 2:3, which is possibly due to the presence of O vacancies in Ga$_2$O$_3$. It should be noted that the content of Ga in the S4 sample is higher than that in the other samples, which indicates that S4 has more O vacancies to affect the carrier concentration and defect-related luminescence properties.

Table 1. The results of HR-XRD for four β-Ga$_2$O$_3$:Nb samples.

| Samples | S1 | S2 | S3 | S4 |
|---------|----|----|----|----|
| Crystal faces | 2θ | FWHM | 2θ | FWHM | 2θ | FWHM | 2θ | FWHM |
| (400) | 30.12 | 0.110 | 30.12 | 0.108 | 30.20 | 0.094 | 30.14 | 0.072 |
| (600) | 45.89 | 0.130 | 45.9 | 0.139 | 45.99 | 0.174 | 45.85 | 0.095 |
| (800) | 62.58 | 0.190 | 62.57 | 0.158 | 62.68 | 0.153 | 62.57 | 0.09 |
| (1200) | 102.29 | 0.281 | 102.26 | 0.203 | 102.49 | 0.299 | 102.32 | 0.21 |

Figure 1. High-resolution x-ray diffraction (HR-XRD) 2θ-ω patterns for the Nb doped β-Ga$_2$O$_3$.

Figure 2. (a) The wide-scanning X-ray photoelectron spectroscopy (XPS) spectra of samples S1, S2, S3, S4. (b) O 1s fitting results. (c) Ga 2p fitting results.
Table 2. The O 1s and Ga 2p atomic percentages and bonding analysis of S1, S2, S3, and S4. (In table, the unit of Area is CPSeV, CPS is counts per second)

| Sample | Ga 2p 1/2 | Ga 2p 3/2 | Ga | O 1s | O |
|--------|-----------|-----------|----|------|---|
|        | B.E. (eV) | Area      | B.E. (eV) | Area | Ratio% | B.E. (eV) | Area | Ratio% |
| S1     | 1145.7    | 18250     | 1118.7 | 36435 | 41.4 | 530.7   | 77453 | 58.6 |
| S2     | 1145.4    | 23873     | 1118.5 | 47134 | 41.6 | 530.48  | 99503 | 58.4 |
| S3     | 1145.5    | 22035     | 1118.6 | 43616 | 41.5 | 530.52  | 92349 | 58.5 |
| S4     | 1145.8    | 23697     | 1118.9 | 46686 | 42.3 | 530.86  | 96144 | 57.7 |

3.2. Bandgap and Defect-Related Luminescence

The OT measurements were performed to obtain the bandgap energies of the four β-Ga2O3:Nb samples and the recorded transmission spectra is shown in Figure 3. The bandgap energies are calculated by using the following expression [16]

\[
\alpha = B' (h\nu - E_g)^{1/2}
\]

where \(\alpha\) represents the absorption coefficient, \(h\nu\) denotes the incident photon energy, \(B'\) is related to the valence and conduction bands and \(E_g\) signifies the bandgap energy. In Equation (1), if \(h\nu\) is zero, the square of absorption coefficient becomes equal to the \(E_g\). By linear extrapolation, the bandgap energies of the four samples are obtained as 4.72 eV (S1), 4.73 eV (S2), 4.81 eV (S3), 4.68 eV (S4), respectively. The absorption shoulder located near 4.5 eV is usually considered as the perturbation caused by Ga\(^{3+}\) vacancies (V\(_{\text{Ga}^{3+}}\)) [17].

Figure 3. The optical transmission spectra of four samples of Nb-doped β-Ga2O3 at room temperature, and the bandgap of the four samples calculated results.

The band-to-band transitions and defect-related luminescence were also investigated by using PLE and PL techniques. As shown in Figure 4a, the band-to-band absorptions of the four samples are about 4.7 eV, which coincide with the results of OT measurements. For the S3 sample, the PLE spectrum revealed two peaks with an energy level difference of 0.23 eV, suggesting that this is either caused by the split of an energy level or related to the energy levels of a shallow donor.

To further analyze the defect-related luminescence features of the four Nb doped samples, we used a high power with a laser source of wavelength 213 nm to excite the samples. We used the Gaussian peak fitting method to perform analyses of the PL spectra and reported the best fitting results in Table 3. The defect-related luminescence spectra of β-Ga2O3:Nb mainly consist of three parts: the first one is an ultraviolet band with a relatively higher intensity. According to earlier reports [18–20], Ga2O3 luminescence in the ultraviolet band is independent of the impurity, which is related to the combination of free electrons and self-trapping holes (STHs). Another one is in the blue light region, which is mainly caused by the recombination of the deep-level donor-acceptor-pairs. These deep-level donors are attributed to the material’s intrinsic defects, such as the oxygen vacancies (V\(_O\)).
gallium interstitials (Ga$_i$), and the acceptors are gallium vacancies (V$_{Ga}$), gallium-oxygen vacancy pairs complex (V$_{O}$-V$_{Ga}$), respectively [19,21,22]. It can be noted from Table 3 that the peak positions of ultraviolet and blue lights in S1 and S2 samples are almost the same, while the peaks of S3 showed blue shift and the peaks of S4 displayed red shift. The last part is red light near 700 nm with relatively weak intensity. In references [23,24], the red band was attributed to the nitrogen impurities but the study in references [25] suggested that the oxygen vacancies could participate in the PL as a hole trap, which give rise to emission between 1.6 and 2.0 eV. Since there was no N element in our samples from the XPS results, the red band might originate from holes trapped at the intrinsic defects of O vacancies at trigonal sites [25]. Unlike several reports, we noticed no green bands in the PL spectra of our samples [18,23,24,26]. We also calculated the intensity ratio of the three peaks in our samples, which are 1:0.8:0.41 (S1), 1:0.63:0.33 (S2), 1:0.29:0.17 (S3), and 1:1.15:0.102:0.73 (S4), respectively. It was noted that the intensity ratio of the blue light and red light decreased with the increase of Nb doping for samples S1–S3, for sample S4; however, the intensity ratio of red light increased significantly, which we attribute it to the interstitial oxygen.

![Figure 4](image_url)

**Figure 4.** (a) Room Temperature photoluminescence excitation (PLE) and photoluminescence (PL) spectra of samples S1, S2, S3, and S4. (b) Deconvoluted PL spectra of samples S1, S2, S3, and S4.

**Table 3.** PL analysis results.

| Simples | S1      | S2      | S3      | S4      |
|---------|---------|---------|---------|---------|
| Peaks (eV) | 3.25    | 2.69    | 1.77    | 3.23    |
| FWHM (nm) | 80.8    | 14      | 183     | 80.6    |
| Ratio of Area | 1:0.8:0.41 | 1:0.63:0.33 | 1:0.29:0.17 | 1:1.15:0.102:0.73 |

### 3.3. Electronic Energy Band Structures

In order to determine the $E_F$ and work function, the UPS study was performed on the four $\beta$-Ga$_2$O$_3$:Nb samples. By calibrating the Fermi level ($E_F$) of sample and testing stage in the same level, we measured the ultraviolet photoelectron spectra of four samples and the results were shown in Figure 5. Using the linear extrapolation method, we calculated the distances between the $E_F$ and the top of valance band (i.e., the valance band minimum, VBM) for four samples, which were 4.05 eV, 4.35 eV, 4.44 eV, and 4.29 eV, respectively. The cutoff
edges ($E_{\text{cutoff}}$) of the four samples were 16.24 eV, 16.23 eV, 16.24 eV, 16.26 eV, respectively, as shown in Figure 5. The work functions are calculated by the following expression [27]

$$W_f = h\nu - E_{\text{cutoff}}$$

(2)

where $W_f$ is the work function, represented the ionization energy of the electrons from $E_F$ to the vacuum level ($E_{\text{vacuum}}$); and $h\nu$ is the photon energy of light source ($h\nu = 21.22$ eV) [28,29]. The calculated $W_f$ values of the four samples by expression (2) were 4.98 eV (S1), 4.99 eV (S2), 4.98 eV (S3), and 4.96 eV (S4), respectively. Obviously, the $W_f$ of four samples varied slightly with the increase of Nb contents. The band diagrams of the four samples were drawn in Figure 6. It was noted that the distance between the Fermi level and the top of valance band first decreases and then increases with the increase of Nb dopants. The energy difference between conduction band minimum (CBM) and $E_F$ ($\Delta E_C$) for samples S1, S2, S3, and S4 were 0.67 eV, 0.38 eV, 0.37 eV, and 0.39 eV, respectively. The sample S3 has the highest $E_F$ and the lowest $\Delta E_C$.

Figure 5. The ultraviolet photoelectron spectroscopy (UPS) spectra of S1, S2, S3, S4 samples.

Figure 6. Schematics of energy level structure for Nb doped $\beta$-$\text{Ga}_2\text{O}_3$ samples.
4. Conclusions

In summary, comprehensive investigations of the structural, optical, and electronic traits are reported on a series of Nb doped β-Ga2O3 crystals by using XRD, OT, PLE, PL, XPS, and UPS techniques. Four β-Ga2O3:Nb crystals grown by the OFZ method exhibited good monoclinic structure. While the Nb doping slightly affected the bandgap and work function characteristics of the four samples, it certainly played an important role influencing the defect luminescence and energy band structures. The PL spectra have revealed Nb doping inhibited the green light luminescence. With the increase of Nb doping, the distance between Fermi level and the bottom of the conduction band first decrease and then remain almost unchanged. We strongly feel that the structural, optical, and electronic features reported here are quite useful to help design Nb doped β-Ga2O3 optoelectronic devices.

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