精密 X 線回折法による高品質 EFG β-Ga_2O_3 単結晶の格子定数の決定

Determination of Lattice Constants of High-quality Monoclinic β-Ga_2O_3 Single Crystals by Precise X-ray Diffraction Measurements

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1. Introduction

Beta-Gallium Oxide (β-Ga_2O_3) is an ultra-wide bandgap semiconductor material that has a bandgap energy of about 4.5 eV and a breakdown electric field of about 8 MV/cm, which makes this material preferable for high-power electronic devices. To design the layered material for electronic devices, it is crucial to determine the accurate lattice parameters of the crystal.

In this study, we conducted the 2θ/ω scan for symmetric and asymmetric diffraction conditions and calculated the lattice parameters *a*, *b*, *c*, and *β* of the unit cell precisely.

2. Experimental Method

We measured un-doped (UID), Sn-doped, and Fe-doped EFG grown EFG grown (010) wafers. EFG grown (010) wafers were cut from bulk crystals and polished by the chemical mechanical polishing (CMP) technique. Here, a high-resolution X-ray diffraction system (RIGAKU SmartLab) is used where Ge (440) 4-bounce monochromator is installed. 2θ/ω scan is performed for symmetric and asymmetric diffraction (in skew geometry) conditions; (020), (420), (022), (111) and ($\bar{1}$11), and used the following equations to find out the precise lattice constants:

$$\lambda = 2d\ sin\theta_B \qquad (1)$$

$$\frac{1}{{d_{hkl}}^2} = \frac{1}{sin^2\beta}\left(\frac{h^2}{a^2} + \frac{k^2 sin^2\beta}{b^2} + \frac{l^2}{c^2} - \frac{2hlcos\beta}{ac}\right) \qquad (2)$$

We assumed CuKα_1 X-ray wavelength λ = 1.5405929Å.

3. Results and Discussion

Fig. 1 (a) – (e) represents the 2θ/ω-scan results for (420), (020), (022), (111) and ($\bar{1}$11) diffractions respectively for the UID sample. From these results, we calculated the values of d-spacing in Table. I for all the conditions and calculated the accurate lattice parameters *a*=12.23413923Å, *b*=3.039962730Å, *c*=5.800822962Å, and *β*=103.6696273° using the equations (1) and (2).

Table 1: Measured Bragg angle (θ_B) and obtained *d*-spacing for respective *hkl* diffractions of UID β-Ga_2O_3.

hkl	Bragg angle θ_B	d-spacing(Å)
020	30.44820°	1.519981365
420	34.69560°	1.353257688
022	35.15485°	1.337812118
111	17.58320°	2.549880302
$\bar{1}$11	16.73245°	2.675542096

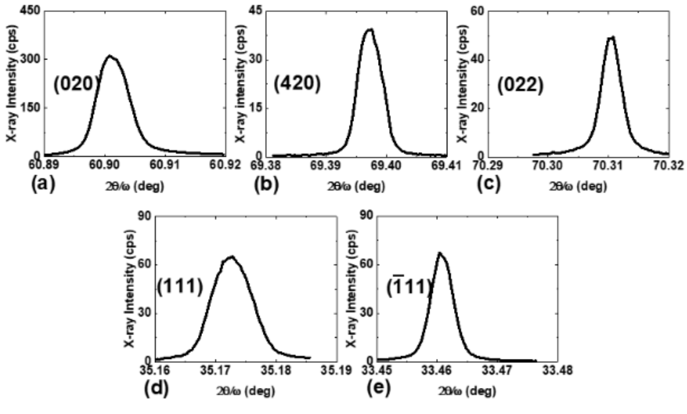

Fig. 1 (a) – (e): 2θ/ω-scan results for 020, 420, 020, 022, 111 and $\bar{1}$11 diffraction conditions of EFG UID β-Ga_2O_3 sample.

References

[1] S. Geller, J. Chem. Phys. **33**, 676 (1960).

[2] J. Åhman, G. Svensson, and J. Albertsson, Acta Cryst. Sect. C **52**, 1336 (1996).