Metal–organic Chemical Vapor Deposition of ε-Ga_2O_3 Thin Film Using N_2O Precursor

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Section S1. XRD rocking curves measurement

Figure S1 shows XRD rocking curves of Ga_2O_3 (004) plane grown with different conditions (temperatures and VI/III ratios). Experimental rocking curves are fitted with Gaussian function. The extracted FWHM values are listed in Table S1.

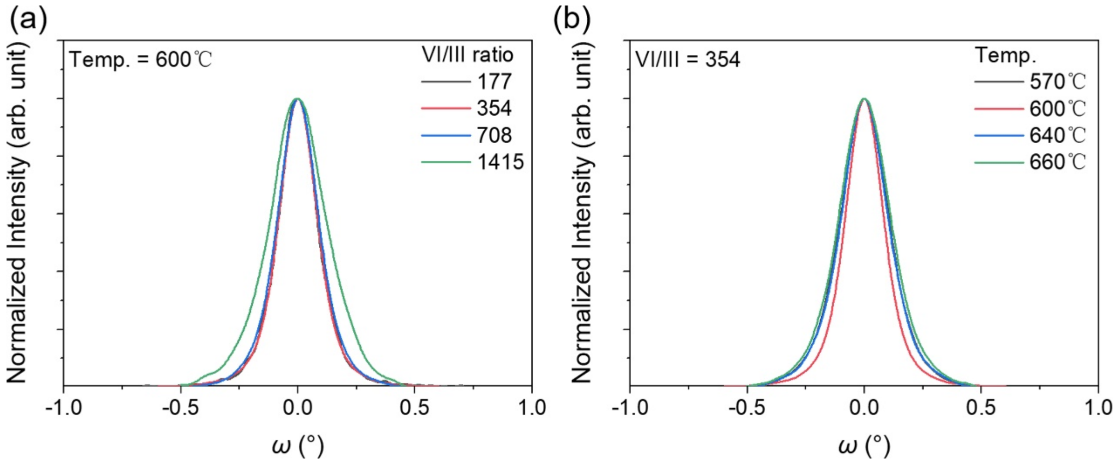

Figure S1. XRD rocking curves of Ga_2O_3 (004) plane grown with (a) various temperatures and (b) various VI/III ratios.

Table S1. The fitted FWHM of rocking curve of Ga_2O_3

Sample	*Growth T (°C)*	*VI/III ratio*	*FWHM(°)*
A	600	177	0.200
B	600	354	0.197
C	600	708	0.207
D	600	1415	0.281
E	570	354	0.243
F	640	354	0.237
G	660	354	0.258

Section S2. Measurement of lattice parameter of ε-Ga_2O_3

In order to calculate the lattice parameters more accurately, Bragg angle correction was performed at first by the measurement of the diffraction patterns of (004) and (006) plane. According to the Bragg's law, the following equation can be deduced [1]:

$$\frac{4\lambda}{2\sin(\theta_{004-meas}+\Delta\theta)}=\frac{6\lambda}{2\sin(\theta_{006-meas}+\Delta\theta)} \qquad (1)$$

where λ is the wavelength of X-ray (λ = 0.1542 nm), $\theta_{004-meas}$, $\theta_{006-meas}$ are the measured Bragg angle, and $\Delta\theta$ is the Bragg angle correction due to the zero setting of instrumental alignment. Thus, $\Delta\theta$ is calculated as -0.148° from Eq. (1). Then, the lattice spacing (d_{hkl}) of the crystal plane (*hkl*) can be calculated from Eq. (2).

$$d_{hkl}=\frac{n\lambda}{2\sin(\theta_{hkl-meas}+\Delta\theta)} \qquad (2)$$

Using d_{004}, d_{013} and d_{133}, we can deduce the lattice parameters (a, b and c) using the following equation (Eq. (3)).

$$\frac{1}{d_{hkl}^2}=\frac{h^2}{a^2}+\frac{k^2}{b^2}+\frac{l^2}{c^2} \qquad (3)$$

Figure S2 shows the result of *2θ*-scan: ε-Ga_2O_3 (004), ε-Ga_2O_3 (006), ε-Ga_2O_3 (013) and ε-Ga_2O_3 (133). The χ angle of (013) and (133) are 19.63° and 50.96°, respectively. All peak positions were obtained by fitting a Gaussian function to the experimental curve. The measured Bragg angle ($\theta_{hkl-meas}$) of ε-Ga_2O_3 (600 °C, VI/III = 354) and the corresponding lattice spacing (d_{hkl}) are listed in Table S2. According to the Eq. (1), Eq. (2) and Eq. (3), we obtain: a = 0.503 nm, b = 0.872 nm, c = 0.928 nm.

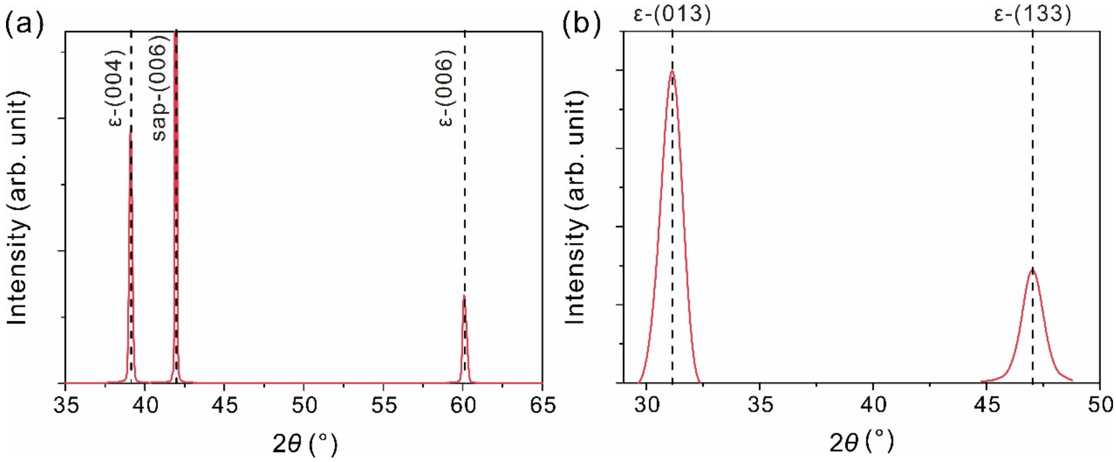

Figure S2. Diffraction peaks of ε-Ga_2O_3 films from XRD *2θ*-scan mode.

Table S2. The measured Bragg angle and the calculated lattice spacing

crystal plane	*(004)*	*(006)*	*(013)*	*(133)*
$\theta_{hkl\text{-}meas}$ (°)	19.550	30.035	15.573	23.515
d_{hkl} (nm)	0.232	0.155	0.292	0.195

Section S3. SEM analysis of growth rate under different growth conditions

The thickness of the Ga_2O_3 thin films with the growth temperatures and VI/III ratio was measured by SEM. The cross-sectional SEM images are shown in Figure S3. The growth rate can be extracted as follow:

growth grate(nm/min) = [epilayer(nm) – nucleation layer(nm)] / growth time(min). Here, the nucleation layer thickness is about 30 nm.

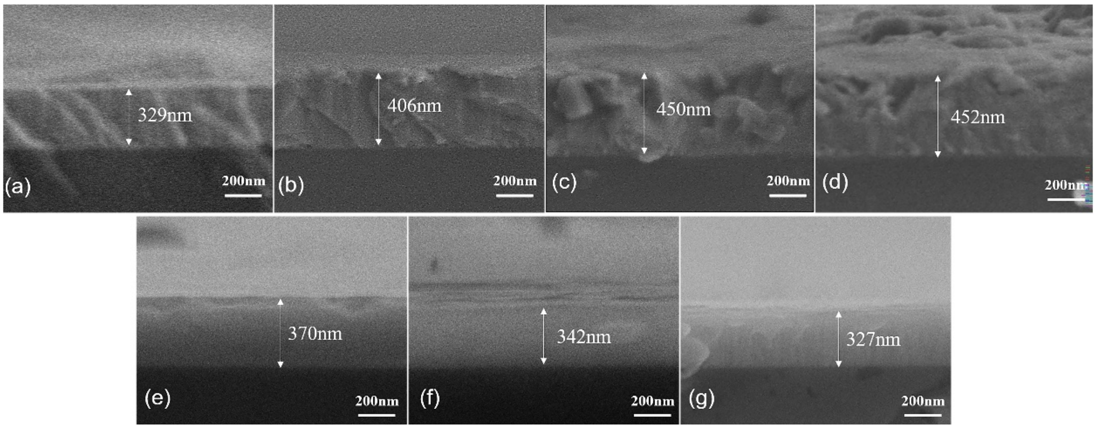

Figure S3. The cross-sectional SEM image of Ga_2O_3 thin film grown at 600 ^{o}C with VI/III ratio of (a) 177, (b) 354, (c) 708, (d) 1415 and growth with VI/III ratio of 354 at (e) 570 ℃, (f) 640 ℃ and (g) 660 ℃, respectively.

1. X. Zheng, Y. Wang, Z. Feng, H. Yang, H. Chen, J. Zhou and J. Liang, *Journal of Crystal Growth*, 2003, **250**, 345-348.