Electronic Supplementary Material (ESI) for CrystEngComm.

High-quality heteroepitaxy of ε-Ga2O3 films on 4H-SiC substrates via MOCVD

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Section 1. Twist extraction

The tilt and twist are extracted from the FHMWs of the measured X-ray rocking curves (XRCs) of symmetric (004) and skew symmetric (131), (133), (135) and (136) reflections. The XRCs are shown in Fig. S1 (a)-(d) and the FWHM (W) of different reflections for different samples is shown in Table S1. The tilt and twist of ε-Ga_2O_3 on 4H-SiC were calculated by following formula: [1]

$$W^{tilt}(\chi) = cos^{-1}[cos^2(\chi)\cos(W_{out}) + sin^2(\chi)]$$

$$W^{twsit}(\chi) = cos^{-1}\left[sin^2(\chi)\cos(W_{in}) + cos^2(\chi)\right]$$

$$W^{tilt}_{eff}(\chi) = W^{tilt}(\chi)\exp\left(-m\frac{W^{twsit}(\chi)}{W^{twsit}(90)}\right)$$

$$W^{twist}_{eff}(\chi) = W^{twsit}(\chi)exp\left(-m\frac{W^{tilt}(\chi)}{W^{tilt}(0)}\right)$$

$$W(\chi) = \{[W^{tilt}_{eff}(\chi)]^n + W^{twist}_{eff}(\chi)]^n\}^{\frac{1}{n}}$$

where χ is the angle of inclination between crystal plane of interest and the surface normal, W_{out} and W_{in} are the out-plane tilt and in-plane twist angle. *m* is a parameter to characterize the interdependence between the tilt and the twist. The constant $n = 1 + (1 - f)$ depends on the fraction (f) of the Lorentzian character in the XRD rocking curves in terms of the pseudoVoigt (PV) function, $PV(x) = (1 - f)G(x) + fL(x)$,where $G(x)$ and $L(x)$ represent the Gaussian and Lorentz functions, respectively.

As shown in Fig. S2, good fittings of $W(\chi)$ as a function of χ are obtained for all samples and the values of W_{out} and W_{in} are obtained, listing in Table S2.

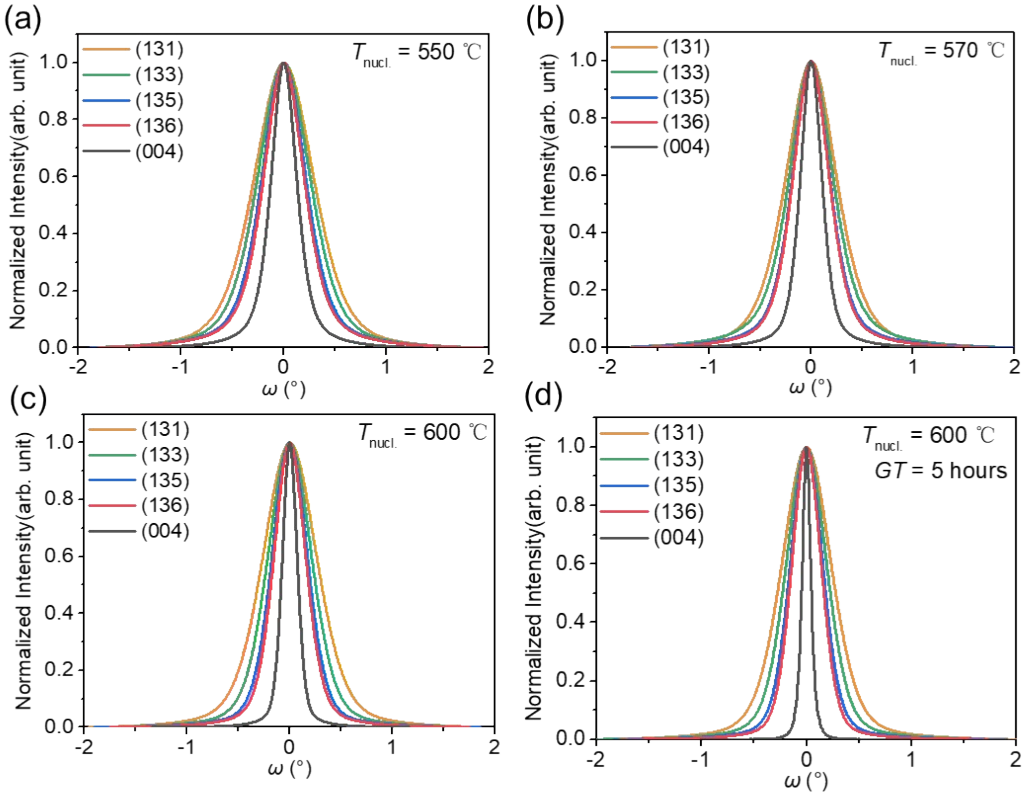

FIG. S1. X-ray rocking curves (XRCs) of different planes under symmetric and skew symmetric geometries. (a) $T_{necl.}$ = 550 °C samples, (b) $T_{necl.}$ = 570 °C samples, (c) $T_{necl.}$ = 600 °C samples and (d) $T_{necl.}$ = 600 °C, 5 hours samples.

Table S1. Details on the XRC FWHM of different reflection s for different samples.

Reflection	2θ (°)	χ (°)	FWHM (°)			
			550 °C	570 °C	600 °C	600 °C(5h)
(131)	18.28	74.87	0.70	0.60	0.62	0.56
(133)	22.95	50.96	0.61	0.52	0.51	0.46
(135)	30.61	36.50	0.51	0.43	0.41	0.36
(136)	35.24	31.66	0.47	0.42	0.37	0.33
(004)	38.94	0	0.30	0.25	0.17	0.09

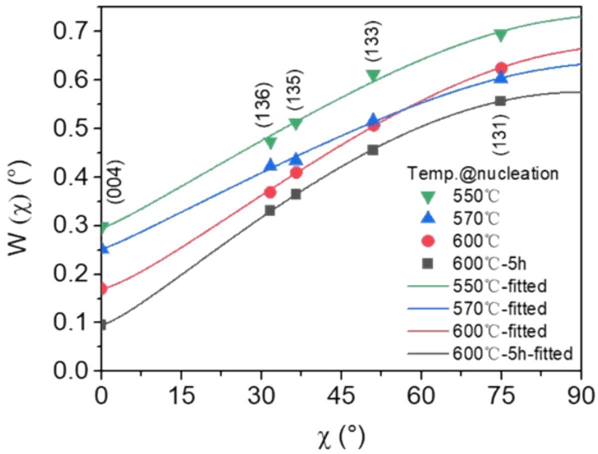

FIG. S2. $W(\chi)$ as a function of inclination angle χ. The lines are fitting results using a model developed by Srikant et al.

Table S2. The tilt and twist for different samples extracted from the mosaic model

$T_{nucl.}$(°C)	**Growth T. (h)**	**W_{out}(°)**	**W_{in}(°)**
550	2	0.30	0.73
570	2	0.25	0.63
600	2	0.17	0.66
600	5	0.09	0.58

[1] V. Srikant, J. S. Speck, and D. R. Clarke, "Mosaic structure in epitaxial thin films having large lattice mismatch," *J. Appl. Phys.*, vol. 82, no. 9, pp. 4286-4295, 1997, doi: 10.1063/1.366235.