



(110)- and (−134)-faceted surface morphology of halide vapor phase epitaxy-grown β -Ga₂O₃ homoepitaxial layers on (011) substrates

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The surface morphology of the homoepitaxial layer grown on a (011) β -Ga₂O₃ substrate by HCl-based halide vapor phase epitaxy was investigated using atomic force microscopy (AFM) and transmission electron microscopy (TEM). The surface consisted of (110) and (−134) facets elongated along [1−11], with facet coverage ratios of 0.207:0.793 (AFM) and 0.210:0.790 (TEM), in close agreement with the geometrically expected ratio of 0.219:0.781. Thus, the surface can be regarded as being composed of (110) macrosteps and (−134) terraces. These findings indicate that growth kinetics and impurity incorporation should be discussed based on the actual (110) and (−134) faceted morphology, rather than the nominal (011) substrate orientation. © 2026 The Author(s). Published on behalf of The Japan Society of Applied Physics by IOP Publishing Ltd

β -Ga₂O₃ has gained significant attention as a promising ultrawide-bandgap semiconductor for high-power applications.¹⁾ This interest is primarily driven by its breakdown electric field, which is estimated to be approximately 8 MV cm^{−1}, resulting in a Baliga's figure of merit significantly higher than those of wide-bandgap SiC and GaN.²⁾ Furthermore, the availability of high-quality, large-area substrates up to 6 inches in diameter, enabled by high-speed melt growth methods, provides a distinct cost advantage for industrial scalability.^{1,3,4)}

In high-voltage and high-current applications, vertical device architectures are preferred, requiring thick epitaxial drift layers with low impurity concentrations. Halide vapor phase epitaxy (HVPE) has become a key technique for forming such layers due to its high growth rates and ability to produce high-purity epitaxial films.^{5–10)} Accordingly, HVPE-grown epiwafers have been widely used as platforms for demonstrating vertical high-power devices, including Schottky barrier diodes (SBDs),¹¹⁾ metal-oxide-semiconductor field-effect transistors (MOSFETs),¹²⁾ and heterojunction p-n diodes.¹³⁾

The (001)-oriented plane has primarily been chosen for epiwafers due to its relatively high growth rate in HVPE.⁸⁾ However, (001) surfaces often suffer from significant morphological issues, such as deep pits or streaky grooves elongated along the [010] direction.⁸⁾ These pits, which originate from dislocations propagating from the substrate, often require costly chemical mechanical polishing (CMP) before device fabrication.^{7,14)} Notably, nearly half of the epilayer thickness may need to be removed by CMP to planarize the surface.¹⁴⁾ Additionally, chlorine (Cl), which acts as a shallow donor,¹⁵⁾ is readily incorporated into (001) epitaxial layers during HVPE, making it difficult to achieve low-donor concentrations less than 8×10^{15} cm^{−3}.¹⁶⁾

Recently, the (011) plane has emerged as a superior alternative to overcome these morphological and Cl-incorporation issues. Goto et al. discovered that a pit-free homoepitaxial surface can be achieved on (011) substrates by Cl₂-based HVPE, in which GaCl precursor is produced by the reaction between Ga and Cl₂, because the (011) plane is

nearly parallel to the dislocations that generate surface pits on the (001) plane.⁸⁾ This suppresses the inheritance of substrate defects into the epitaxial layer. Although the growth rate of Cl₂-based HVPE is limited to approximately 2.8 μ m h^{−1} to prevent the deposition of particles produced by parasitic reactions,⁸⁾ the rate can be increased to approximately 14 μ m h^{−1} using HCl-based HVPE, in which GaCl precursor is produced by the reaction between Ga and HCl, together with the additional introduction of HCl etching gas to suppress parasitic reactions.^{9,17,18)} However, this additional HCl supply in HCl-based HVPE induces slit-like pits that are not observed in Cl₂-based HVPE,⁹⁾ and thus the HCl flow rate must be optimized to suppress both particle deposition and pit formation. Moreover, for both Cl₂- and HCl-based HVPE, the (011) orientation effectively suppresses Cl incorporation, enabling low Cl concentrations of around 1×10^{15} cm^{−3}, roughly one order of magnitude lower than those typically measured for the (001) orientation.^{9,16)}

These advantages have already led to high-performance device demonstrations on (011) epiwafers, including vertical multi-fin MOSFETs with breakdown voltages exceeding 10 kV¹⁶⁾ and vertical SBDs reaching 3.7 kV with ultra-low leakage current.¹⁹⁾ Furthermore, other studies related to the (011) orientation, such as bulk crystal growth,²⁰⁾ metal-organic chemical vapor epitaxy,²¹⁾ plasma-free HCl-gas etching,²²⁾ and killer-defect characterization,²³⁾ have been reported, highlighting the growing interest in the (011) orientation as a promising platform for β -Ga₂O₃ epitaxy and device fabrication.

In this study, we focus on the surface morphology of HVPE-grown (011) homoepitaxial layers. In our previous study, we observed that the surface exhibited step-bunched macrosteps and terraces rather than an atomically flat morphology, even in pit-free flat areas, as evidenced by scanning electron microscopy (SEM) observations [Fig. 1].⁹⁾ This observation suggests that crystallographic facets other than the (011) plane develop on the surface. However, the faceted structures were not investigated in detail. Therefore, in this study, we further investigated the surface morphology



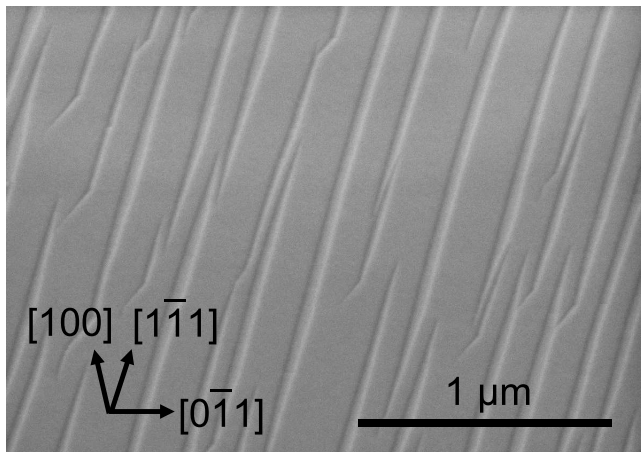


Fig. 1. Plan-view SEM image of a homoepitaxial layer grown on a (011) β -Ga₂O₃ substrate.

using nanometer-scale characterization techniques, including atomic force microscopy (AFM) and transmission electron microscopy (TEM), to identify the facets forming the macrosteps and terraces.

For this investigation, we used a 3.6 μm thick homoepitaxial layer grown on the (011) substrate using HCl-based HVPE, with detailed growth conditions reported previously.⁹⁾ The layer was single-crystalline, and its tilt and twist spreads were comparable to those of the substrate. Furthermore, unintentional Cl incorporation was sufficiently low, with a concentration of $1.7 \times 10^{15} \text{ cm}^{-3}$. Therefore, this homoepitaxial layer is considered suitable for power device applications.

The surface morphology of the homoepitaxial layer was first examined by AFM, as shown in Fig. 2. The surface consisted of macrosteps and terraces elongated along the $[1\bar{1}1]$ direction. Owing to the presence of macrostep-and-terrace structures, the root-mean-square (RMS) roughness values were somewhat large for a homoepitaxial layer, with values of 8.0 and 7.2 nm for $3 \mu\text{m} \times 3 \mu\text{m}$ and $1 \mu\text{m} \times 1 \mu\text{m}$ scan areas, respectively [Figs. 2(a) and 2(b), respectively]. In contrast, the macrostep and terrace surfaces were relatively smooth, with local RMS roughness values of 0.2–0.6 nm and 0.1–0.5 nm, respectively, indicating the development of well-defined crystallographic facets.

To estimate the possible macrostep and terrace facets, a height profile perpendicular to the $[1\bar{1}1]$ direction was extracted from Fig. 2(b), as shown in Fig. 2(c). Linear fitting of the corresponding regions yielded inclination angles of 23° and 7° for the macrosteps and terraces, respectively. Although these inclination angles may include uncertainties due to the finite cantilever-tip size and slight scan-tracking deviations, they are still useful as screening indicators for narrowing down possible facet orientations.

The possible macrostep and terrace planes were considered as follows. Assuming that the intersection line between the macrostep and terrace planes is parallel to the $[1\bar{1}1]$ direction, these (hkl) planes can be regarded as zone planes belonging to the $[1\bar{1}1]$ zone axis. Thus, they satisfy the zone law, $h - k + l = 0$, or equivalently, $k = h + l$. Among the relatively low-index planes satisfying this relationship in the vicinity of (011), (110) and (132) are possible step-plane candidates, with calculated inclination angles of 28.27° and 8.74° , respectively; whereas $(\bar{1}34)$ and $(\bar{1}12)$ are possible

terrace-plane candidates, with calculated inclination angles of 7.66° and 19.73° , respectively. Here, the lattice parameters used for the calculations are $a = 12.214 \text{ \AA}$, $b = 3.0371 \text{ \AA}$, $c = 5.7981 \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 103.83^\circ$, and $\gamma = 90^\circ$.²⁴⁾ The selection of these candidate planes can be intuitively understood from the TEM diffraction pattern shown later [Fig. 3(c)]. Based on their consistency with the experimentally observed inclination angles, the (110) and $(\bar{1}34)$ planes are considered to be the most plausible candidates for the macrostep and terrace facets, respectively.

Additionally, the surface coverage ratio of the macrostep and terrace facets was calculated by analyzing the AFM topography data. Figure 2(d) shows a histogram of the local surface inclination angles over the entire scan area shown in Fig. 2(b). The histogram exhibited two peaks at 23.1° and 7.1° , consistent with the inclination angles of the macrosteps and terraces obtained from the line profile. The corresponding peak areas (blue and red regions), obtained after subtraction of the linear background, were used to estimate the respective areas projected onto the (011) plane. The projected area (A_{pro}) can be converted into the actual surface area (A_{act}) using $A_{\text{act}} = A_{\text{pro}}/\cos \theta$, where θ is the inclination angle. The resulting actual surface coverage ratio of the macrosteps and terraces was determined to be 0.207:0.793.

To further examine the macrostep and terrace planes, we analyzed the cross-sectional surface profile of the homoepitaxial layer using TEM, as shown in Fig. 3. Figures 3(a) and 3(b) are bright-field TEM images acquired with low and high magnifications, respectively. The electron incidence direction was $[1\bar{1}1]$, and the acceleration voltage was 200 kV. The observed macrostep and terrace profiles were linear, indicating that these facets were flat.

Figure 3(c) shows the corresponding electron diffraction pattern, in which each hkl diffraction spot represents the direction normal to the (hkl) plane. By comparing the normal directions of the observed macrostep and terrace facets in the TEM image with the directions of the hkl diffraction spots, their facets could be assigned to (110) and $(\bar{1}34)$, respectively. Here, the angular deviation between the step-surface normal and the 110-diffraction spot was $\sim 0.7^\circ$, whereas the angular deviation between the terrace-surface normal and the $\bar{1}34$ -diffraction spot was $\sim 0.8^\circ$. These assignments are consistent with the facet candidates inferred from the AFM analysis.

The (110) and equivalent $(\bar{1}10)$ facets are known to appear on the surfaces of homoepitaxial layers grown on (010) substrates,²⁵⁾ as the (110) surface is energetically more stable than the (010) surface.²⁶⁾ In addition, smooth homoepitaxial growth of (110) β -Ga₂O₃ with an RMS roughness of 0.4 nm has been reported.²⁷⁾ Thus, the development of the (110) facet on our epilayer surface is reasonable. In contrast, the $(\bar{1}34)$ facet has not yet been reported in β -Ga₂O₃ studies. Because the $(\bar{1}34)$ plane is a high-index vicinal plane, its surface atomic structure, including possible surface terminations and dangling-bond configurations, is not straightforwardly defined. Therefore, further theoretical studies, including detailed surface-energy calculations, are required to clarify the origin of its stabilization.

The surface coverage ratio of the (110) and $(\bar{1}34)$ facets was also evaluated from the cross-sectional TEM image. The widths of the macrostep and terrace regions in Fig. 3(a) were separately summed and compared, using seven step-terrace

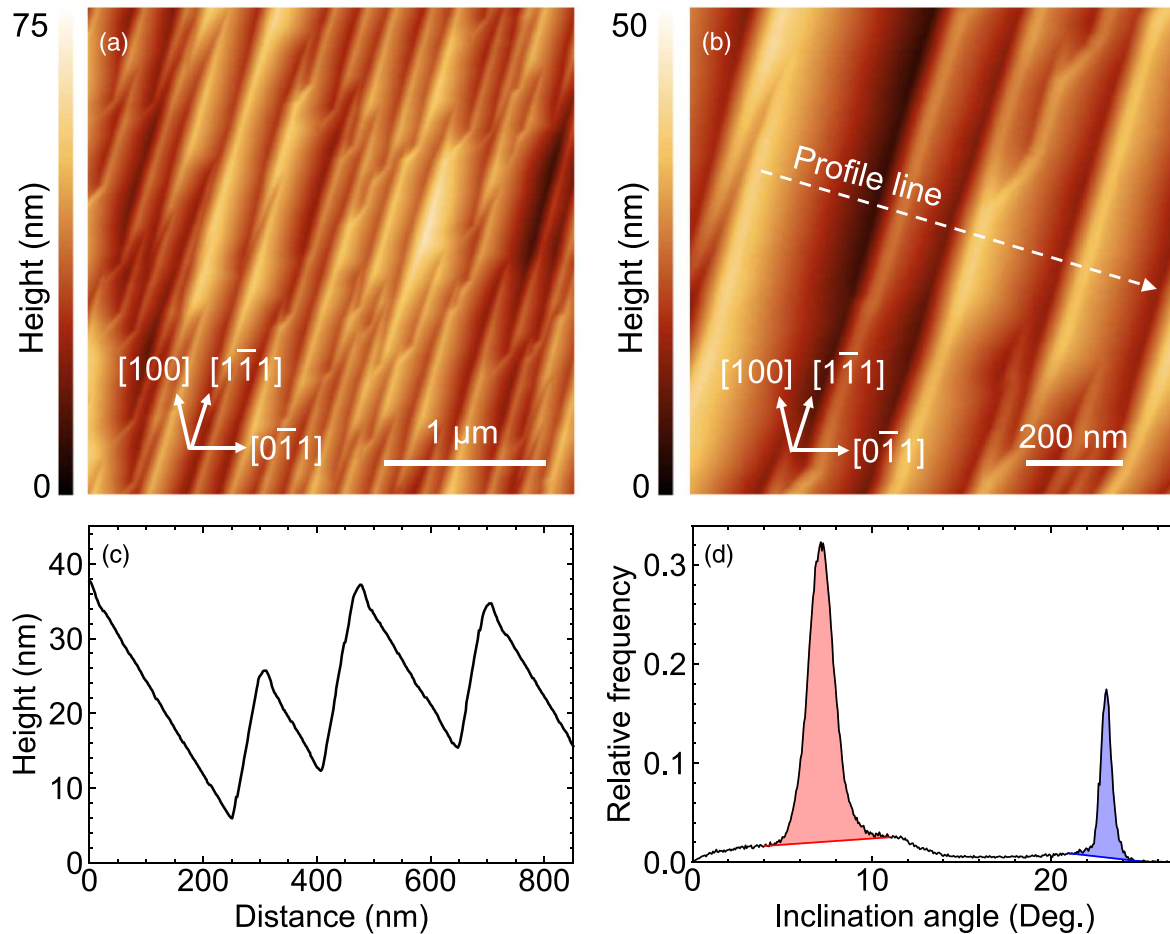


Fig. 2. AFM images of the homoepitaxial layer grown on the (011) β -Ga₂O₃ substrate, acquired over scan areas of (a) $3\ \mu\text{m} \times 3\ \mu\text{m}$ and (b) $1\ \mu\text{m} \times 1\ \mu\text{m}$. These topographic images were leveled over the entire area. (c) Height profile taken along the arrow indicated in (b). (d) Relative frequency of local inclination angles obtained from (b).

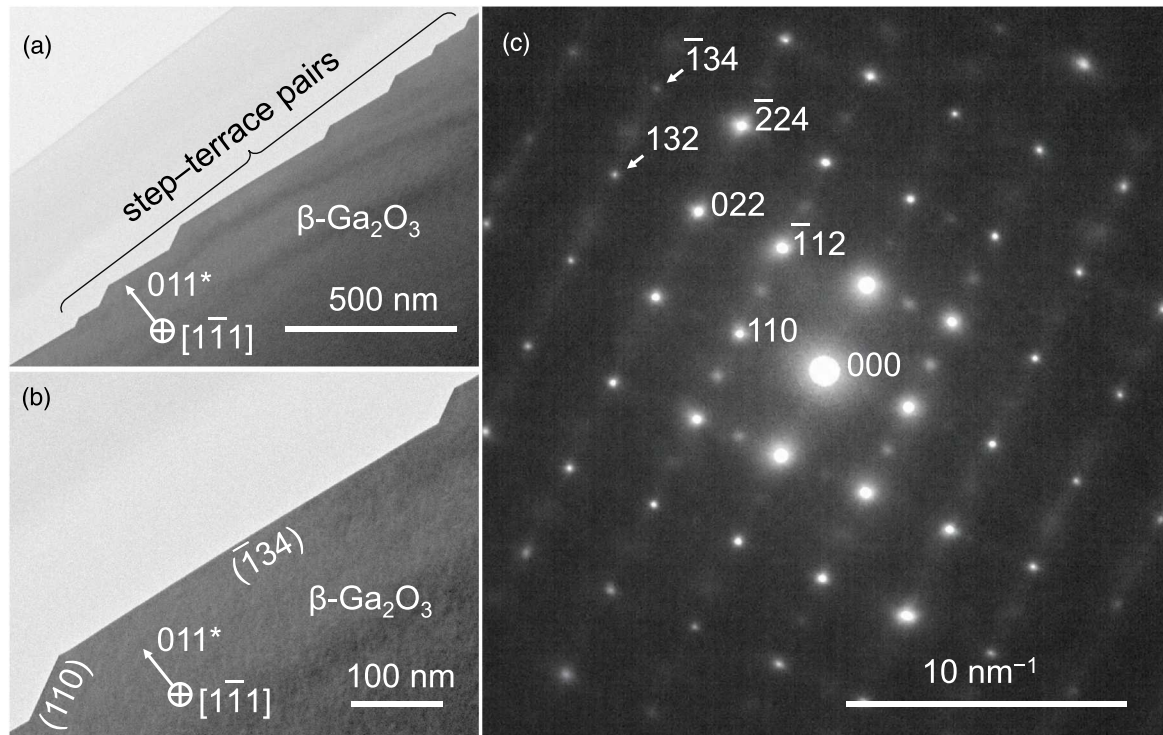


Fig. 3. Cross-sectional TEM images of the homoepitaxial layer on the (011) β -Ga₂O₃ substrate viewed along the $[1\bar{1}1]$ direction, acquired at different magnifications: (a) low-magnification image and (b) high-magnification image. Note that hkl^* denotes the direction normal to the (hkl) plane. The seven step-terrace pairs indicated by a curly brace in (a) were used for the calculation of the step-terrace surface coverage ratio (see the text for details). (c) Electron diffraction pattern acquired from the same specimen orientation as that used for the TEM observations.

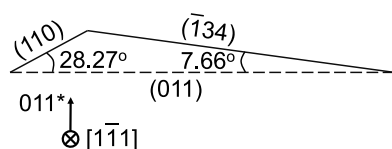


Fig. 4. Schematic illustrating the orientation relationship among the (011), (110), and ($\bar{1}34$) planes.

pairs for which both ends were fully contained within the image. The surface coverage ratio was determined to be 0.210:0.790.

Finally, to examine the validity of the surface coverage ratios experimentally determined from the AFM and TEM results, we compared these values with the geometrically expected ratio. As shown in Fig. 4, we considered a triangular cross section bounded by the (011), (110), and ($\bar{1}34$) planes. Based on a simple trigonometric calculation, the length ratio of the (110) and ($\bar{1}34$) segments was calculated to be 0.219:0.781, which agrees well with the experimentally determined values of 0.207:0.793 (AFM) and 0.210:0.790 (TEM), supporting the validity of our facet identification.

In conclusion, we found that the homoepitaxial surface on the (011) β -Ga₂O₃ substrate was characterized by (110) macrosteps and ($\bar{1}34$) terraces elongated along the $[1\bar{1}1]$ direction, with facet coverage ratios of 0.207:0.793 (AFM) and 0.210:0.790 (TEM), in good agreement with the theoretical ratio of 0.219:0.781. This faceted morphology is expected to influence growth kinetics and impurity incorporation, including Cl incorporation, during HVPE growth. These findings therefore provide useful insights into the morphology and growth behavior of HVPE-grown (011) β -Ga₂O₃ homoepitaxial layers. Furthermore, the present results suggest that facet-level flatness may also be attainable in HVPE-grown homoepitaxial layers on (110)- and ($\bar{1}34$)-oriented substrates, offering a promising route toward CMP-free epiwafers.

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