Refining *m*-plane α-Al_2O_3 Substrates for Conductive α-$(Al_xGa_{1-x})_2O_3$ Thin Films

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Abstract

α-Gallium oxide (α-Ga_2O_3) grown on α-aluminum oxide (α-Al_2O_3) substrates has attracted significant attention for its potential as an emerging ultra-wide bandgap semiconductor. As of late, the highest conductivity for α-Ga_2O_3 has been realized using suboxide molecular beam epitaxy (*S*-MBE) and because of its high breakdown voltage and low on-resistance, theory suggests that α-Ga_2O_3 also has a higher Baligas Figure of Merit (BFOM) than the previously studied ultra-wide bandgap semiconductor β-Ga_2O_3, increasing the interest in optimizing α-Al_2O_3 substrate preparation for high quality thin film growth.

Introduction

α-Aluminum oxide (α-Al_2O_3) is a widely sought after material in the semiconductor industry due to its affordability, thermal stability, high structural quality, and ultra-wide bandgap. Its corundum structure makes for great compatibility with α-Ga_2O_3, which also has corundum symmetry.
Among the different orientations such as *c*-plane, *r*-plane, and a-plane, the *m*-plane has garnered attention for its ability to remain phase-pure whereas the *c*-plane and *r*-plane display challenges with nucleating the β-phase and the *a*-plane has shown to contain β-Ga_2O_3 impurities.

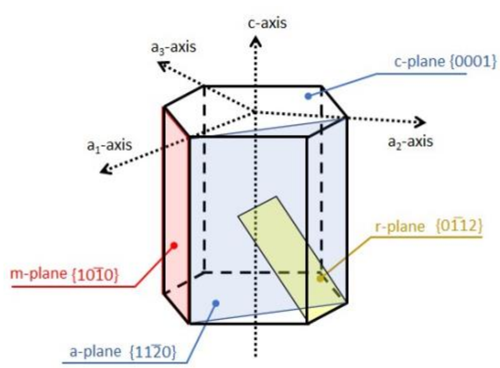

Figure 1. The general 3-dimensional view of the α-Al_2O_3 crystal at the atomic level demonstrating the corundum structure. [1].

However, achieving atomic-level flatness and uniformity needed for high quality epitaxial thin films requires careful surface preparation. Annealing α-Al_2O_3 substrates to promote step formation, formally called "Step-Flow Growth", on the surface helped greatly as deposited atoms are more stable at step edges, plus vicinal surfaces with atomic steps may produce higher quality thin films. A vicinal surface describes a miscut angle of the substrate—an angle at which the surface is cut from the plane. The deviations may introduce regularly spaced atomic steps on the surface which can promote step-flow growth.

Furthermore, the company the α-Al_2O_3 substrates are purchased from has a ± 0.1° margin of error that may affect the direction the steps grow in. The 0° miscut growth direction is completely random, the 0.1° miscut grows primarily toward the a-plane, and the 0.2° and 0.4° miscuts are always oriented toward the a-plane. While the 0.2° and 0.4° miscuts seem to be optimal choices, it is important to note that a higher miscut angle can promote step-bunching—atomic steps clustered together.

Methods

The core approach to this project involved thermally annealing sapphire substrates with four different miscut angles: 0°, 0.1°, 0.2°, and 0.4°. These substrates were annealed in the MBE chamber using a CO_2 laser heating system. Initially, each miscut was tested using literature [2], as well as using suggested parameters based on prior annealing done in the lab. These early runs served to establish baseline responses for each angle. After observing general trends, the methodology was refined to optimize annealing parameters for one miscut at a time, rather than testing all at once. The results from one miscut guided adjustments to the next.

A challenge faced while annealing was cracking. Cracking was observed during extreme ramp or cool rates or by simply overheating the substrate. This obstacle was attributed to thermal shock such as rapid heating/cooling or uneven heating/cooling. To combat this, a set rotation speed of 20rpm was implemented for all substrates as well as testing slower ramp rates, however it is important to note that too slow of a ramp rate can lead to faceting.

Results and Discussion

Surface morphology after annealing was characterized using atomic force microscopy (AFM). This allowed for visualization of the step height, terrace width, and roughness features—critical indicators of whether step formation had been achieved. Parameters such as temperature, ramp, dwell time, and cool rate were adjusted as needed to improve the surface for each miscut.

In general, the 0.2° and 0.4° miscut substrates promoted easier step formation at lower temperatures, while the 0° and 0.1° miscut substrates required higher annealing temperatures to induce visible steps. Below are AFM images to best help describe the projected optimal parameters.

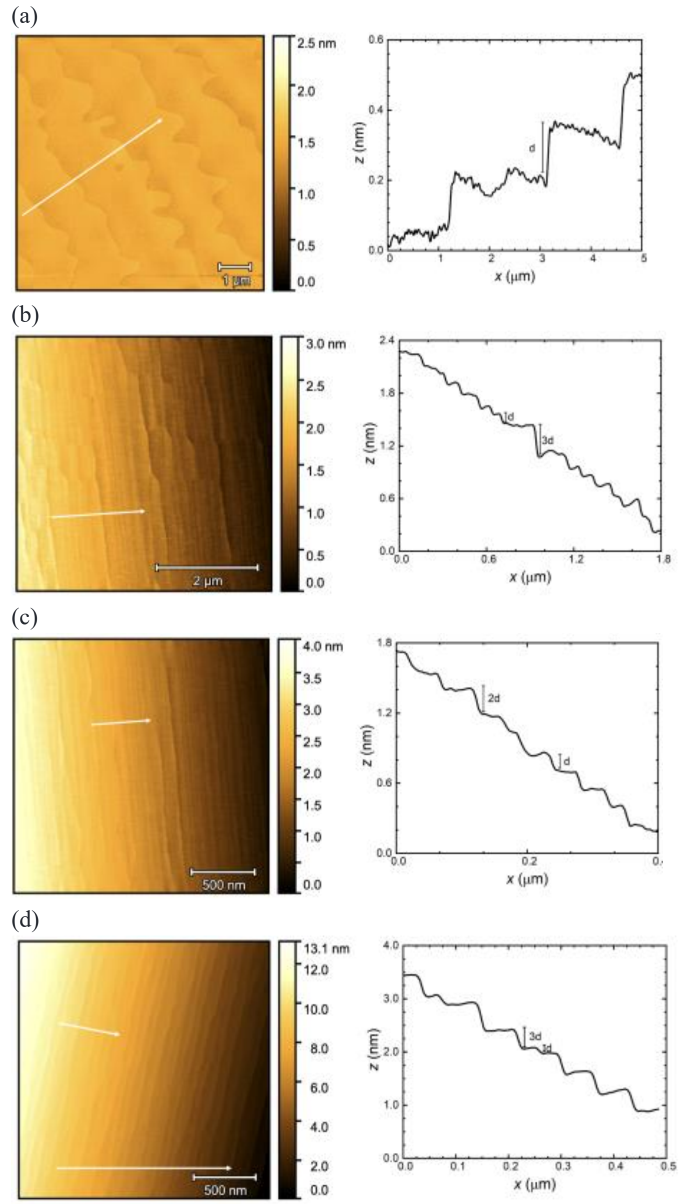

Figure 2. a) A 0° miscut α-Al_2O_3 substrate showcasing mostly single-step heights with consistent terrace widths and slight surface roughness on the surface. Parameters - Temperature:1450°C, Ramp:500°C/min, Time:5 min., Cool Rate: Quenched[1]. b) A 0.1° miscut α-Al_2O_3 substrate with mostly single steps except for step-bunching noted as "3d" on the graph, indicating three steps clustered together. There is mostly even terrace width and low surface roughness. Parameters – Temperature:1420°C, Ramp:500°C/min, Time:5min., Cool Rate:Quenched. c) A 0.2° miscut α-Al_2O_3 substrate showing single step formation, even terrace width and low surface roughness apart from two steps clustered together marked as "2d" on the graph. Parameters – Temperature:1225°C, Ramp:100°C/min, Time:5min., Cool Rate: 100°C/min. d) Lastly, a 0.4° miscut with mostly "3d" step heights evenly across the surface. Although the steps aren't single steps, a trend of uniform step height is still observed with mostly even terrace width and low surface roughness. Parameters – Temperature:1200°, Ramp:500°C/min, Time:5min, Cool Rate: 500°C/min

Conclusions and Future Work

Table I. Projected Optimal Parameters for Each Miscut

Miscut	Temp.	Ramp	Time	Cool Rate
0°	1400-1450°C	500°C /min	5 min.	quenched
0.1°	1400-1420°C	500°C /min	5 min.	quenched
0.2°	1200-1225°C	100°C /min	5 min.	quenched
0.4°	≥1200°C	500°C /min	5 min.	quenched

The results presented reflect the progress made within a two-month research period and represent the beginning of a broader effort to fully optimize the annealing parameters for *m*-plane α-Al_2O_3 substrates. This initial phase has provided valuable insights into the effect of miscut angle and thermal conditions on step formation, but further refinement is encouraged to achieve consistent and ideal surface morphologies across all substrate types. Future work will focus on perfecting parameters for each miscut, growing α-Ga_2O_3 thin films on α-Al_2O_3 substrates to see how electrical properties and surface quality compare, demonstrating consistency on projected optimal parameters, and allowing for new applications of α-Al_2O_3 substrates.

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[1] Quenching – the act of an immediate stop or rapid cooling of a chemical reaction