

Epitaxial Growth of Highly Conductive α -Ga₂O₃ by Suboxide Molecular-Beam Epitaxy

Julianne Chen¹, Jacob Steele², and Darrell G. Schlom^{2,3,4}

¹*Department of Materials Science and Engineering, The Pennsylvania State University, State College, 16802, Pennsylvania, USA*

²*Department of Materials Science and Engineering, Cornell University, Ithaca, 14853, New York, USA*

³*Kavli Institute at Cornell for Nanoscale Science, Ithaca, 14853, New York, USA*

⁴*Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany*

August 18, 2024

Abstract

Growth of alpha Ga₂O₃ on flat m-plane sapphire (Al₂O₃) substrates was achieved through a thin, high temperature alpha Ga₂O₃ buffer with 8% aluminum and growth conditions such as 480C film growth temperature and high ozone pressure of 5×10^{-6} torr. Record breaking results such as symmetrical rocking curve FWHM (0.167°), resistivity ($1.67 \times 10^{-3} \Omega\text{cm}$), mobility ($81.7 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$), and dislocation density ($2.48 \times 10^8 \text{ cm}^{-2}$) were achieved.

I. Introduction

The Baliga figure of merit (BFOM) is a metric for semiconductors which correlates device power dissipation to intrinsic material properties such as mobility or critical electric field.^[1] Ultrawide bandgap semiconductors such as Ga₂O₃ or diamond have been researched as their higher BFOM values allow for more efficient high voltage devices.

There are many different phases of Ga₂O₃ that have been studied, with the most thermodynamically stable being the β phase, but the metastable α -Ga₂O₃ phase has garnered interest for its bandgap of 5.3 eV that can be extended to 8.6 eV by alloying with Al₂O₃.^[2]

Molecular beam epitaxy (MBE) is a thin film growth technique which heats metal sources in an ultra-high vacuum which allows for molecules to be deposited on a substrate atomic layer by layer. Growth of α -Ga₂O₃ with conventional MBE requires a two-step process with the gallium reacting with background ozone to form an intermediate being the rate-limiting step.

Suboxide MBE (*S*-MBE) supplies oxide intermediates instead of metal sources, skipping the rate-limiting step of materials such as α -Ga₂O₃.

II. Methods

X-ray diffraction (XRD) and X-ray reflectivity (XRR) measurements were performed using a PANalytical Empyrean system. Surface topography was investigated with atomic force microscopy (AFM) using an Asylum Research Cypher Environmental AFM. Growth of α -Ga₂O₃ was conducted via *S*-MBE with a Ga₂O and SiO₂ molecular beam.

10x10 mm² m-plane sapphire (Al₂O₃) substrates were used. Indium metal contacts were soldered onto the corners for Hall measurements.

III. Results & Discussion

M-plane sapphire substrates with nanometer tall steps grew films with respectable electrical properties. When using flat m-plane sapphire substrates, streaks of β -Ga₂O₃ or cracks formed, as shown in the

AFM below, which demonstrated directional conductivity along the steaks. Stepped substrates are not able to be effectively produced, so flat substrates must be used.

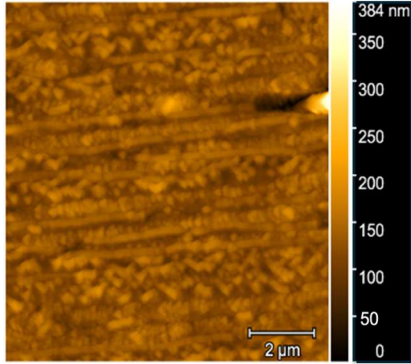


Figure 1: Film growth on flat substrates, RMS of 24.5 nm, 436 nm thick sample

Adding a buffer with low amounts of aluminum would reduce the 4% lattice mismatch between pure Al_2O_3 and $\alpha\text{-Ga}_2\text{O}_3$ and not only prevent cracks from forming but promote $\alpha\text{-Ga}_2\text{O}_3$ growth as $\alpha\text{-Al}_2\text{O}_3$ and $\alpha\text{-Ga}_2\text{O}_3$ are isostructural. The high temperature would allow the buffer to survive relaxation and allow the film to be strained to the buffer, preventing dislocations in the film that would form during the relaxation process. The buffer is thin, around 35 nm, to reduce the amount of growth time in a high temperature where $\beta\text{-Ga}_2\text{O}_3$ is more likely to form.

Films with a $\alpha\text{-(Al,Ga)}_2\text{O}_3$ buffer, $\alpha\text{-Ga}_2\text{O}_3$ buffer with no aluminum, and no buffer were grown at the same conditions.

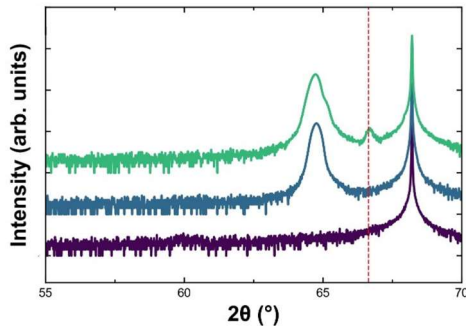


Figure 2: S1 has no buffer, S2 has a $\alpha\text{-Ga}_2\text{O}_3$ buffer, and S3 has a $\alpha\text{-(Al,Ga)}_2\text{O}_3$ buffer

$\alpha\text{-Ga}_2\text{O}_3$ did not grow on the flat substrate without a buffer. Adding aluminum in the buffer increased mobility and lowered resistance. A hybrid peak, a peak created through interactions with the film and substrate which is associated with high order, was present in the film with aluminum in the buffer.

Property	$\alpha\text{-Ga}_2\text{O}_3$	$\alpha\text{-(Al,Ga)}_2\text{O}_3$
ρ	64.2 Ω/\square	49 Ω/\square
μ	61.6 $\text{cm}^2/(\text{V}\cdot\text{s})$	78.8 $\text{cm}^2/(\text{V}\cdot\text{s})$
FWHM	0.283°	0.167°

Table 1: Properties of different buffer compositions

Film growth temperature and ozone growth pressure were varied to optimize flat substrate films for conductivity. High pressures and low film temperatures resulted in a lower resistivity and FWHM than stepped substrates.

Property	Stepped	Flat
ρ	$7.4 \times 10^{-3} \Omega/\square$	$1.9 \times 10^{-3} \Omega/\square$
FWHM	0.352°	0.167°

Table 2: ρ and FWHM of flat and stepped substrates

The source temperature of SiO_2 was varied to control the carrier concentration. With decreased carriers, ionization scattering limits mobilities. However, the measurable points with our current contacts seem to indicate the typical mobility curve has been increased and shifted to the left. The high mobilities could be attributed to the high structural quality of our films, although better contacts would be needed to confirm our suspicions. Our films have exceeded the current literature records.

Parameter	Records	AlGa722	AlGa726
FWHM	0.27 [3]	0.167	0.185
R (Ω/\square)	7.4×10^{-2} [4]	2.01×10^{-3}	1.67×10^{-3}
μ ($\text{cm}^2/\text{V}\cdot\text{s}$)	65 [5]	78.8	81.7
Dislocations (cm^{-2})	$10^{11}\text{-}10^{12}$ [7, 8]	3.72×10^8 [6]	2.48×10^8

Table 3: Records versus our best films' properties

IV. References

- [1] B.J. Baliga, *Fundamentals of Power Semiconductor Devices*, 2nd ed. (Springer, 2019).
- [2] R. Jinno, C.S. Chang, T. Onuma, Y. Cho, S.-T. Ho, D. Rowe, M.C. Cao, K. Lee, V. Protasenko, D.G. Schlom, D.A. Muller, H.G. Xing, and D. Jena, “Crystal orientation dictated epitaxy of ultrawide-bandgap 5.4- to 8.6-eV α -(AlGa)₂O₃ on m-plane sapphire,” *Sci. Adv.* 7(2), eabd5891 (2021).
- [3] M. Lee et al., *Materials Science in Semiconductor Processing*, vol. 123, no. 123, pp. 105565–105565, Mar. 2021, doi: <https://doi.org/10.1016/j.mssp.2020.105565>.
- [4] S. Vogt et al., *Physica Status Solidi*, vol. 220, no. 3, Jan. 2023, doi: <https://doi.org/10.1002/pssa.202200721>.
- [5] Akaiwa et al., *Physica Status Solidi*, vol. 217, no. 3, Jan. 2020, doi: <https://doi.org/10.1002/pssa.201900632>.
- [6] J. E. Ayers, *Journal of Crystal Growth*, vol. 135, no. 1–2, pp. 71–77, Jan. 1994, doi: [https://doi.org/10.1016/0022-0248\(94\)90727-7](https://doi.org/10.1016/0022-0248(94)90727-7).
- [7] K. Kaneko et al., *Japanese Journal of Applied Physics*, vol. 51, no. 2R, pp. 020201–020201, Jan. 2012, doi: <https://doi.org/10.1143/jjap.51.020201>.
- [8] T. C. Ma et al., *Applied Physics Letters*, vol. 115, no. 18, Oct. 2019, doi: <https://doi.org/10.1063/1.5120554>.

V. Supplementary Figures

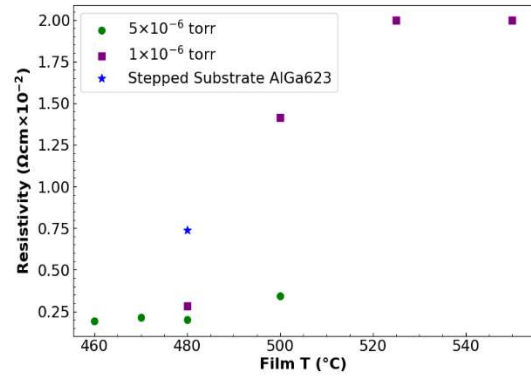


Figure 3: film T and P_{O₃} versus ρ

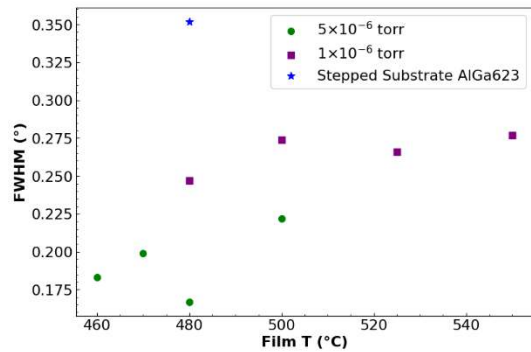


Figure 4: film T and P_{O₃} versus FWHM

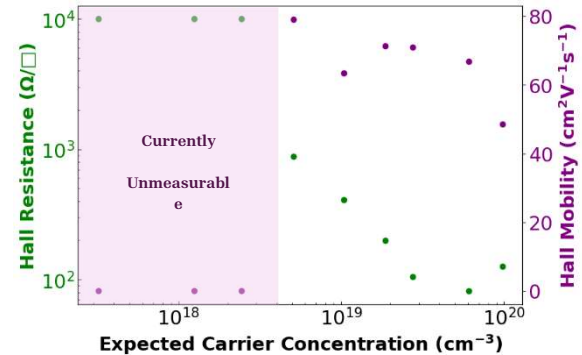


Figure 5: Changing SiO₂ versus R and μ

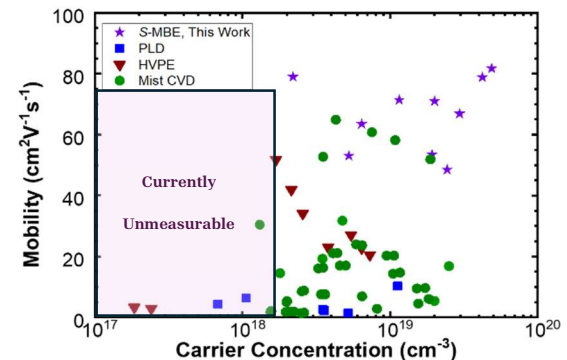


Figure 6: Our work versus current literature μ