

Strain relaxation and dislocation annihilation with graded $\alpha\text{-(Al}_x\text{Ga}_{1-x})_2\text{O}_3$ layer for high quality epitaxial $\alpha\text{-Ga}_2\text{O}_3$ thin films

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Introduction

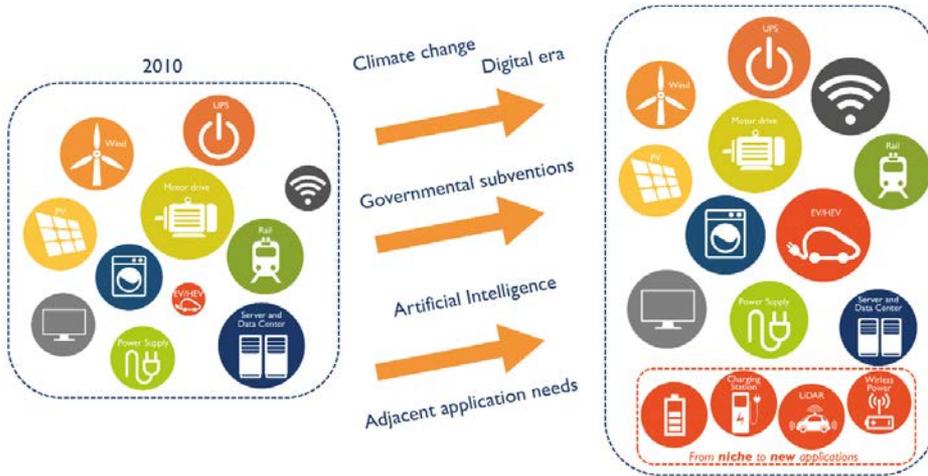
- ✓ Issue of power devices & wide band gap materials
 - ✓ Ga₂O₃ material properties
-

Experiment & results

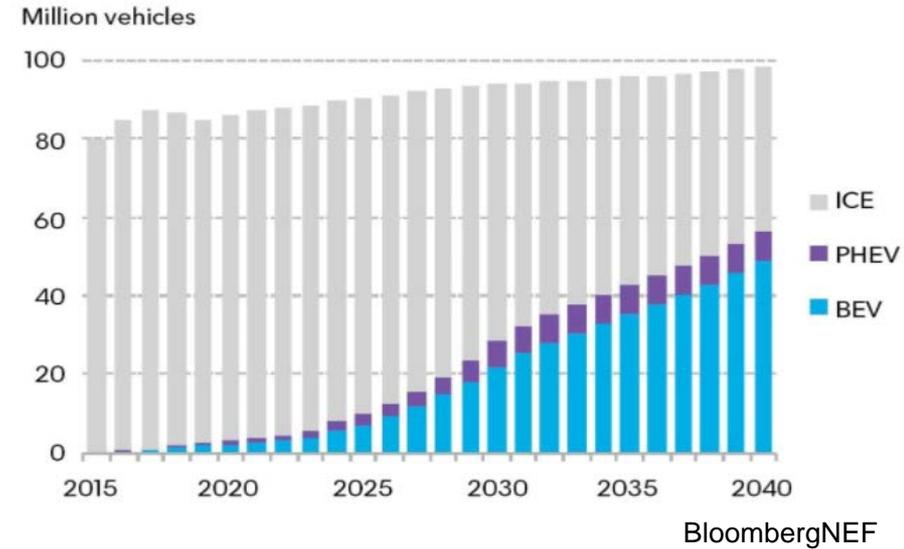
- ✓ Hetero-epitaxial growth of α -Ga₂O₃ / α -(Al_xGa_{1-x})₂O₃ on sapphire substrate
 - ✓ Structure properties of α -Ga₂O₃ / α -(Al_xGa_{1-x})₂O₃ / c-sapphire hetero structure
 - Strain state & dislocation annihilation in α -(Al_xGa_{1-x})₂O₃ / c-sapphire
 - Threading dislocation density in α -Ga₂O₃ layer
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Summary

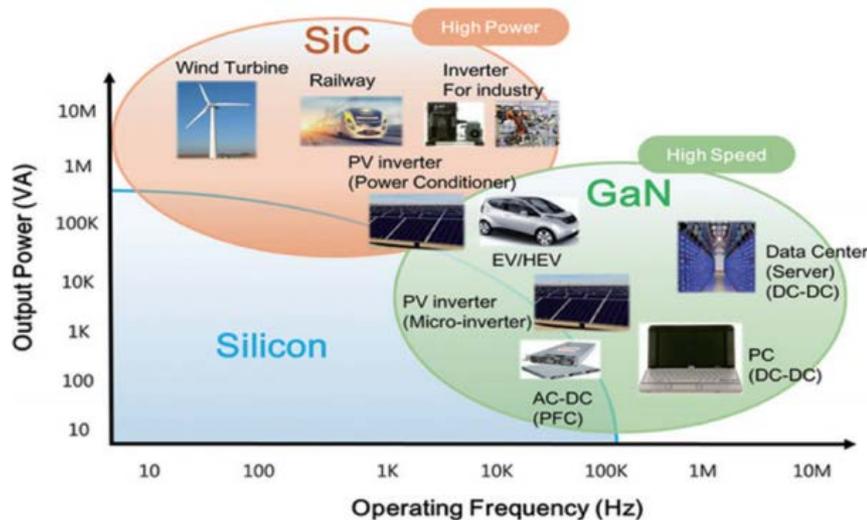
- Expansion of power electronic field



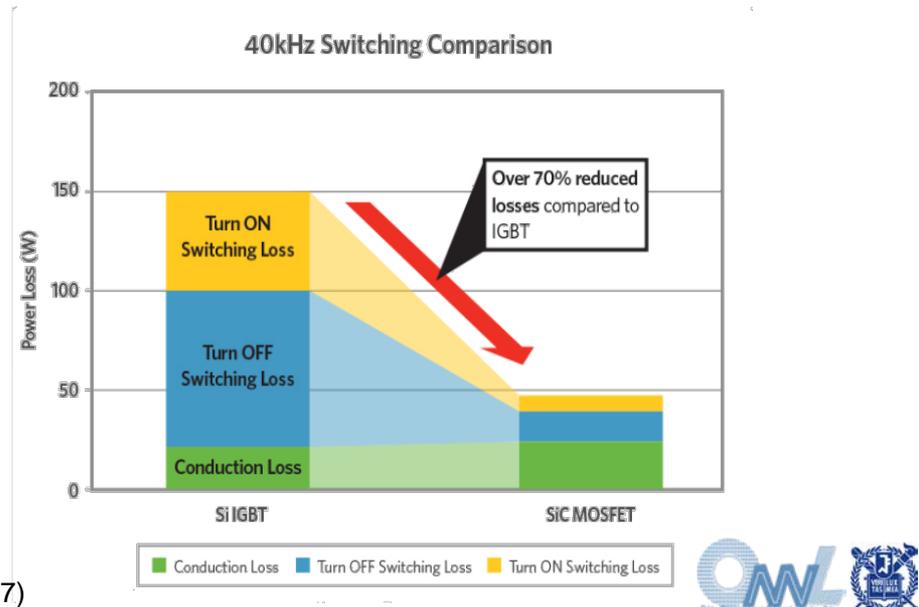
- Global long-term vehicle sales market



- Challenge of silicon-based power devices



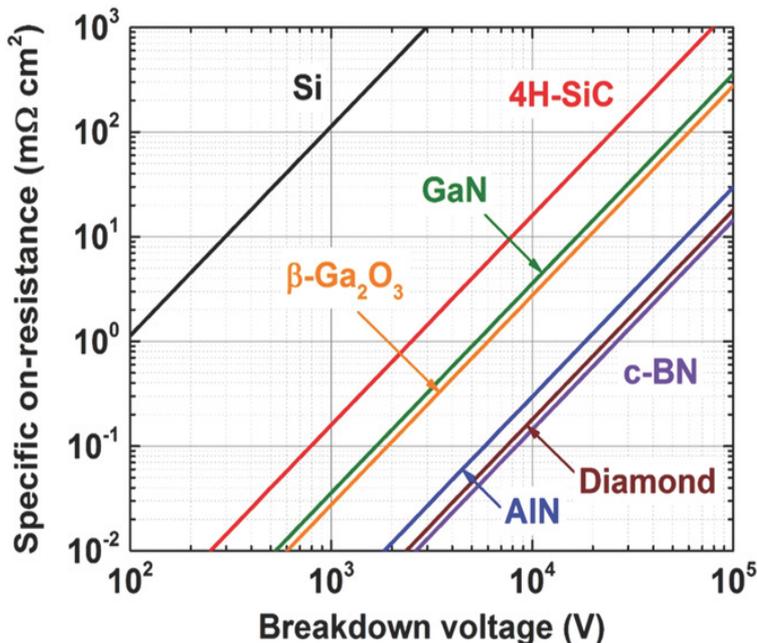
Yole Development (2017)



- Candidate materials for power semiconductor

Name of materials	Si	SiC	GaN	$\beta\text{-Ga}_2\text{O}_3$	$\alpha\text{-Ga}_2\text{O}_3$
Band gap (eV)	1.1	3.3	3.4	4.8	5.3
Mobility (cm ² /VS)	1400	1000	1200 2000 (2DEG)	200~300 1000 (2DEG)	200
Breakdown field (MV/cm)	0.3	2.5	3.3	6.5	9.5
Relative dielectric constant	11.8	9.7	9	10	10
Baliga's FOM	1	340	870	1231	3844

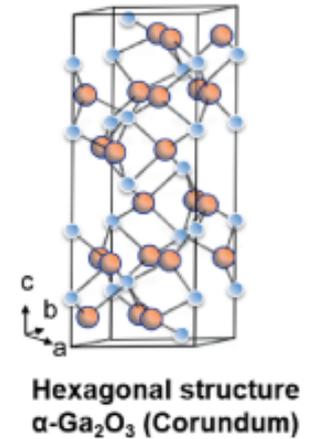
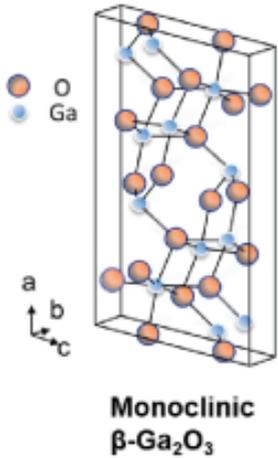
- Baliga figure of merit(BFOM) : V_{BR}^2 / R_{on} (V_{BR}^2 : Break down voltage R_{on} : specific on-resistance)



- ✓ The higher the Baliga figure of merit(BFOM)
 - The higher the voltage the device can block at off state.
 - The higher its conductance per unit area at on state.
- ✓ Ga₂O₃ has merit in availability native substrate compare to other materials.

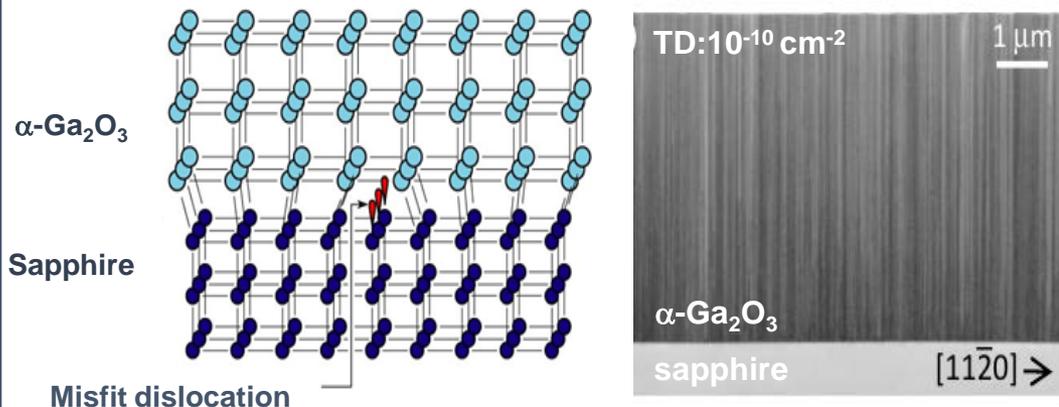
- Comparison between material properties & technological maturity of β , α -phase

	β -phase (stable state)	α -phase (meta-stable state)
Crystal structure	Monoclinic	Corundum
E_g (Band gap)	4.8 eV	5.0 eV
Electron mobility	300 cm ² /Vs	200 cm ² /Vs
E_{br}	6.5 MV/cm	9.5 MV/cm
Substrate	β -Ga ₂ O ₃ (melt-grown)	Sapphire
n-type doping	Si, Ge, Sn	Si, Sn
p-type doping	No report	No report
Hetero junction – (Al _x Ga _{1-x}) ₂ O ₃	x < 18% (phase segregation)	x < 90% (This work)
Epitaxial growth technique	MOCVD, PLD, MBE, HVPE (Homo-epi) (Hetero-epi)	Mist-CVD , HVPE (Hetero-epi)
Application	SBD, FET, Photo detector	FET, SBD



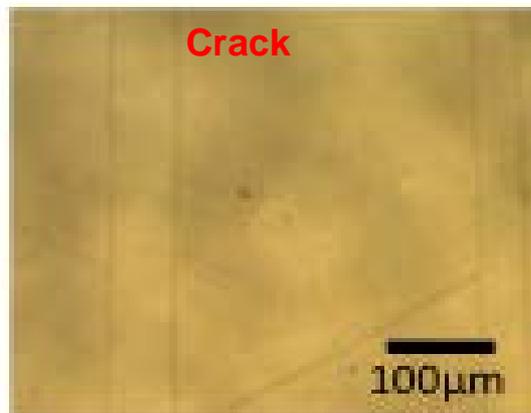
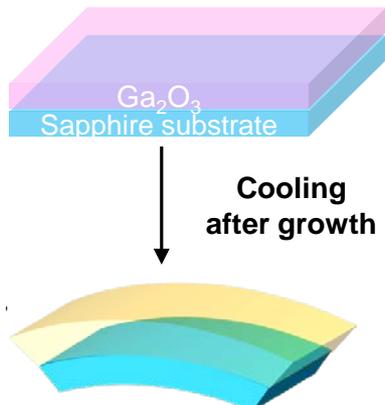
- ✓ The availability of the bulk substrate is main advantage of β - phase over α - phase.
→ Native β -Ga₂O₃ substrate cost is very expensive. (cost limitation)
- ✓ The advantage of α - Ga₂O₃ is corundum structure which allows band gap engineering (3.8eV ~ 8.8eV) with α -Al₂O₃ and α - In₂O₃.

- α -Ga₂O₃/sapphire lattice mismatch: 4.6%
 → High threading dislocation density (TDD)

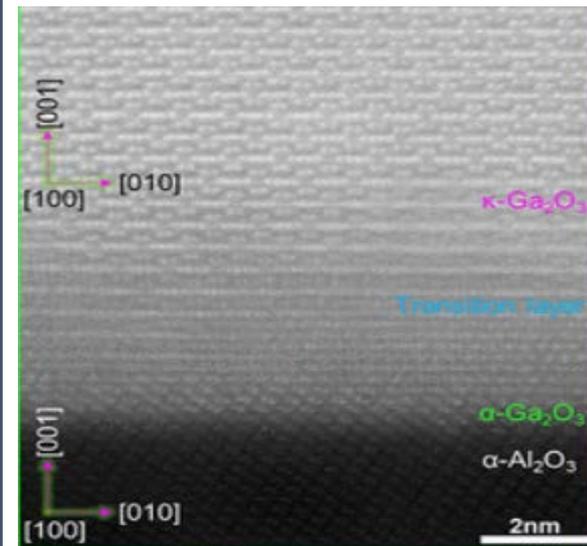
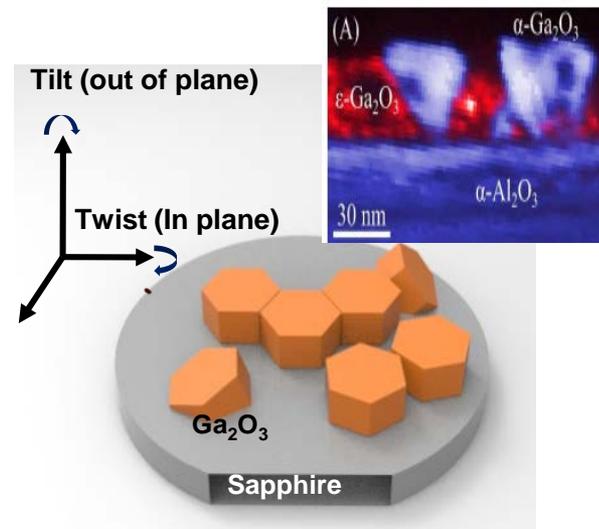


T.C.Ma *et al.*, Appl. Phys. Lett. **115**, 182101 (2019)

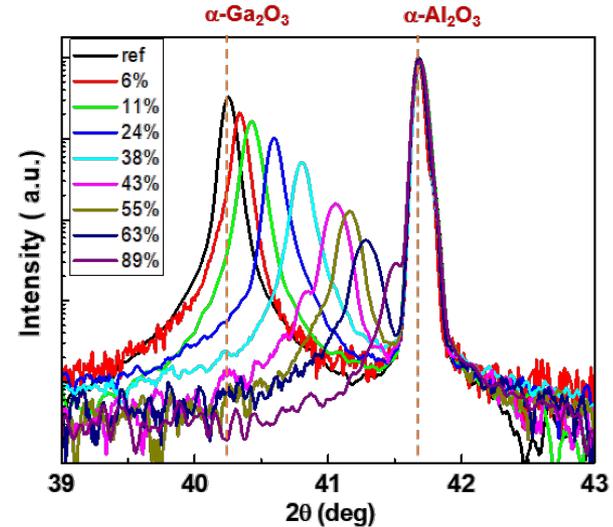
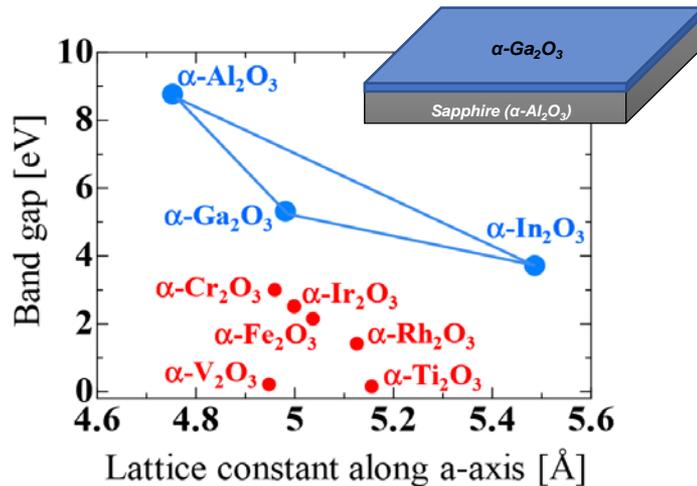
- Difference in thermal expansion coefficient
 → Thermal stress , wafer bow



- Metastable phase epitaxy



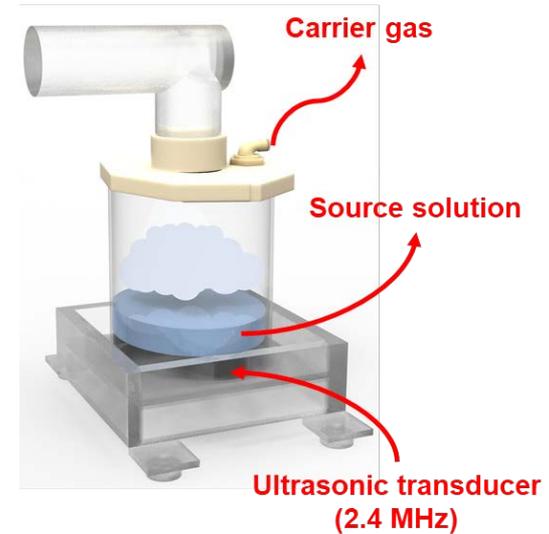
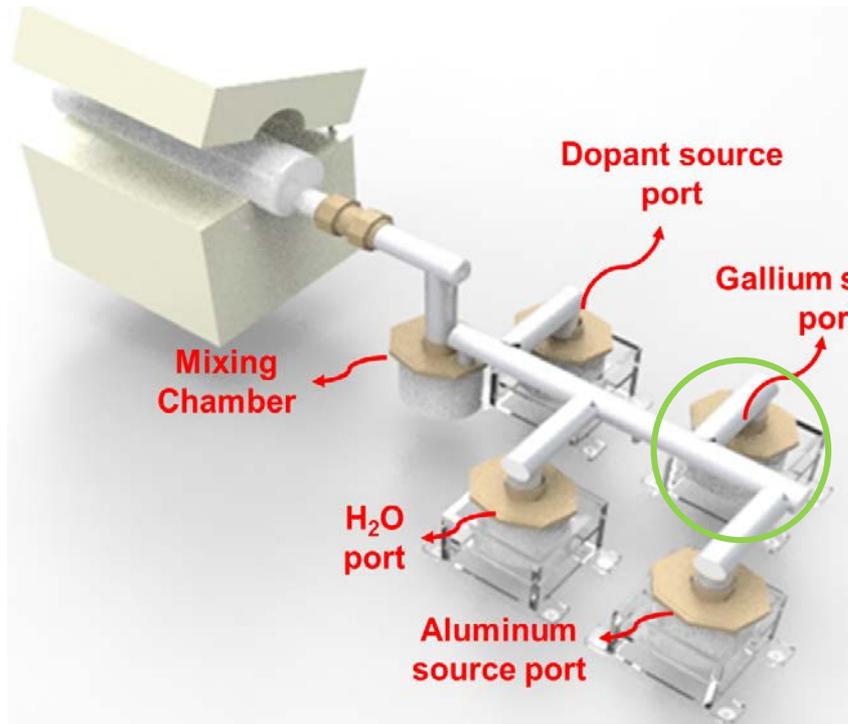
Epitaxial grown α -(Al_xGa_{1-x})₂O₃ buffer layer



- ✓ α -(Al_xGa_{1-x})₂O₃ lattice constant is intermediate between α -Ga₂O₃ (4.98(Å)) and α -Al₂O₃(4.76(Å)).



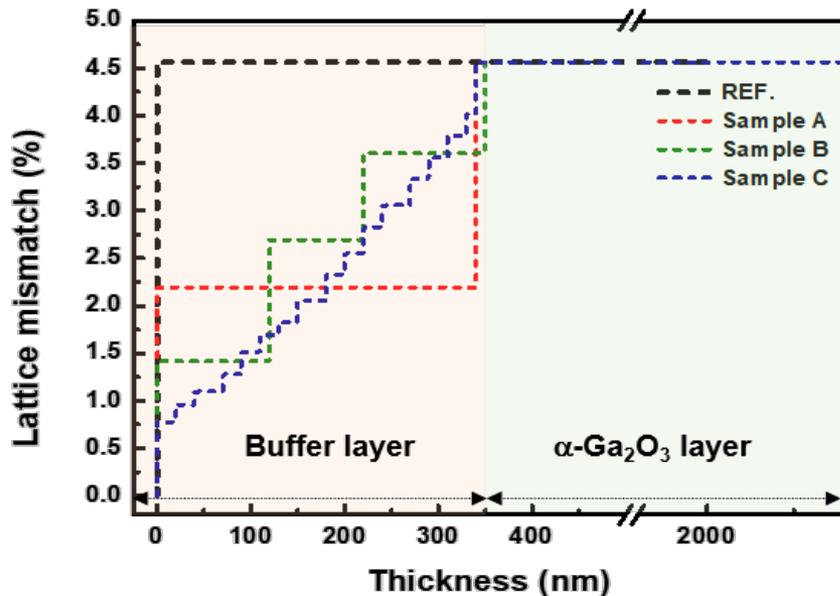
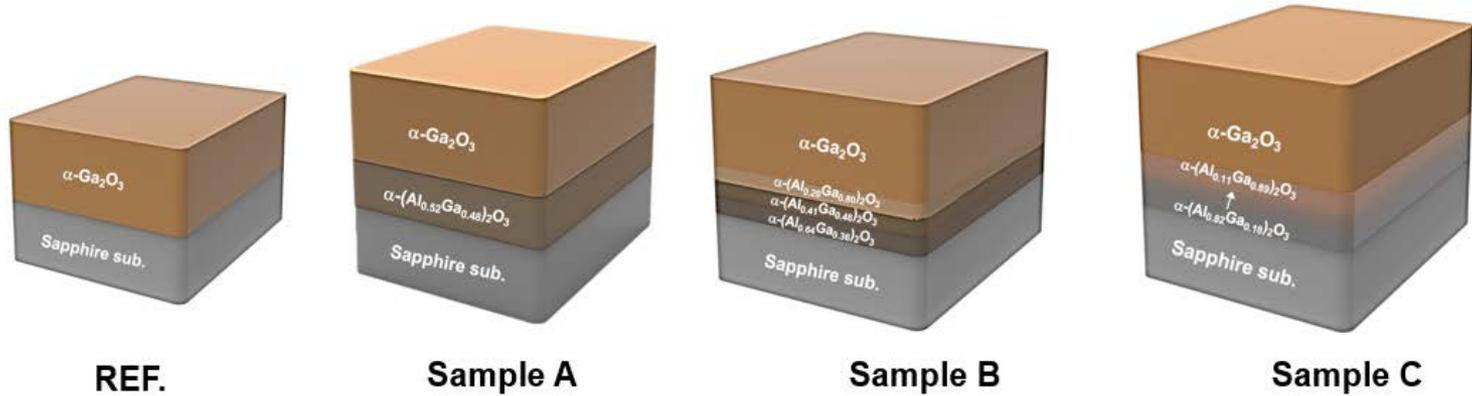
- ✓ Epitaxial α -Ga₂O₃ with reduced TD density could be demonstrated in graded α -(Al_xGa_{1-x})₂O₃ layer on c- sapphire hetero structure.



Source	substrate	Carrier gas	Flow rate (carrier/dilution)
GaCl ₃	Al(acac) ₃ Half of 2-inch sapphire	N ₂	3slm/0.5slm

- ✓ Liquid solution of precursors is ultrasonically atomized to form aerosol particles, and these mist are transferred onto heated substrates.

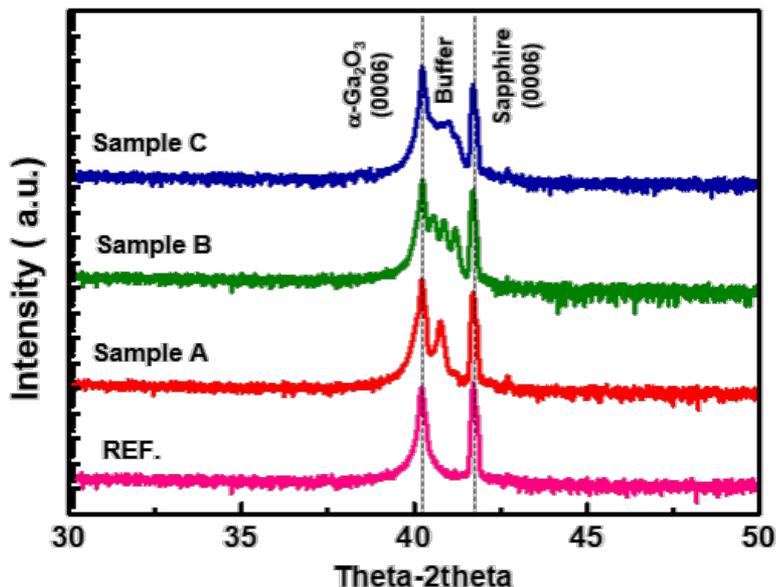
- Schematic $\alpha\text{-Ga}_2\text{O}_3 / \alpha\text{-(Al}_x\text{Ga}_{1-x})_2\text{O}_3 / \text{c- sapphire}$ hetero structure



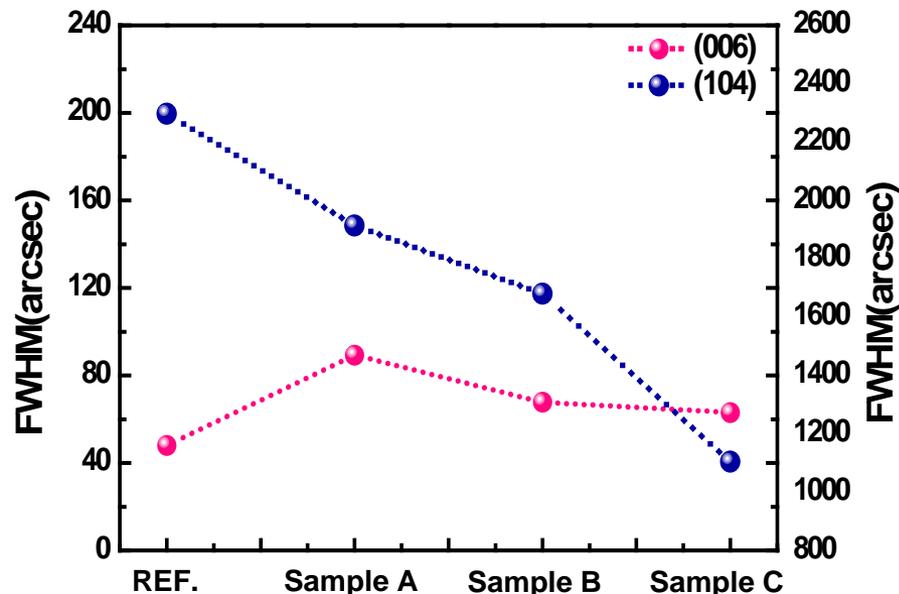
- Growth conditions of $\alpha\text{-Ga}_2\text{O}_3 / \alpha\text{-(Al}_x\text{Ga}_{1-x})_2\text{O}_3$

	$\alpha\text{-(Al}_x\text{Ga}_{1-x})_2\text{O}_3$	$\alpha\text{-Ga}_2\text{O}_3$
Al composition (%)	11~ 82	0
Thickness (um)	0.35	2
Growth temp. (°C)	525	500
Carrier gas	N ₂	N ₂

- Omega-2theta scan profile



- FWHMs of ω -rocking curves



Buffer layer (0.35 μm)

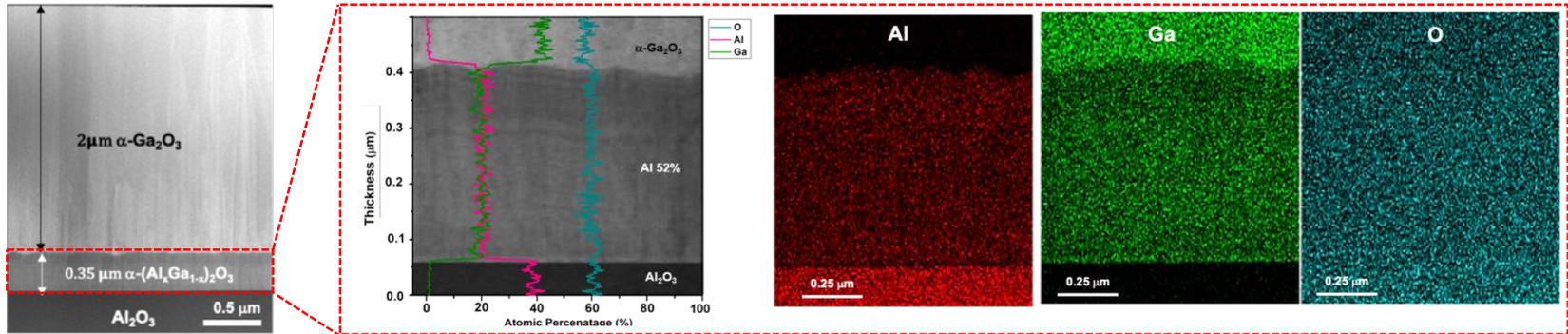
$\alpha\text{-Ga}_2\text{O}_3$ layer (2 μm)

ω - rocking curve FWHM (arcsec)

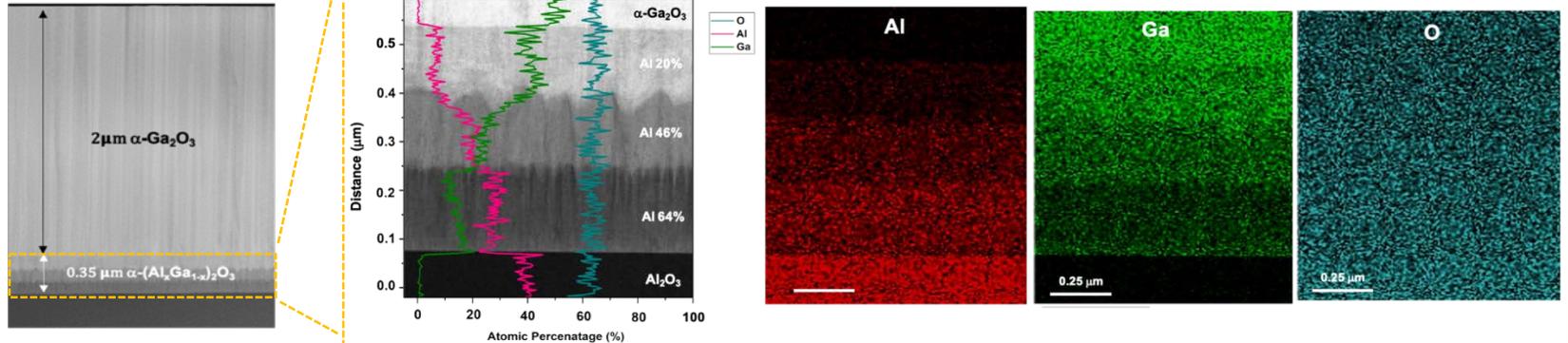
	Buffer configuration	Al composition (%)	In-plane misfit (%)	ω - rocking curve FWHM (arcsec)	
				Symmetric plane (0006)	Asymmetric plane (10 $\bar{1}4$)
REF	-	-	~ 4.6	48.06	2286.43
Sample A	1-layer	52	~ 2.4	89.31	1913.57
Sample B	3-layer	64,41,20	~ 0.92	67.72	1499.97
Sample C	Graded layer	82→60→52→24→11	~ 0.5	62.97	1174.28

Reduced by 42%

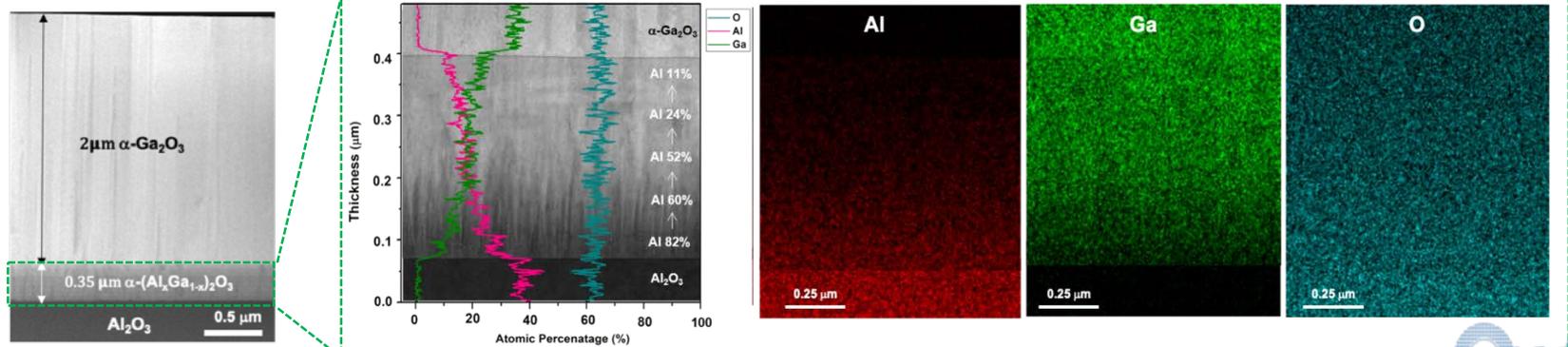
Sample A

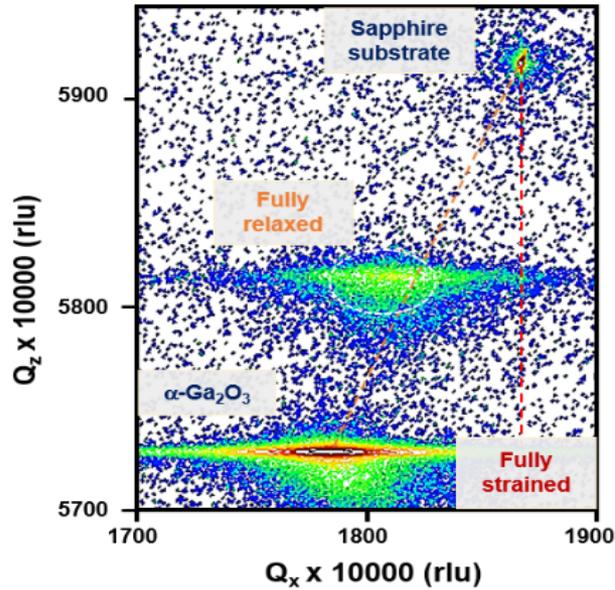
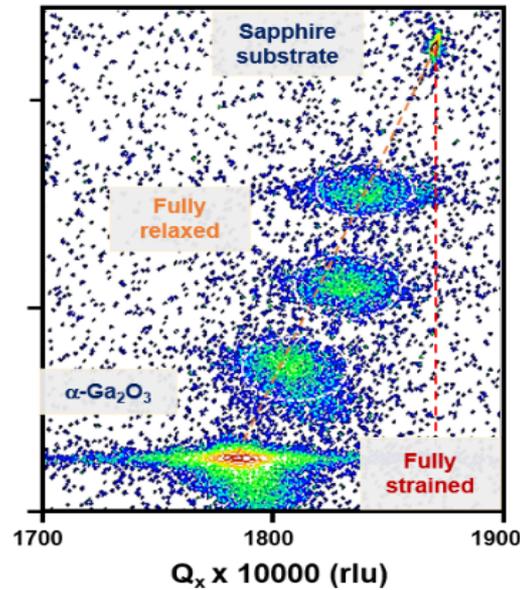
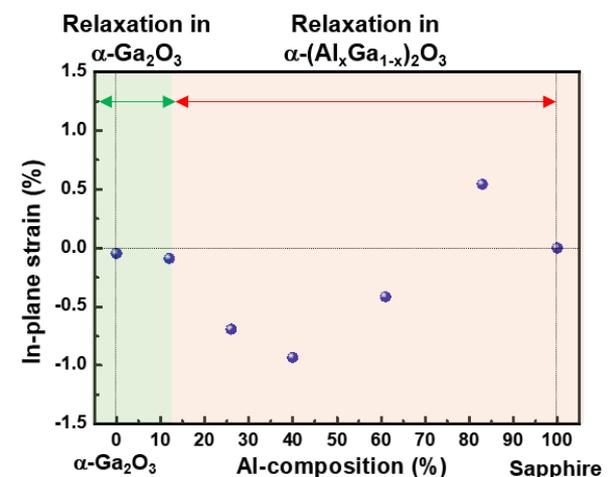
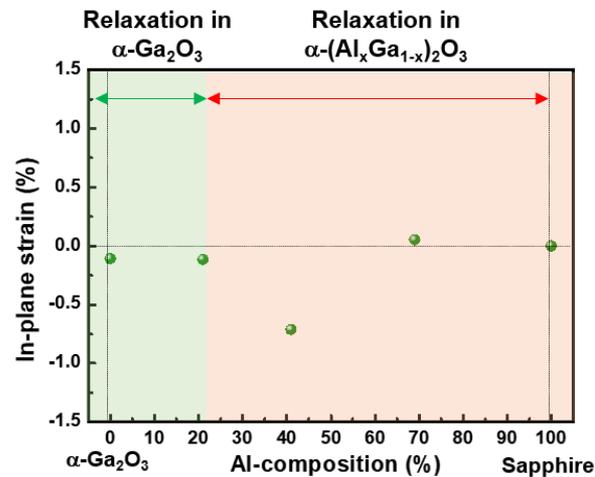
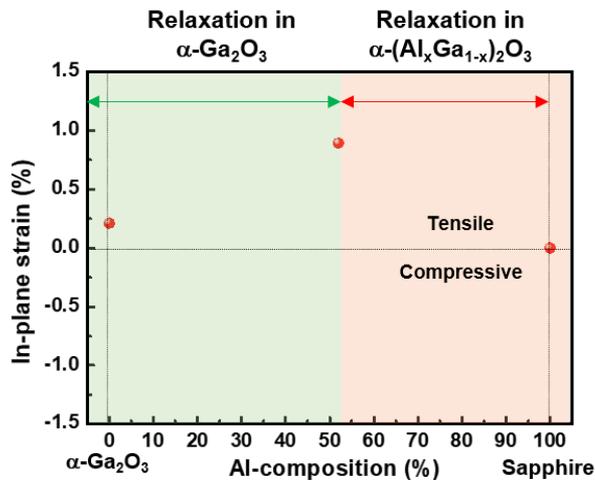
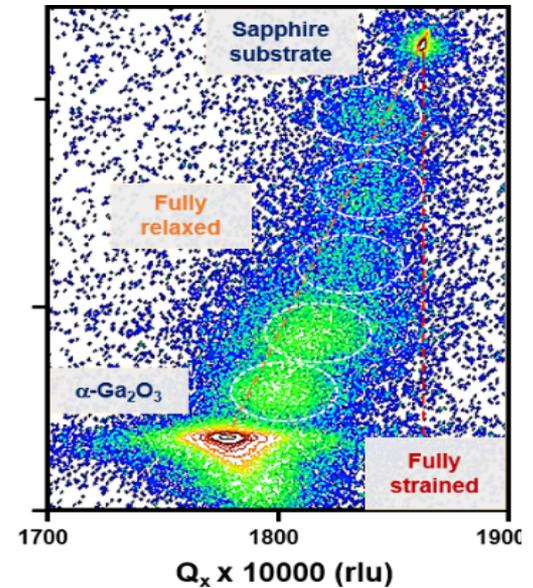


Sample B



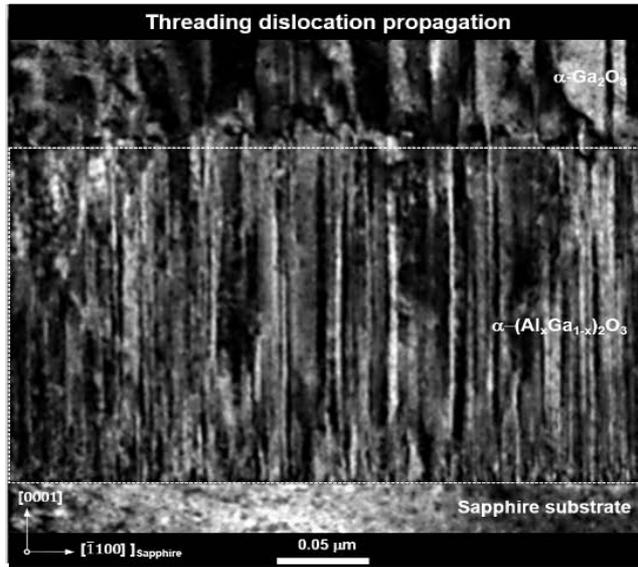
Sample C



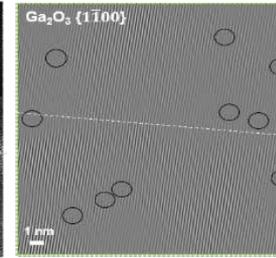
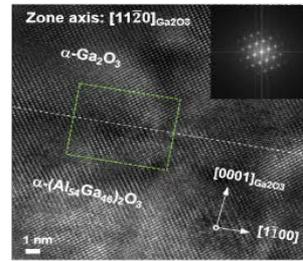
Sample A

Sample B

Sample C


Fully-relaxed state

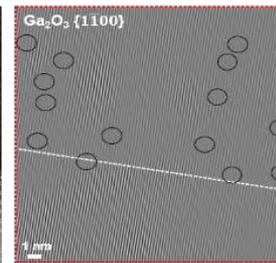
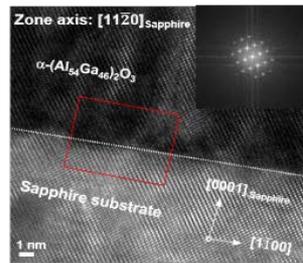
Cross-section TEM



HR-TEM

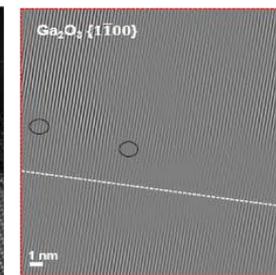
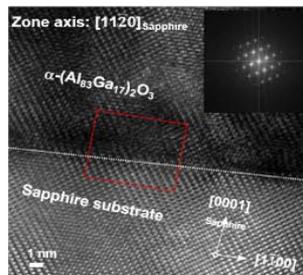
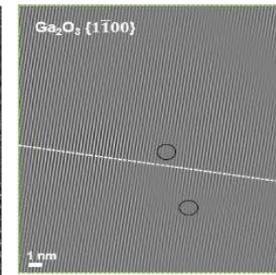
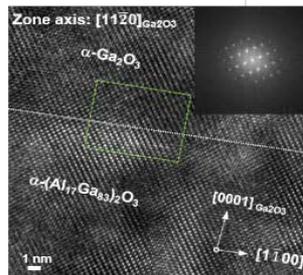
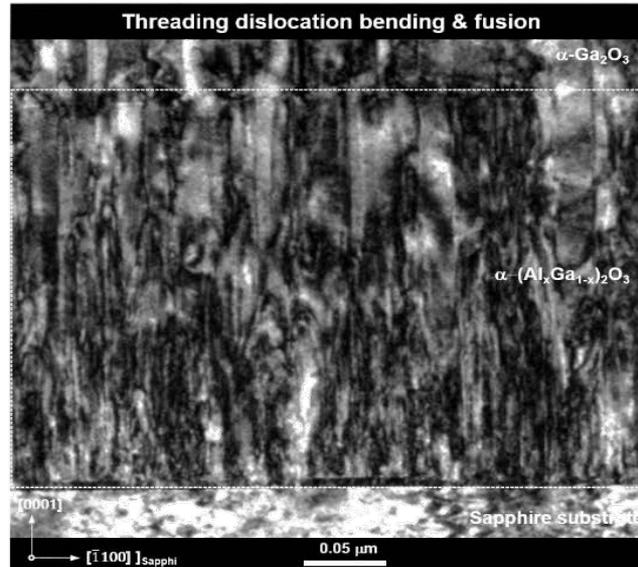


SAED



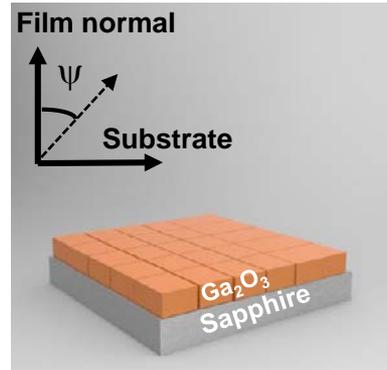
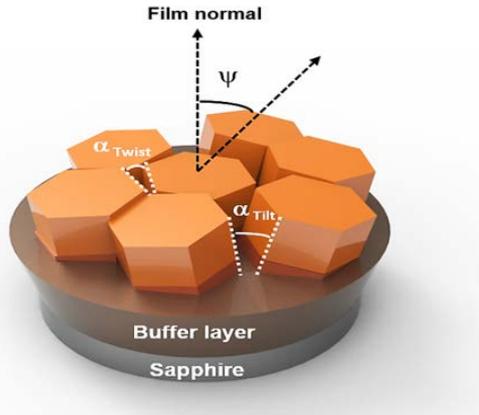
Gradually strain state

Threading dislocation bending & fusion



- Mosaic tilt, twist angle calculation

Srikant model fitting



$$W(\Psi) = \left\{ [W^{tilt}(\Psi)]^n + [W^{twist}(\Psi)]^n \right\}^{1/n}$$

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

$$W^{twist}(\Psi) = \cos^{-1} [\sin^2(\Psi)\cos(W_{in}) + \cos^2(\Psi)]$$

Tilt angle

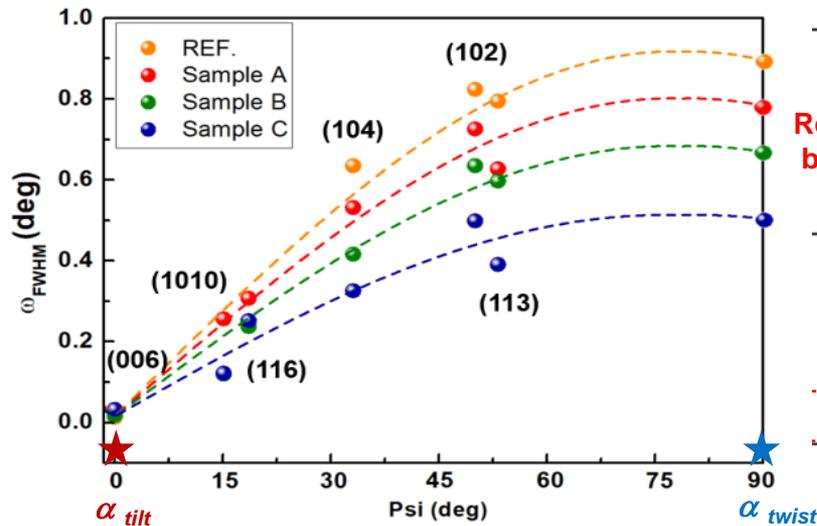
Twist angle

$$N_S = \frac{\alpha_S^2}{4.35b_S^2}$$

$$N_E = \frac{\alpha_E^2}{4.35b_E^2}$$

$$b_S = \langle 0001 \rangle \quad b_E = \frac{1}{3} \langle 2\bar{1}10 \rangle$$

- Threading dislocation density



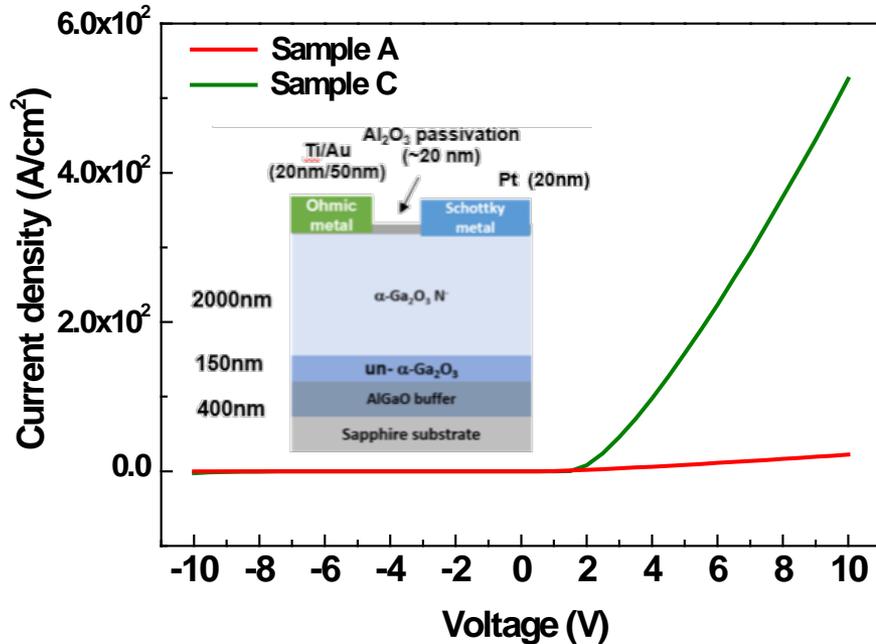
Reduced by 43%

	Crystalline distortion		Dislocation density	
	α_{tilt} (deg)	$\alpha_{twisted}$ (deg)	Screw- dislocation density (cm ⁻²)	Edge-dislocation density (cm ⁻²)
REF	0.013	0.896	1.91 X 10 ⁶	2.08 X 10 ¹⁰
Sample A	0.024	0.783	3.54 X 10 ⁶	1.13 X 10 ¹⁰
Sample B	0.018	0.669	2.69 X 10 ⁶	9.68 X 10 ⁹
Sample C	0.032	0.503	4.68 X 10 ⁶	7.29 X 10 ⁹

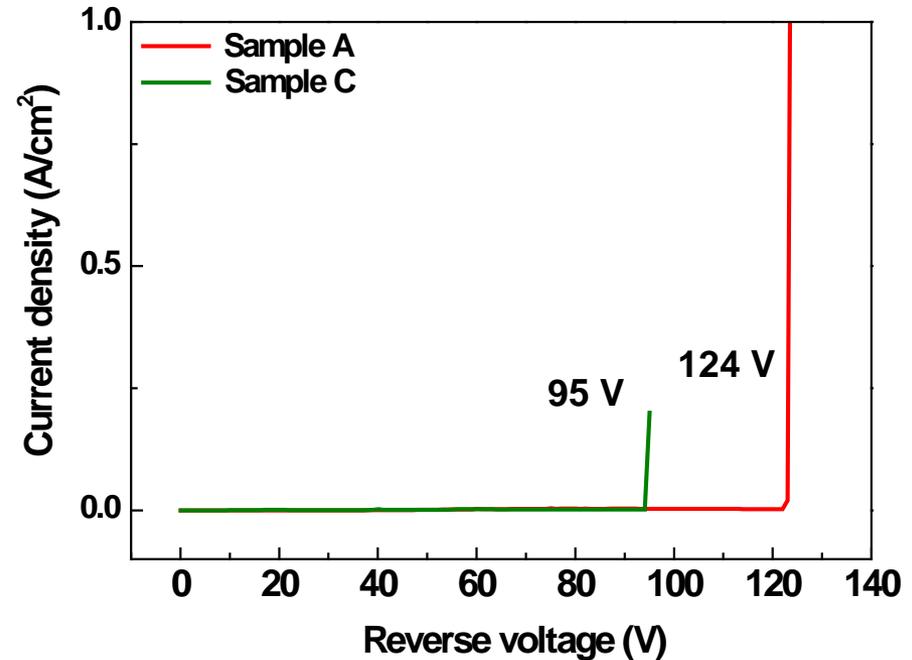
Reduced by 1 order

- ✓ The threading dislocation density of α -Ga₂O₃ grown on graded α -(Al_xGa_{1-x})₂O₃ was reduced by 1 order magnitude compared to that on single α -(Al_xGa_{1-x})₂O₃ layer

• On-resistance



• Breakdown voltage



- Baliga figure of merit(BFOM) : V_{BR}^2 / R_{on} (V_{BR}^2 : Break down voltage R_{on} : specific on-resistance)

	TDD (cm^{-2})	R_{on} ($\Omega \text{ cm}^2$)	V_{BR} (V)	Figure of merit V_{BR}^2 / R_{on} (mw/cm^2)
Sample A	1.13×10^{10}	0.148799	123	733.709
Sample C	7.29×10^9	0.019017	95	4274.577

✓ The figure of merit for the $\alpha\text{-Ga}_2\text{O}_3$ Schottky diode on graded $\alpha\text{-(Al}_x\text{Ga}_{1-x})_2\text{O}_3$ is almost six times larger than that on single $\alpha\text{-(Al}_x\text{Ga}_{1-x})_2\text{O}_3$ layer

- ✓ Epitaxial $\alpha\text{-Ga}_2\text{O}_3$ / $\alpha\text{-(Al}_x\text{Ga}_{1-x})_2\text{O}_3$ hetero structure were successfully grown on c-sapphire substrate by mist-CVD.
- ✓ Compressive strained $\alpha\text{-(Al}_x\text{Ga}_{1-x})_2\text{O}_3$ layer suppressed the propagation of threading dislocation from lattice mismatch.
- ✓ Threading dislocation density were calculated based on mosaic structure with tilt and twist angle.
- ✓ Epitaxial $\alpha\text{-Ga}_2\text{O}_3$ with reduced TD density could be demonstrated in graded $\alpha\text{-(Al}_x\text{Ga}_{1-x})_2\text{O}_3$ layer on c-sapphire hetero structure.
- ✓ The figure of merit for the $\alpha\text{-Ga}_2\text{O}_3$ Schottky diode on graded $\alpha\text{-(Al}_x\text{Ga}_{1-x})_2\text{O}_3$ is almost six times larger than that on single $\alpha\text{-(Al}_x\text{Ga}_{1-x})_2\text{O}_3$ layer

THANK YOU FOR LISTENING
