Investigation of stacking mismatched domain Structure of the γ- Al_2O_3 formed on c-plane sapphire substrate by solid phase epitaxy

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Outline

Introduction

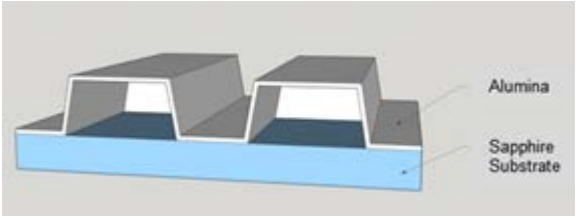
- Growth of GaN on Sapphire (α-Al_2O_3) nano-membrane

Experiments & Analysis

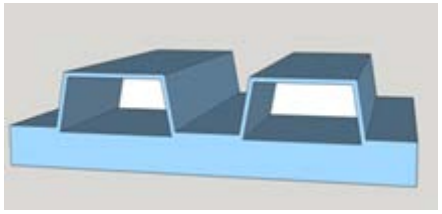
- Fabrication of α-Al_2O_3 / γ-Al_2O_3 nano-membrane
- TEM analysis on the SPE γ-Al_2O_3 layer
- DFT calculation

Growth of GaN on sapphire membrane

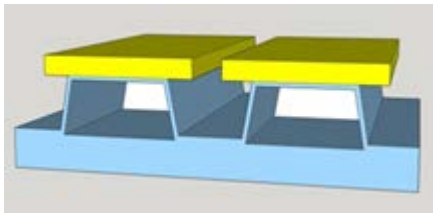
❖ **Growth of GaN on an ultra thin compliant sapphire membrane**



ALD + PR removal

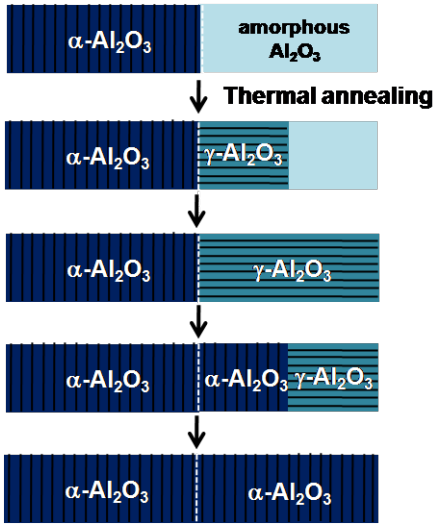


Solid phase epitaxy

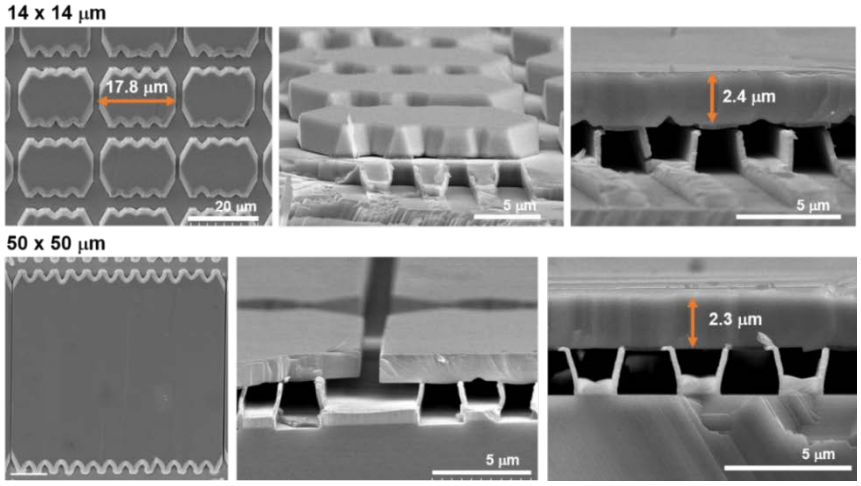


GaN growth

➢ **Solid phase epitaxy of alumina**



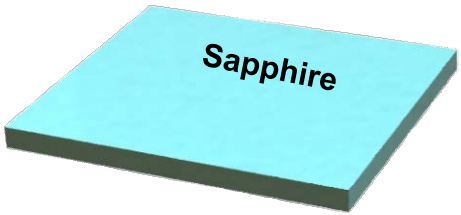
➢ **Micro chip-sized GaN layer**

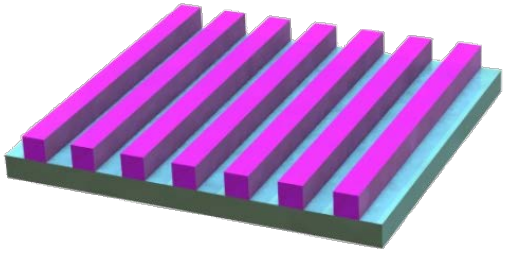


➢ **Understanding the SPE process of the 3D alumina membrane structure is needed.**

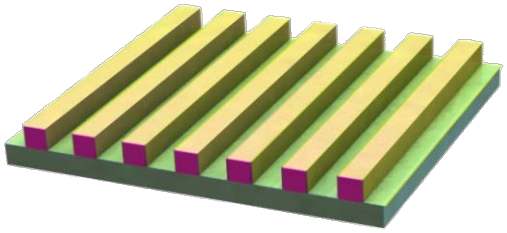
➢ **To obtain high quality α-Al_2O_3, fundamental study on the intermediate γ-Al_2O_3 need to be carried out.**

Experimental details

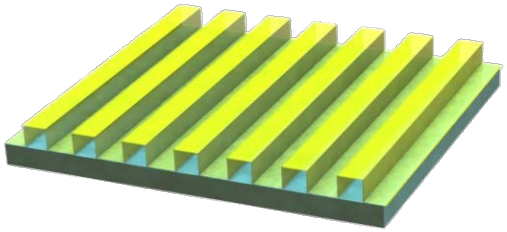




1. Photolithography

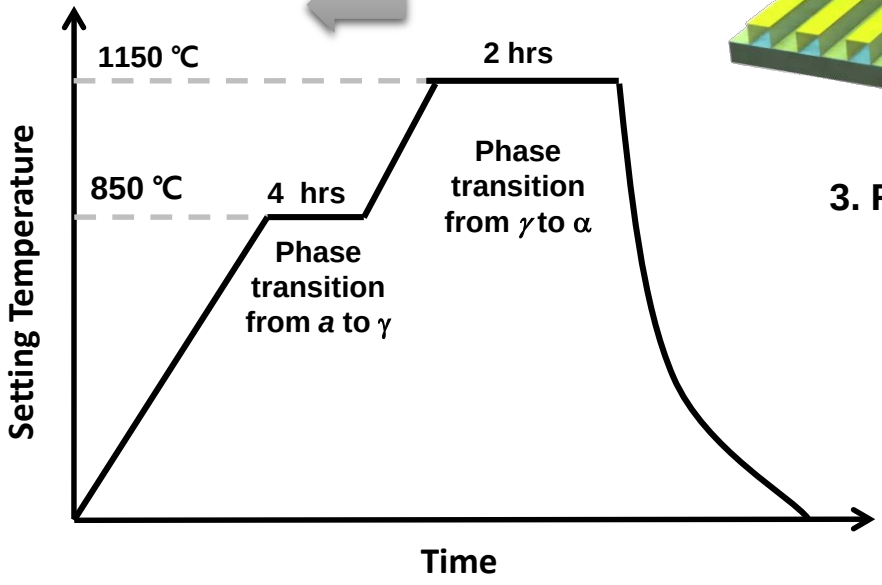


2. Amorphous alumina deposition by ALD

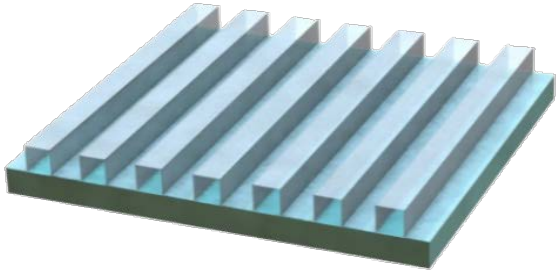


3. Removal of PR

SPE process by thermal treatment



Sapphire nano-membrane

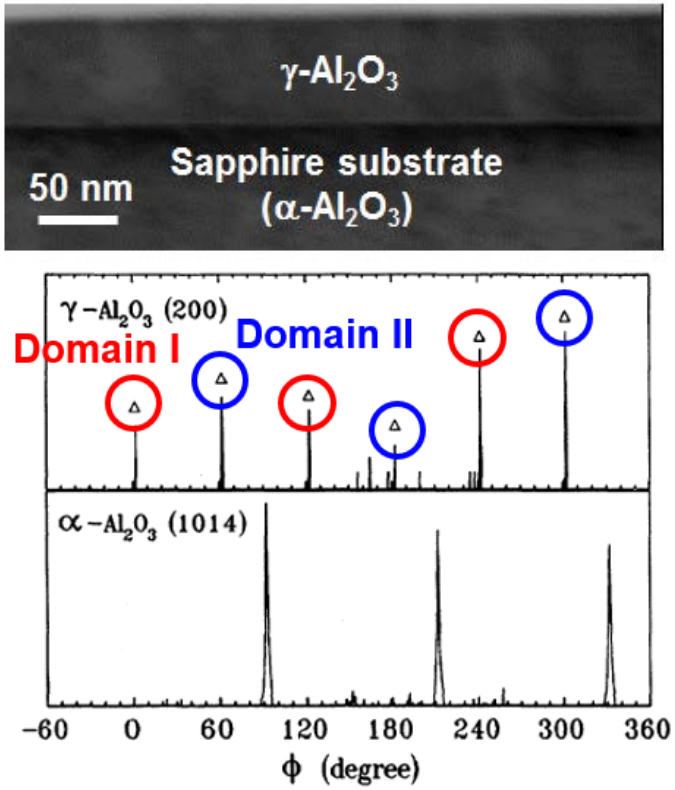


4. Crystallization by thermal treatment

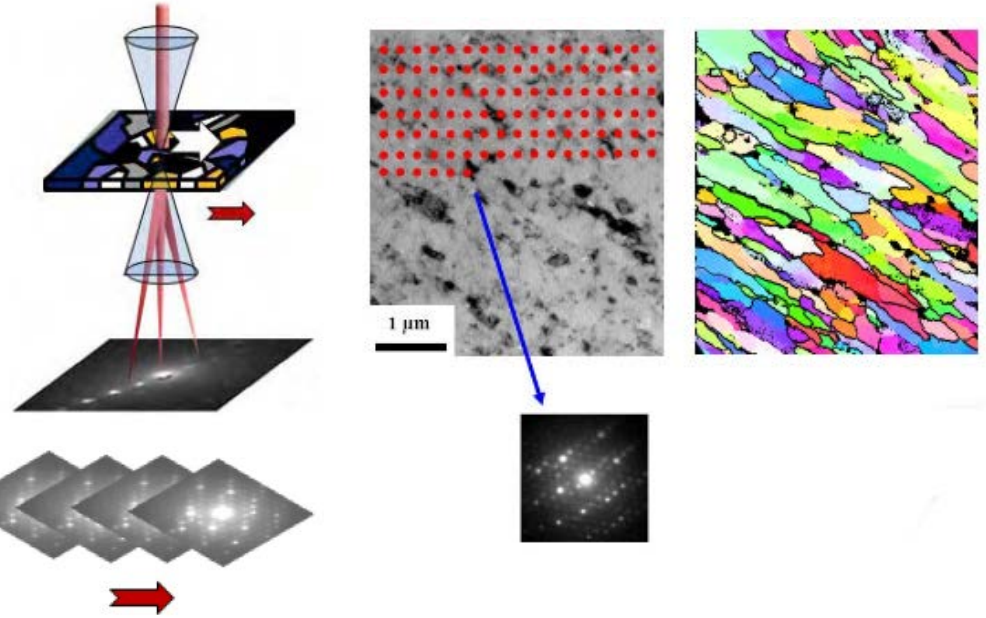
Analysis of γ-Al_2O_3/α-Al_2O_3 interface

- γ-Al_2O_3/α-Al_2O_3 interface_ 850 ^oC 1 hr

<XRD phi scan>



<TEM phase analysis>



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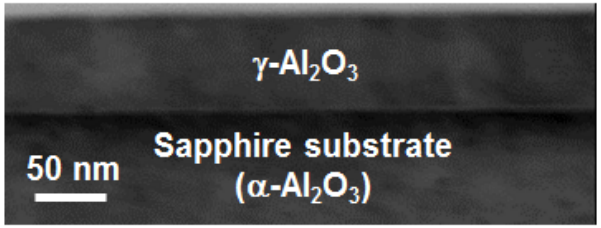
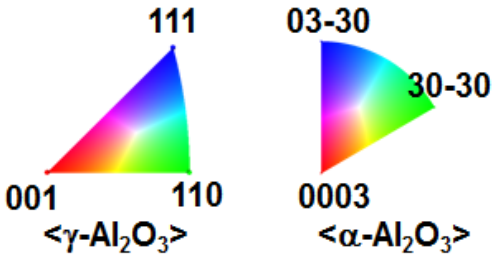
- From the XRD phi scan, γ-Al_2O_3 has two kinds of domain.
- The phase/orientation mapping was conducted for the alumina layer annealed at 850 ^oC for 1 hr.

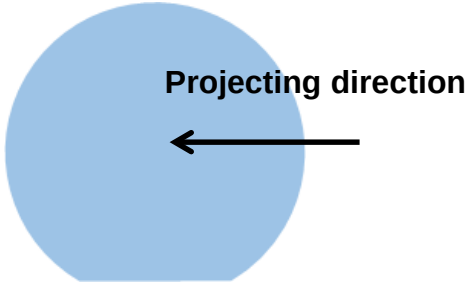
Phase/orientation mapping of γ-Al_2O_3 layer

Projecting direction: <10-10>$_\alpha$ // <110>$_\gamma$

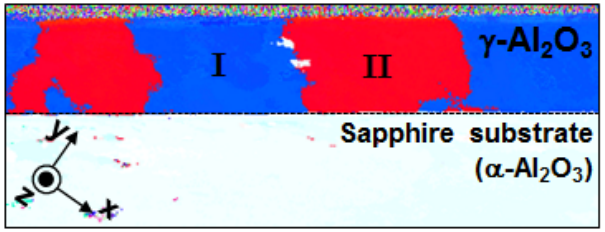
<Virtual bright field image>



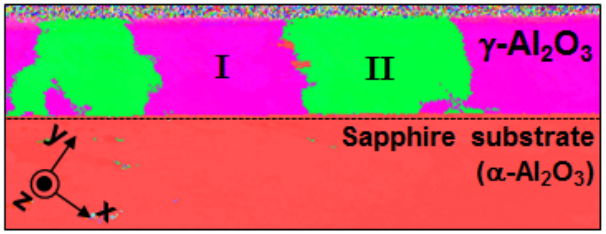




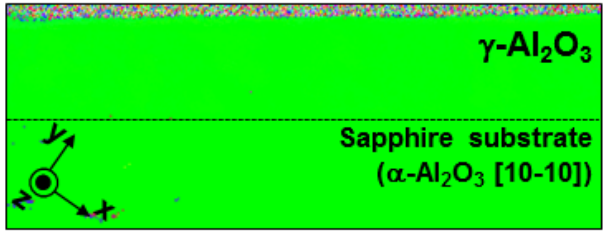
<Phase/orientation map>



x-axis ([-221]$_{\gamma,\,I}$ + [00-1]$_{\gamma,\,II}$)



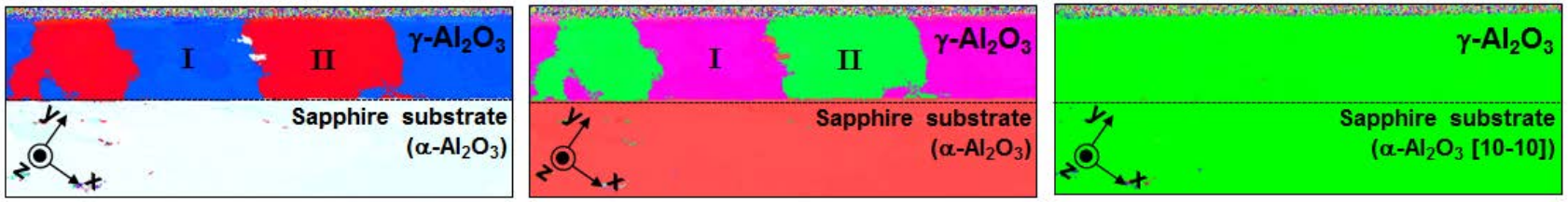
y-axis ([1-14]$_{\gamma,\,I}$ + [1-10]$_{\gamma,\,II}$)



z-axis (<110>$_\gamma$)

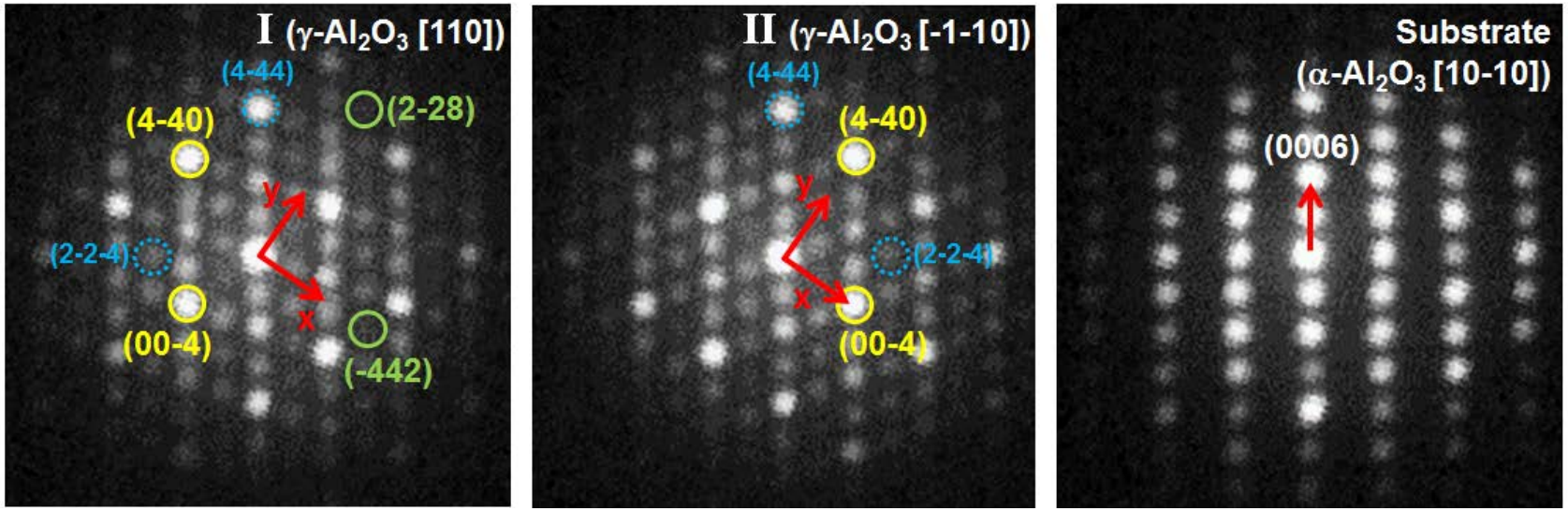
- **Phase/orientation maps show that the γ-Al_2O_3 layer consists of two kinds of domain.**

Phase/orientation mapping of γ-Al_2O_3 layer



x-axis ($[-221]_{\gamma,I}$ + $[00-1]_{\gamma,II}$) y-axis ($[1-14]_{\gamma,I}$ + $[1-10]_{\gamma,II}$) z-axis ($<110>_{\gamma}$)

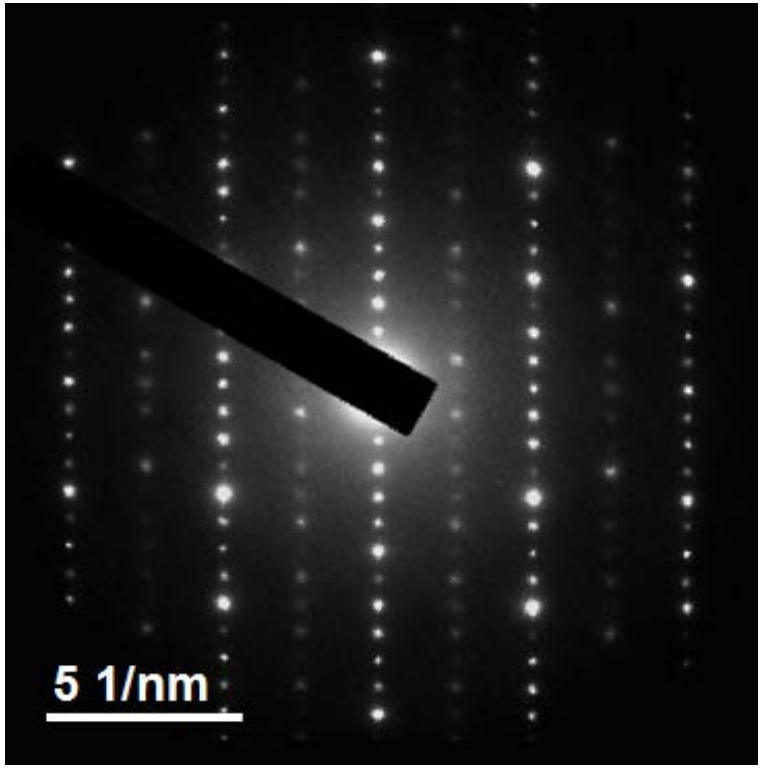
<Nanobeam electron diffraction pattern>

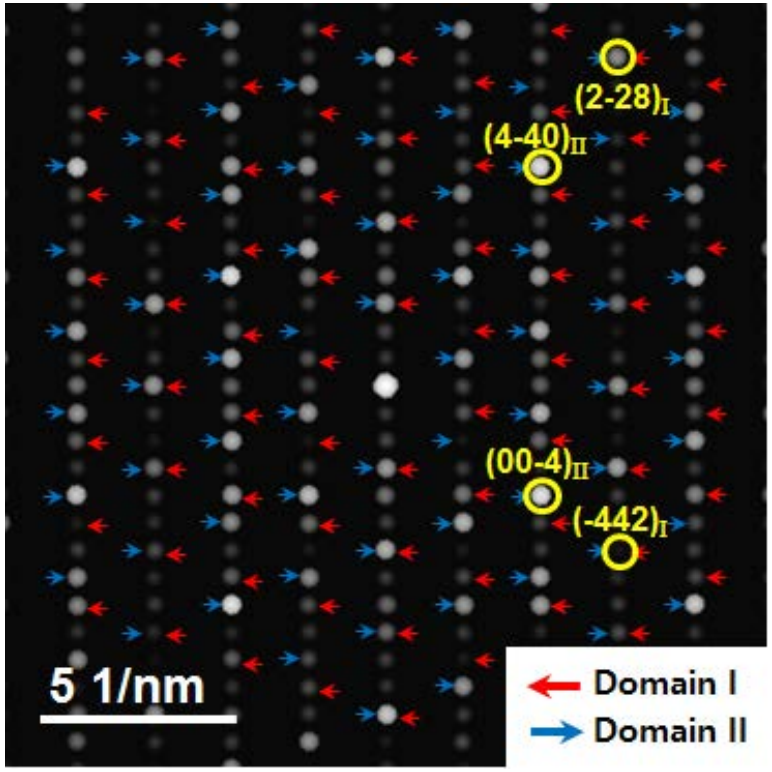


- **The two NPED patterns are in a symmetrical relationship with the virtual vertical line as the symmetry axis, which implies that Domains I and II form twin structure.**

Selected area electron diffraction pattern of γ-Al_2O_3 layer

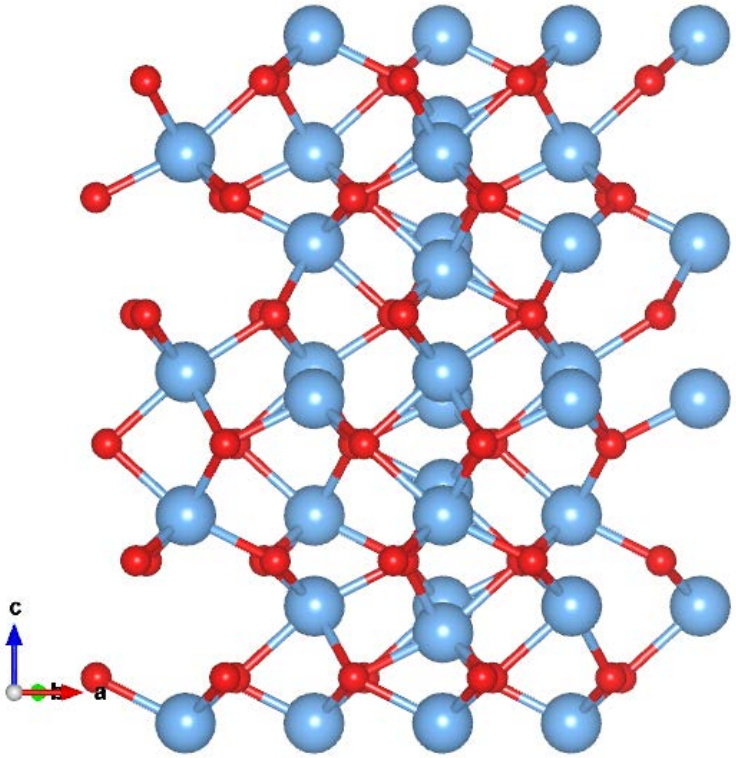
Zone axis: <110>γ

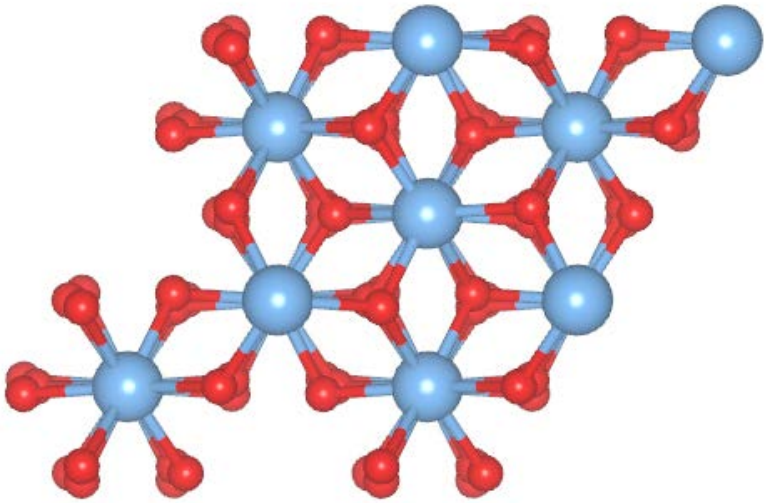


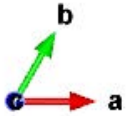


- **The simulated SAED patterns are consistent with the experimental SAED pattern.**

Energetics of γ-Al_2O_3/α-Al_2O_3 interface-DFT

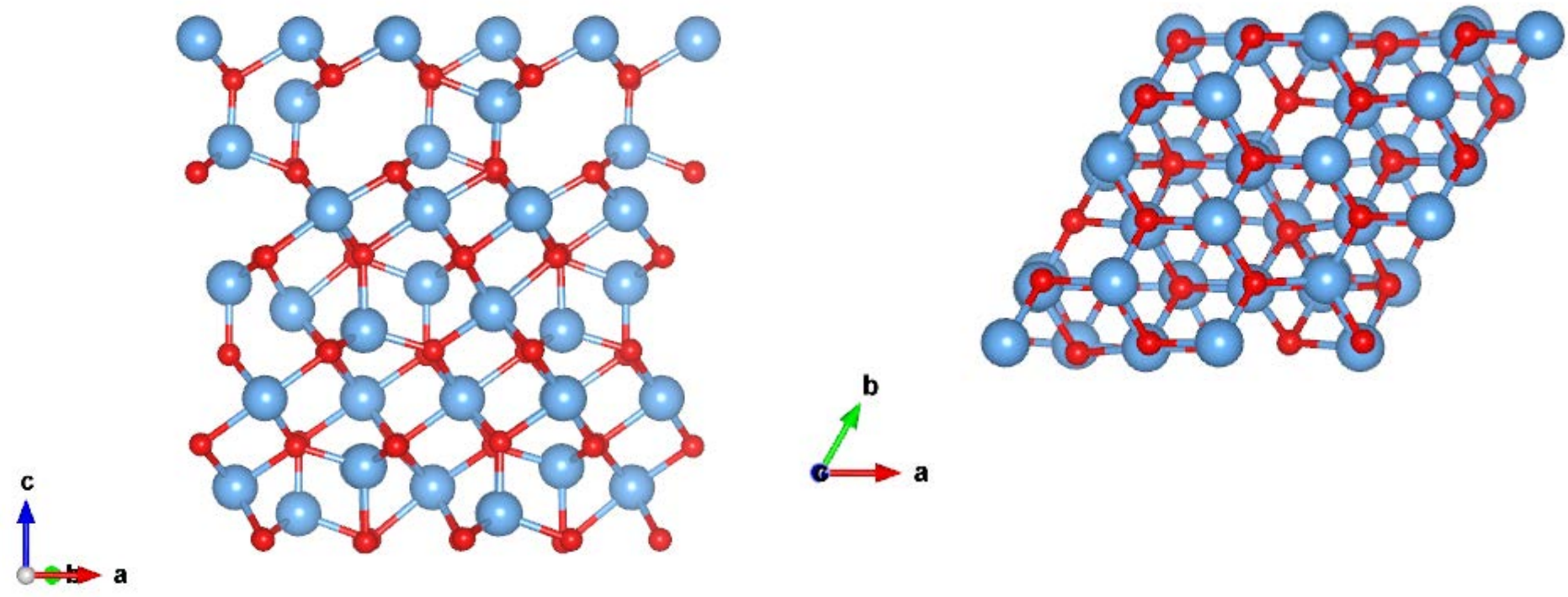






- α-Al_2O_3 unit cell
- Structure of α-Al_2O_3 shown on [10-10], [1-210], [0001], respectively.

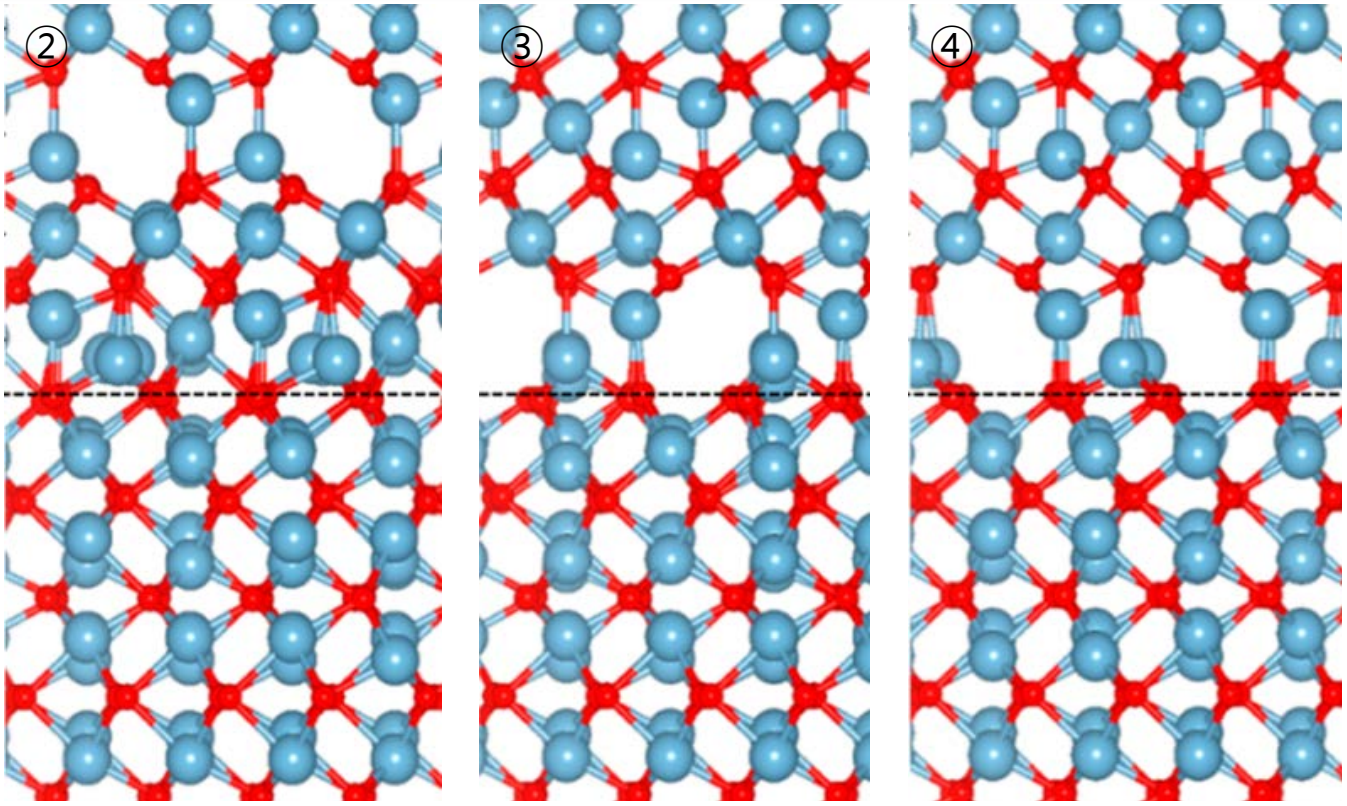
Energetics of γ-Al_2O_3/α-Al_2O_3 interface-DFT



- γ-Al_2O_3 unit cell with [110], [-112], [1-11]
- Spinel-similar structure, but 8/3 cation vacancies must be introduced.

Energetics of γ-Al_2O_3/α-Al_2O_3 interface-DFT

①



- For different heterostructure
- Bottom : α-Al_2O_3 with [10-10], [1-210], [0001] for a, b, c axis.
- Top : γ-Al_2O_3 with [110], [-112], [1-11] for a, b, c axis(① and ③)
  γ-Al_2O_3 with [-1-10], [1-1-2], [1-11] for a, b, c axis(② and ④)

Energetics of γ-Al_2O_3/α-Al_2O_3 interface-DFT

Structure	Energy(relative, eV)
1	0
2	0.11
3	12.35
4	11.39

- **Difference between ①, ③ and ②, ④ : position of Al vacancy**
- **Structure ③ and ④ : are not probable (energetically unfavored)**
- **Structure ① and ② : very small energy difference – both domains are probable in experiment**

Summary

- ✓ **Solid-phase crystallization of 3-D Al_2O_3 membrane structure was investigated, showing the phase transformation sequence from amorphous to γ-(SPE & RNG) and then to α-phase (SPE).**
- ✓ **The epitaxial γ-Al_2O_3 consisted of two stacking-mismatched domains, which can be distinguished at specific directions by XRD scan.**
- ✓ **The simulated SAED patterns are consistent with the experimental SAED pattern, which can confirm both domain I and II**
- ✓ **DFT calculation also confirms that both domain I and II are probable.**

THANK YOU FOR LISTENING