Evaluating the quality of epitaxial In_2O_3 grown by suboxide molecular beam epitaxy

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Suboxide Molecular Beam Epitaxy

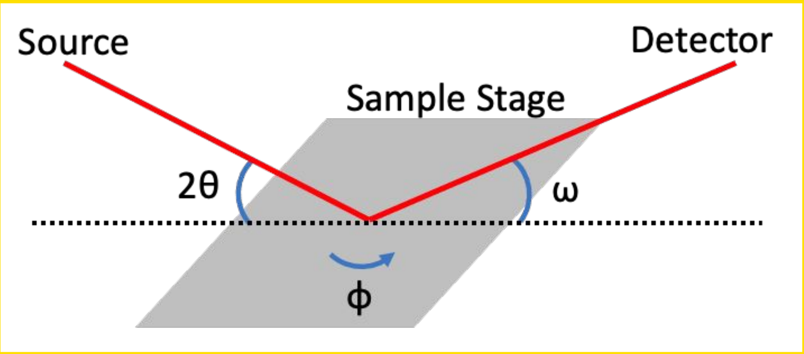
Suboxide molecular beam epitaxy (S-MBE) is a novel technique which can be used to grow high quality epitaxial thin films quickly at back-end-of-line (BEOL) applicable temperatures.[1] One material which can be grown is indium oxide, In_2O_3, which has potential application in transparent thin film transistors (TFTs).[2] In traditional MBE, the oxidation of indium on a substrate surface goes through a two step reaction consisting of a slow step and a fast step:

$$2\,In + 3\,O \xrightarrow{\text{slow step}} In_2O + 2\,O \xrightarrow{\text{fast step}} In_2O_3$$

However, S-MBE starts with an In_2O source rather than an elemental source by utilizing a mixture of indium metal and indium oxide powder resulting in an In_2O beam.[1, 3] Utilizing this technique, we grow epitaxial In_2O_3 thin films on YSZ001 with a growth rate of (0.6 μm/hr) at the BEOL applicable temperature of less than 450ºC. The bulk and surface quality of these films was evaluated by X-ray diffraction (XRD) and atomic force microscopy (AFM).

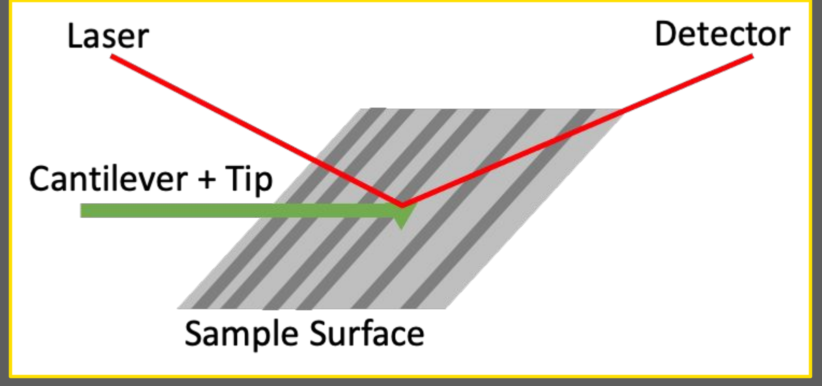
X-Ray Diffraction

XRD is used to measure the crystal structure of the films. The angle between the source and the film surface is 2θ, the angle between the detector and film surface is ω, and the sample stage can be rotated by ϕ.



Atomic Force Microscopy

AFM is used to measure the surface topography and roughness of the films. A tip on a cantilever is repelled by and attracted to the surface and a laser is used to measure the deflection of the tip, providing an image of the surface.



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Bulk Quality

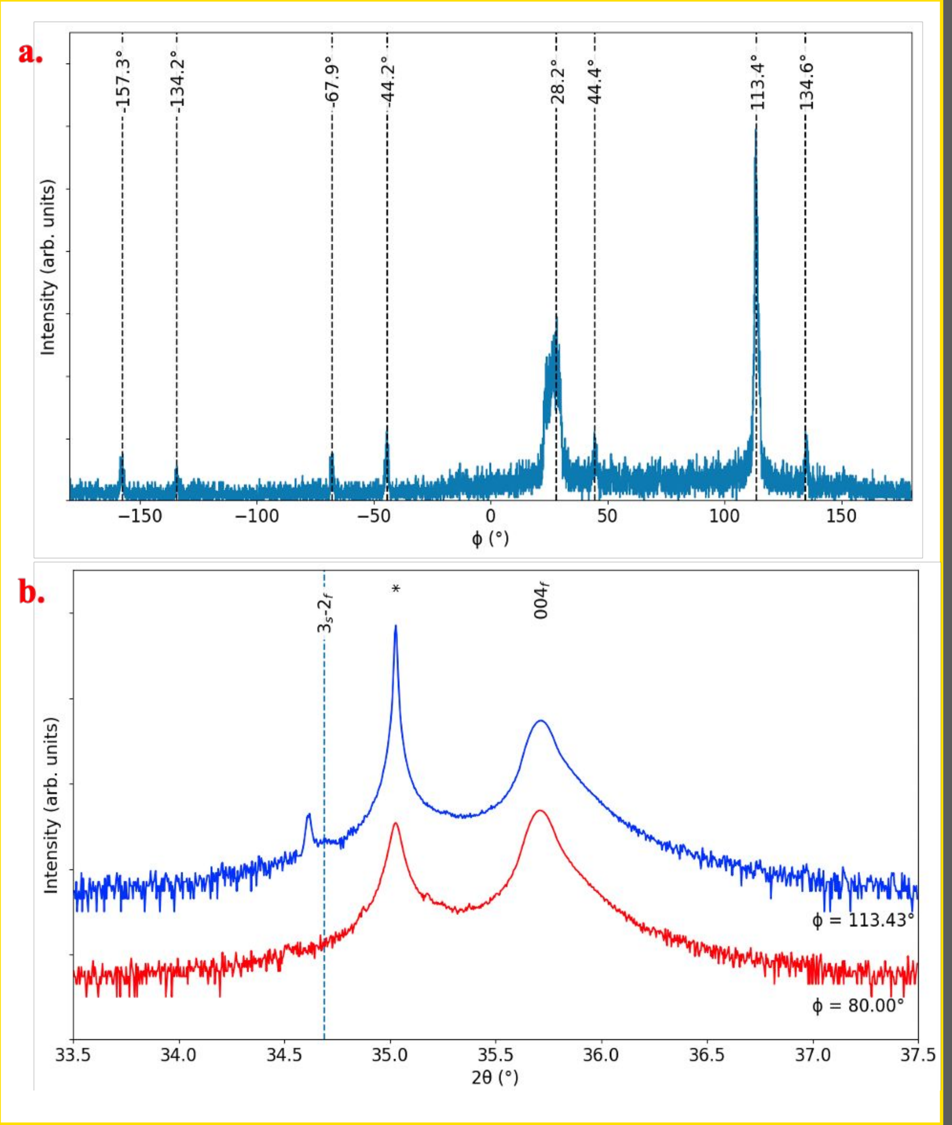
Hybrid Peaks and Full Width Half Maximum

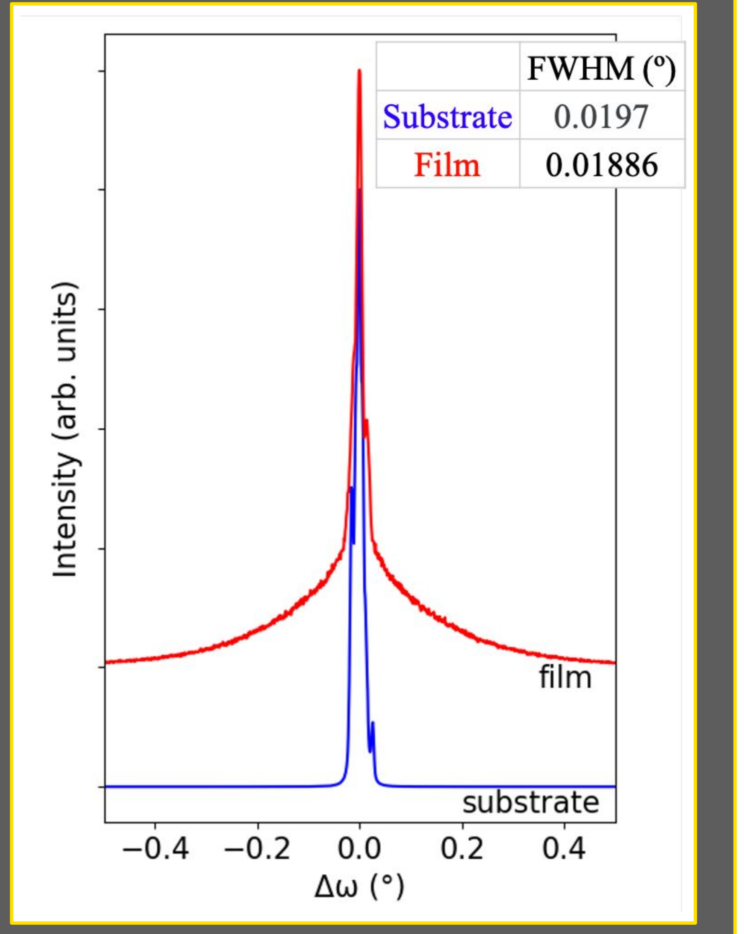
Hybrid reflections can only occur when the bulk film is uniform and phase pure.[5]

- ϕ scan at the angle of the hybrid reflections (2θ = 34.6º) of In_2O_3
- Repeat approximately every 90º - cubic unit cell
- Hybrid reflection ((003) substrate plane interacting with (00$\bar{2}$) film plane) at 2θ = 34.58º
- ϕ dependency confirms it is a hybrid reflection.

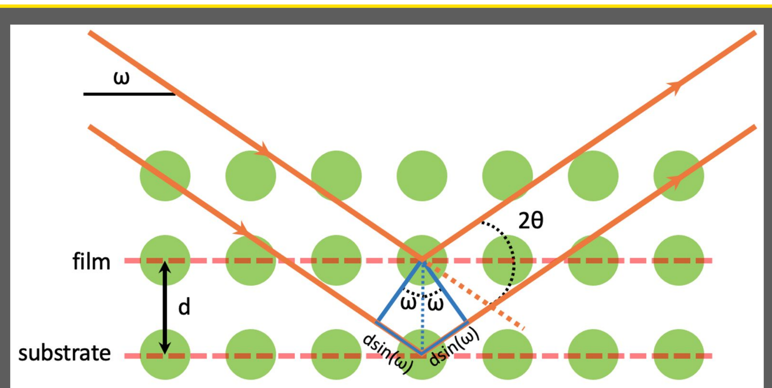
The full width half maximum (FWHM) of the rocking curves of the film and substrate is compared to evaluate the bulk film quality.

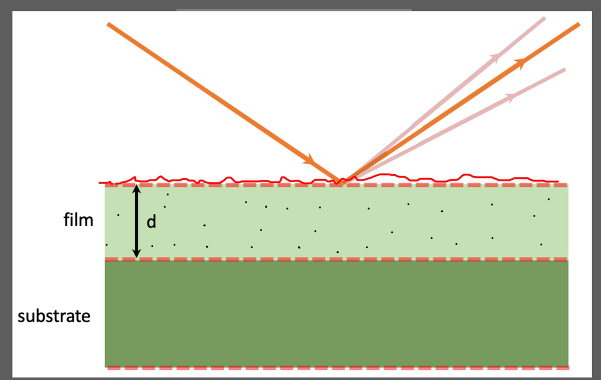
- FWHM of film and substrate are approximately the same
- FWHM of films grown by S-MBE is better than other techniques
- Few defects to broaden peak





T_{growth}	Method	FWHM	Reference[4]
550 °C	RF-sputter	0.54	Lozano *et al*. J.Sol.Mat. 2013
300 °C	MBE	0.08	Taga *et al*. JJAP 1998
550 °C	Mist-CVD	0.231	Nagata *et al*. JJAP 2020
650 °C	MBE	0.11	Bierwagen *et al*. APL 2009
<450 °C	S-MBE	0.0197	



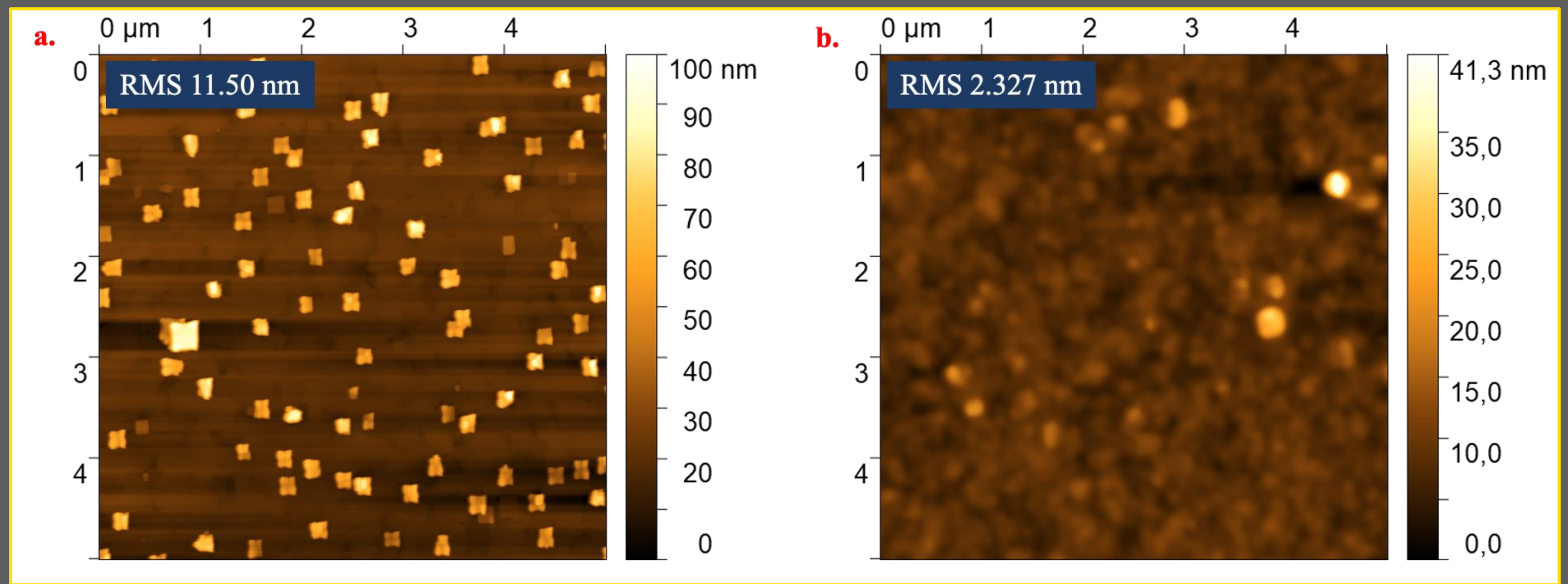


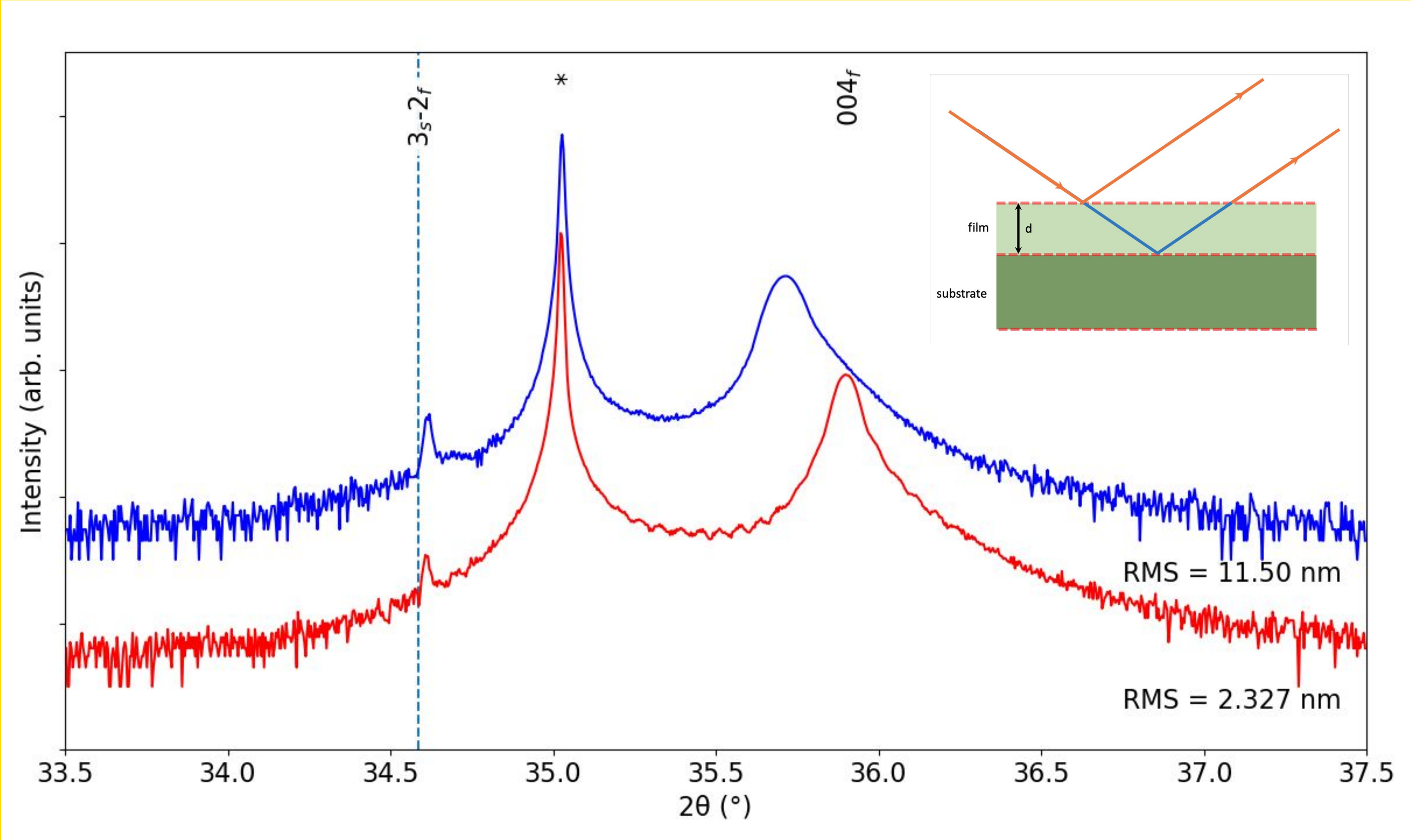
Conclusion

S-MBE can grow high quality films rapidly at BEOL applicable temperatures as evaluated by XRD and AFM. The bulk quality was assessed by the presence of hybrid reflections and the agreement of the FWHM of the film and substrate. The surface quality of the films was assessed by the presence of thickness fringes and topography measurements. Compared to other In_2O_3 films, the speed and quality of growth is unparalleled.

Surface Quality

Atomic Force Microscopy and Thickness Fringes





AFM was used to measure the surface topography and verify the relationship between smooth film surface and the presence of thickness fringes.

- Surface topography of two samples, a rough one and a smooth one
- Rough sample contains islands on its surface, thought to be excess In_2O which

Thickness fringes only occur when the surface of the film is smooth.

- Typically occur at 0º to 8º, but can appear at greater angles if surface is smooth[7]
- Thickness fringes only appear on smooth sample
- Bulk of both samples is highly phase-pure and uniform due to hybrid reflection peak

Future Work

Because S-MBE is able to reach unmatched crystal quality at BEOL applicable temperatures, the next step would be the fabrication of BEOL TFTs using our films. This work would need to consider if the superior crystal quality correlates to superior electronic transport properties and address eventual challenges such as the active control of electronic properties and possible downsizing effects.