First Growth and Characterization of $KTaO_3$ Thin Films Using Molecular-Beam Epitaxy

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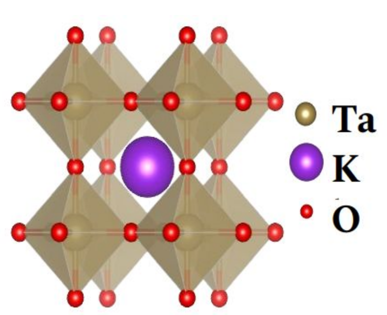
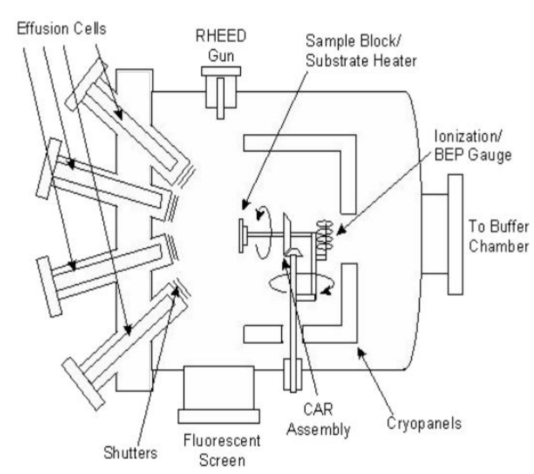
Introduction

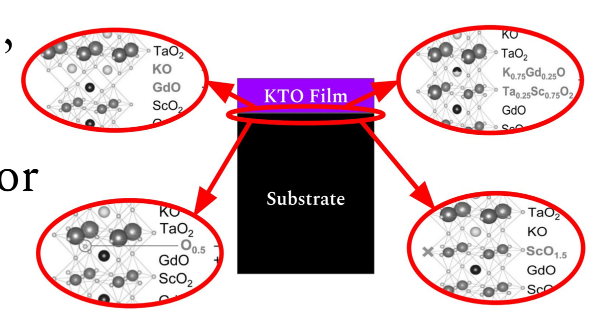


ABO_3-type perovskites can add novel functionalities and performance enhancement to electronics [1]. $KTaO_3$ (KTO) in particular has high spin-orbital coupling with electronic and structural similarities to $SrTiO_3$ (STO) which points to ferroelectricity KTO [2].

Molecular-beam epitaxy uses vacuum deposition of heated sources onto a substrate for epitaxial growth.

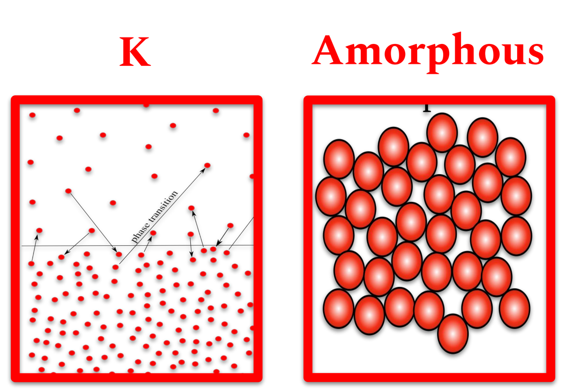


KTO film growth has been dire due to volatile K-atoms and non-volatile Ta-atoms [3]. Oxide MBE offers absorption-controlled growth, high oxidation, enhanced thin-film crystal quality, independent growth parameters, and interfacial control.



Interfacial control of KTO opens the door to several applications in spintronics, memory devices, and photovoltaics.

Experiment Overview

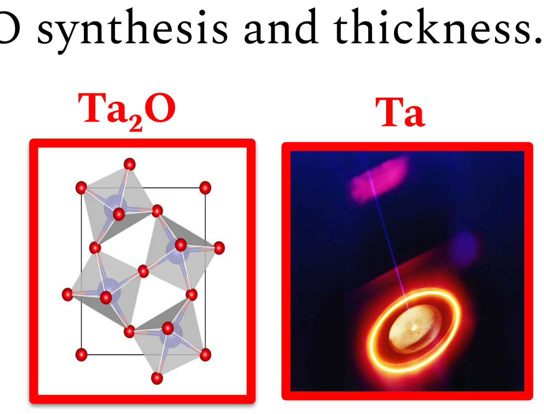


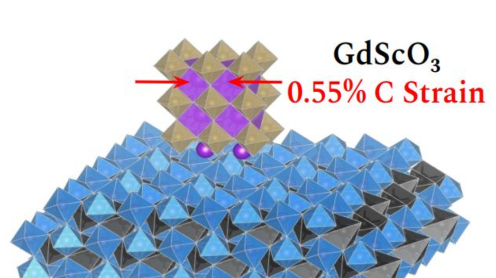
Growth Calibration Adjustments

- Source temperatures for molecular beam flux calibration
- Tsub to balance volatile K-atoms sticking to the film and avoiding amorphous growth.

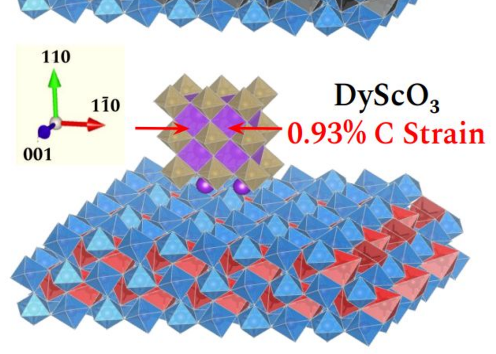
XRD/XRR monitoring to streamline consistent KTO synthesis and thickness.

Films from e-beam heating of a purely Ta source and a source furnace heating of a sub-oxide TaO_2 were compared using 2θ scans, rocking curves, RSM, and AFM.



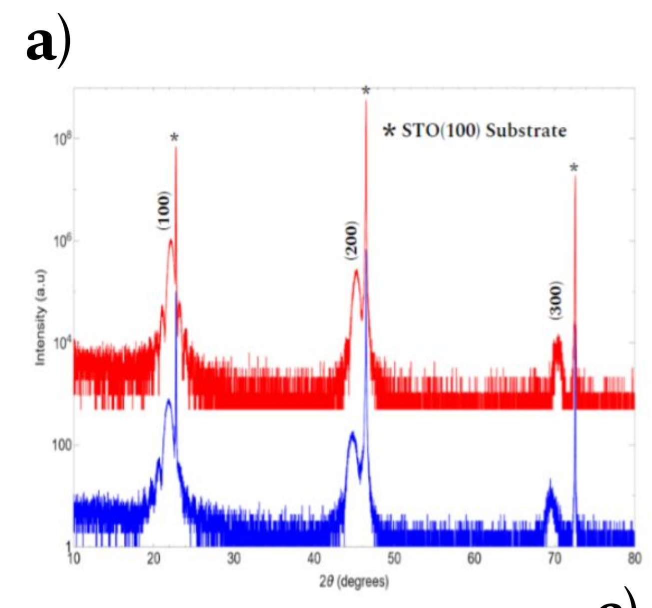


Compressive epitaxial strain using rare-earth scandate (110) crystal substrates that create "cube-on-pseudocube" interfaces with KTO: $GdScO_3$ (GSO) and $DyScO_3$ (DSO)

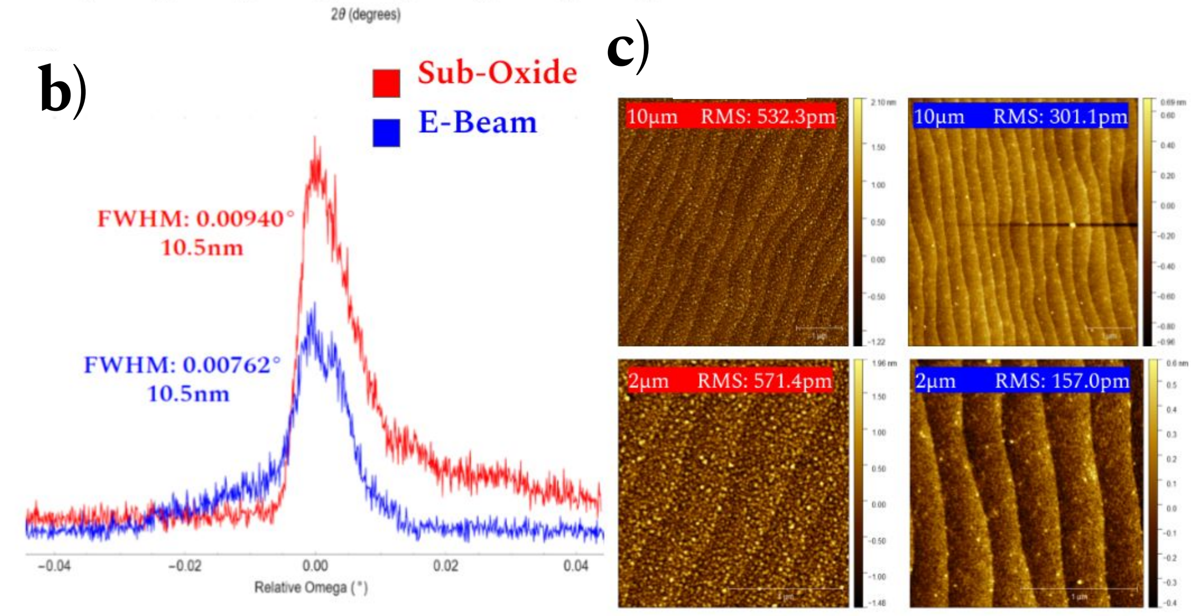


Measured through 2θ scans and RSM such that their crystalline quality and the extent to which compressive strain occurred could be assessed.

Data & Results



Based on the intensity of (100) KTO peaks and fringe character, 10.5nm KTO films derived from both a sub-oxide TaO_2 source and an e-beam Ta source yielded comparable crystallinity — with the sub-oxide films edging by just a small margin (confirmed by extremely similar rocking curves with narrow FWHM).



A 10μm AFM scan revealed a high concentration of impurities on the sub-oxide films compared to e-beam films (further shown in 2μm scan).

Previous literature suggests that these impurities are KO agglomerates [1].

Figure 1: Crystalline and surface comparisons of furnace-heated TaO_2 source (red) and e-beam-heated Ta source KTO films (blue). (a) 2θ scans (logarithmic scale) (b) ω scan rocking curves (linear scale). (c) 10μm and 2μm AFM images and RMS values.

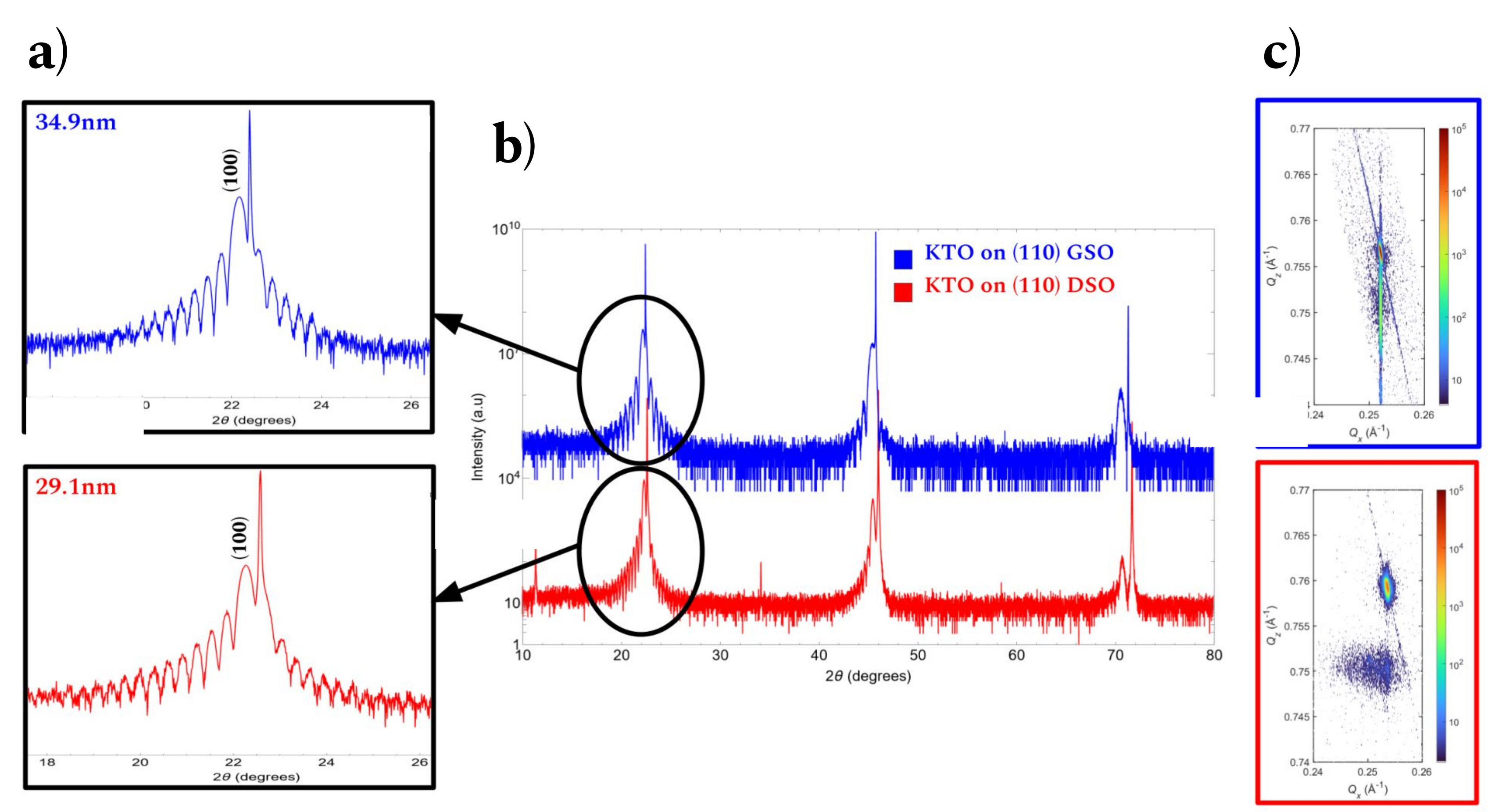


Figure 2: Crystalline and strain analysis of KTO films on (110) GSO and (110) DSO substrates. a) Fine 2θ scans. b) Broad 2θ scans. c) RSM scans (logarithmic scale).

Crystalline quality of KTO films on GSO and KSO excelled, with high intensity (100) peaks and numerous thickness fringes.

Epitaxial strain, for 34.9nm thick KTO films demonstrated full 0.55% compressive strain on GSO substrates (perfect RSM Q_x alignment). RSM scans suggest KTO films on DSO had partial strain (slight RSM Q_x misalignment).

Conclusions

This study has shown a successful growth of KTO using MBE, comparable crystallinity and differing surface character with e-beam and sub-oxide Ta heating methods, as well as full strain with (110) GSO substrates and partial strain with (110) DSO substrates.

Compared to pulsed-laser deposition, MBE grown KTO exhibited better crystallinity, however different GSO substrates were used [4].

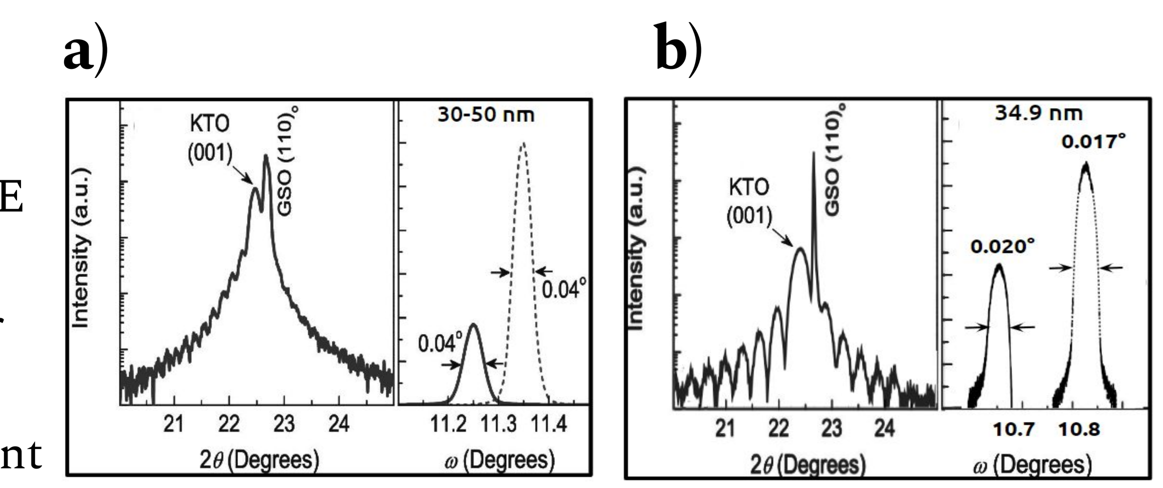
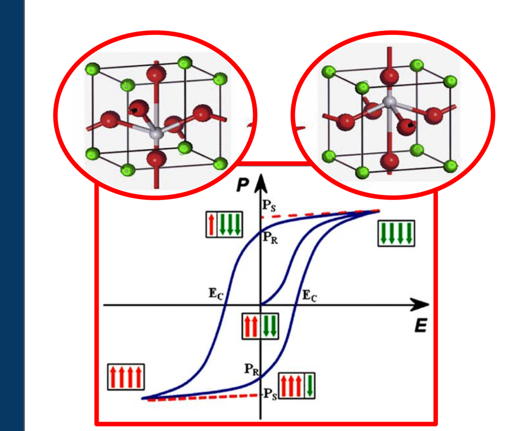


Figure 3: Comparison of MBE and PLD grown KTO through 2θ scans and rocking curves. a) PLD [4]. b) MBE.



Future Work

- Additional RSM analyses with thinner films (further knowledge regarding compressive strain behavior and limitations)
- Ferroelectric behavior of MBE KTO thin films testing (point toward the usability/application of the material)

Acknowledgements

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References

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