

Tunable Insulator-Metal transition in Epitaxial VO₂ thin film *via* strain and defect engineering

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Exposure of (110) plane with respect to (020) out of plane, as shown in Figure S1(a) shows a much better response to X-Ray Diffraction compared to S1(b), which accounts for Phi scan of (110) plane with respect to (002) out of plane.

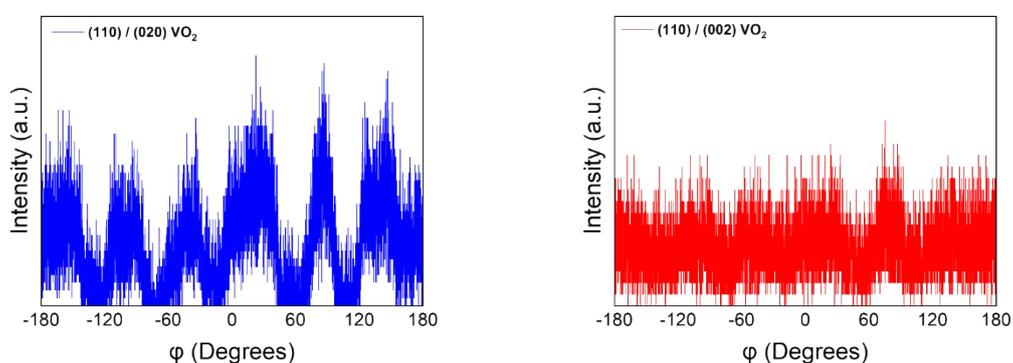


Figure S1 – The Phi scan results of the (110) plane of VO₂, assuming (020) as out of plane orientation in (a), and (002) out-of-plane orientation in (b). The results confirm the (020) out-of-plane orientation, as the (a) is of much better quality

A shift to higher wavelengths signifies lower band gap, the metallic rutile phase being more stable. This correlates well with the XRD results showing more compressive strain along the b-axis present in the film grown at 550°C. The R-T analysis showed the T_c for the VO₂ film grown at 500°C to be 65°C (lowest among all the VO₂ films grown in this study), agreeing with the Reflectivity analysis presented in this article. The direct band gap for the three samples were obtained using the Kubelka–Munk model. $[F(R)hv]^2$ was plotted on the x-axis, and the intercept of the tangent to the plot on this axis was considered as the direct band gap of the sample, where $F(R) = (1 - R)^2/2R$ and hv is the photon energy.¹

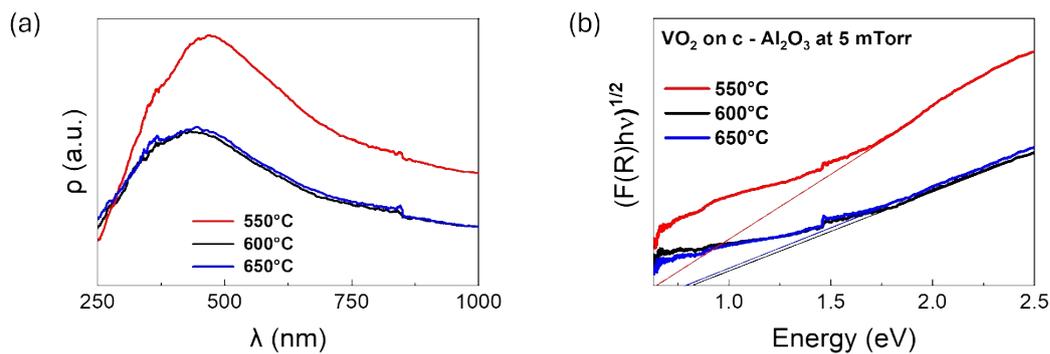


Figure S2 – UV-Vis-Spectroscopy plots for the three VO₂ films grown on (0001) sapphire at 5 mTorr oxygen pressure, with varying substrate deposition temperature (a) is the reflectance plot, while its derivation obtained using the Kubelka-Munk model is shown in (b)

References

- 1 K. Brajesh, S. Ranjan, R. Kumar, R. Gupta, A. Dixit and A. Garg, *Journal of the American Ceramic Society*, 2023, **106**, 6769–6777.