Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary information to 'Atomic Layer Deposition of Vanadium Oxides for Thin-film Lithium-Ion Battery Applications'

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In-situ XRD

To demonstrate the formation of the phases that are examined electrochemically, in-situ X-ray diffraction is done during the formation of the phases. Table 1 shows an overview of the atmosphere, temperature and initial film conditions used to obtain all phases between VO_2 and V_2O_5. Figures 1 to 6 show the resulting isXRD plots on the current collector substrate, demonstrating the successful phase formation.

Table 1: Conversion paths from the as-deposited films to their crystallised and oxidized forms, on the Pt-substrate.

Phase	ALD reactant	Ambient	Temperature (°C)
VO_2 (B)	O_3	He + 3.7 Pa O_2	420
VO_2 (M1)	H_2O	He + 18 Pa O_2	450
V_6O_{13}	O_3	He + 3.7 Pa O_2	550
V_4O_9	H_2O	Ambient air	356
V_3O_7	O_3	He + 48 Pa O_2	560
V_2O_5	H_2O or O_3	Ambient air	500

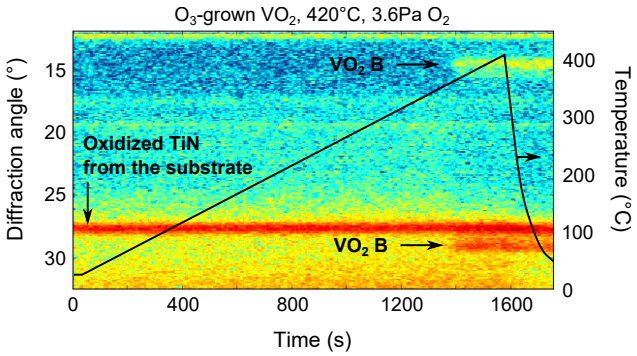

Figure 1: In-situ XRD during the oxidation of ozone-grown amorphous VO_2 to crystalline VO_2 B on the Pt substrate. The temperature was ramped linearly to 420 °C in an ambient consisting of He + 3.6Pa O_2.

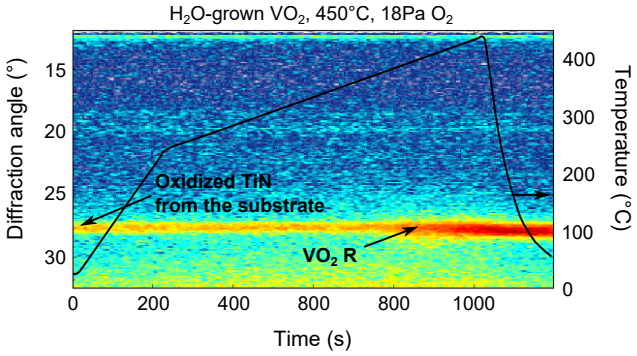

Figure 2: In-situ XRD during the oxidation of water-grown amorphous VO_2 to crystalline VO_2 M1 on the Pt substrate. The temperature was ramped to 450 °C in an ambient consisting of He + 18Pa O_2.

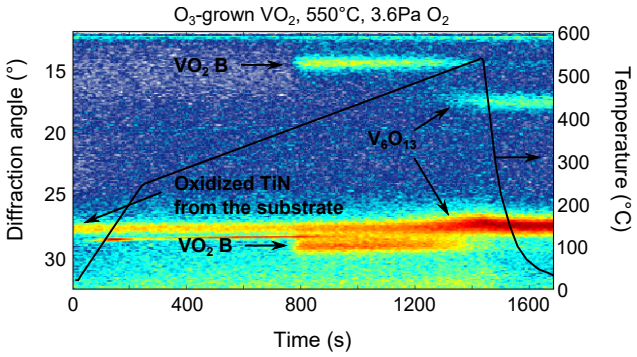

Figure 3: In-situ XRD during the oxidation of ozone-grown amorphous VO_2 to crystalline V_6O_{13} on the Pt substrate. The temperature was ramped to 550 °C in an ambient consisting of He + 3.6Pa O_2.

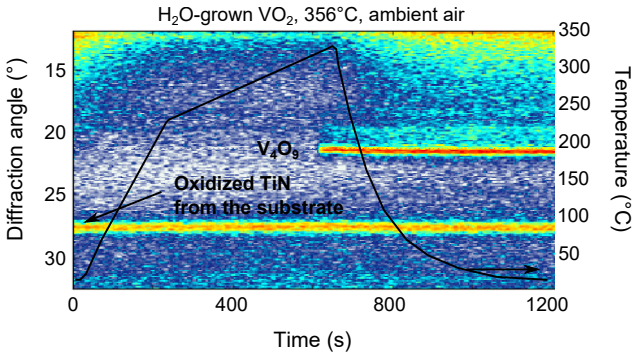

Figure 4: In-situ XRD during the oxidation of water-grown amorphous VO_2 to crystalline V_4O_9 on the Pt substrate. The temperature was ramped to 356 °C in ambient air.

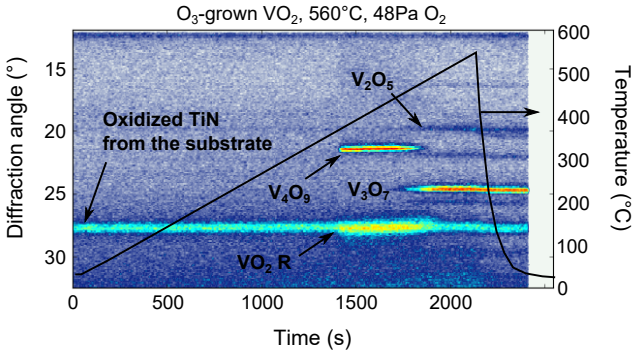

Figure 5: In-situ XRD during the oxidation of ozone-grown amorphous VO_2 to crystalline V_3O_7 on the Pt substrate. The temperature was ramped to 560 °C in He + 48Pa O_2.

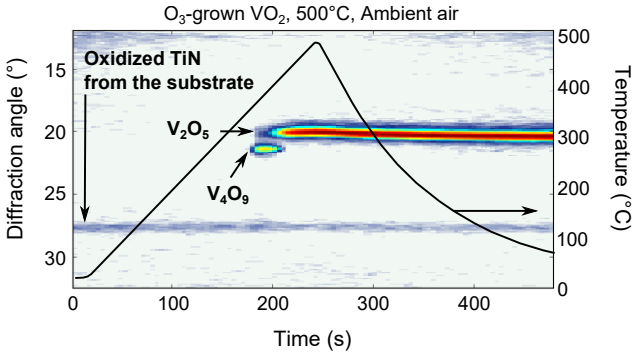

Figure 6: In-situ XRD during the oxidation of ozone-grown amorphous VO_2 to crystalline V_2O_5 on the Pt substrate. The temperature was ramped linearly to 500 °C in ambient air.

Cyclic voltammetry on the Pt substrate and the VO_2 M1 phase

Figure 7 shows the cyclic voltammograms of the VO_2 M1 film and of the uncoated Pt substrate. Some similarities can be seen between the peak positions of both cyclic voltammograms. Furthermore, galvanostatic charge-discharging showed the film displayed almost no storage capacity, indicating almost no bulk energy storage, and thus mostly surface-related electrochemical activity is present for these films.

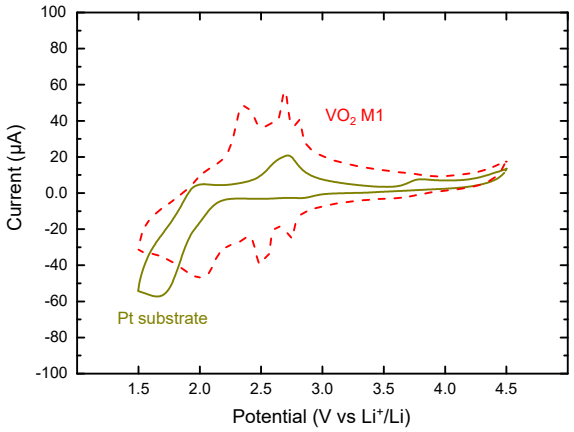

Figure 7: Cyclic voltammetry on the Pt substrate and VO_2 M1 thin film, performed at $10\,\mathrm{mV\,s^{-1}}$ in a 3-electrode setup with lithium as counter and reference electrodes, and 1M $LiClO_4$ in PC as electrolyte.