Supporting information for

Mechanistic insights on electronic properties and electronic/atomic structure aspects in orthorhombic $SrVO_3$ thin films: XANES-EXAFS study

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Experimental details:

X-ray reflectivity (XRR) measurements were carried out by using the high resolution XRD machine (ATX-G Rigaku). An assembly of two-channel-cut Ge (220) crystal was employed to collect the XRR data from all of the thin films. To obtain the thickness, roughness and density of the film material, the XRR data was simulated with *global-fit* software package. Cross-sectional SEM images from the samples were collected by using the FEI/SEM (Helios NanoLab 600), operated at 5 KV.

Results and discussion:

(i) XRR studies

Fig. S1 shows the XRR data (open circles) along with simulated curves (solid red color line). The calculated density, thickness and roughness of the films are provided in each panel of figure. During the fittings of XRR data of pristine and annealed samples, SiO_2 and $SrVO_3$

layers were stacked to simulate the experimental data. The film thickness and density of SiO_2 and $SrVO_3$ layers were gradually decreased in case of annealed thin films. While comparing the XRR results and obtained parameters of all of the samples, it is noticeable that the density of film material is increased and the thickness is decreased upon increasing temperature. This may be due to the densification of film material upon increasing the annealing temperature. Furthermore, the high temperature annealed samples have exhibited higher roughness because of diverse island growth during the heat treatment and can be seen in the cross-sectional SEM results.

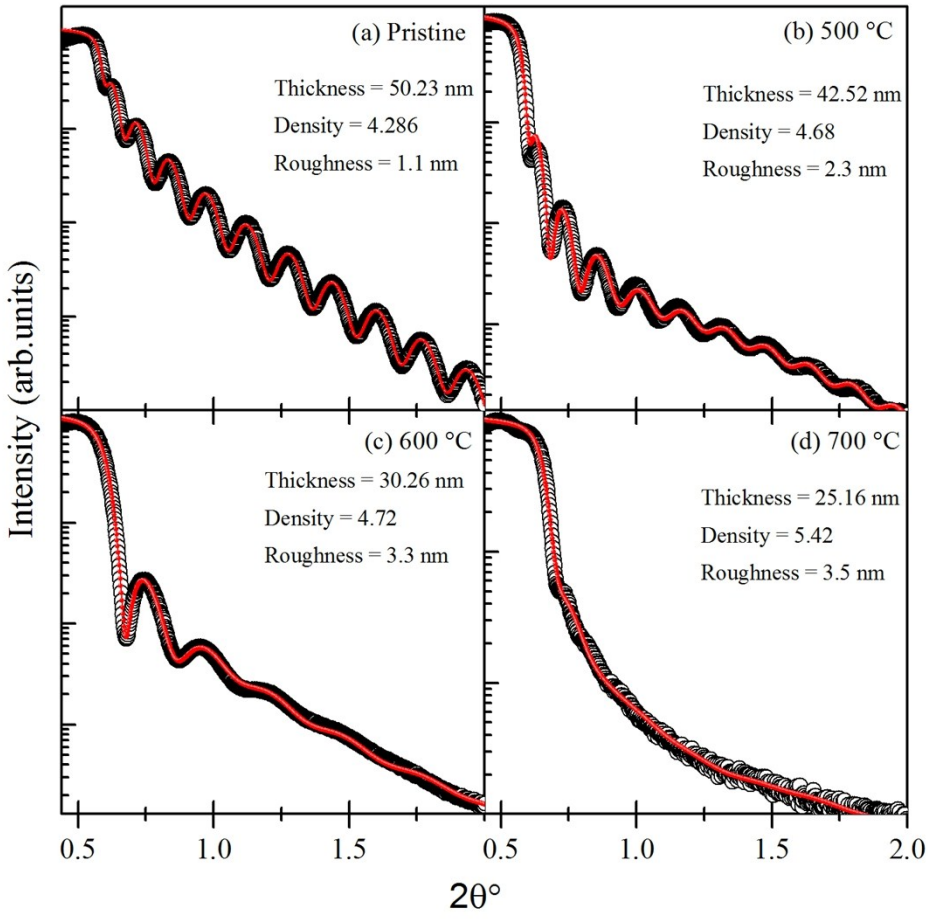

Fig.S1. Experimental and simulated XRR curves of (a) pristine, (b) 500 °C, (c) 600 °C and (d) 700 °C annealed $SrVO_3$ thin films. Film thickness, density and roughness values are also provided in each panel of figure.

(ii) Cross-sectional SEM study

To understand the film thickness and layered structure in the pristine and annealed $SrVO_3$ thin films, systematic, cross-sectional SEM images were collected and are presented in the Fig. S2. It is noticeable from the Fig. S2 (a) that the pristine $SrVO_3$ thin film exhibits few distinct layers. The SiO_2 layer is visible, just above the Si substrate, with thickness of ~ 12 nm (marked by red color arrow).

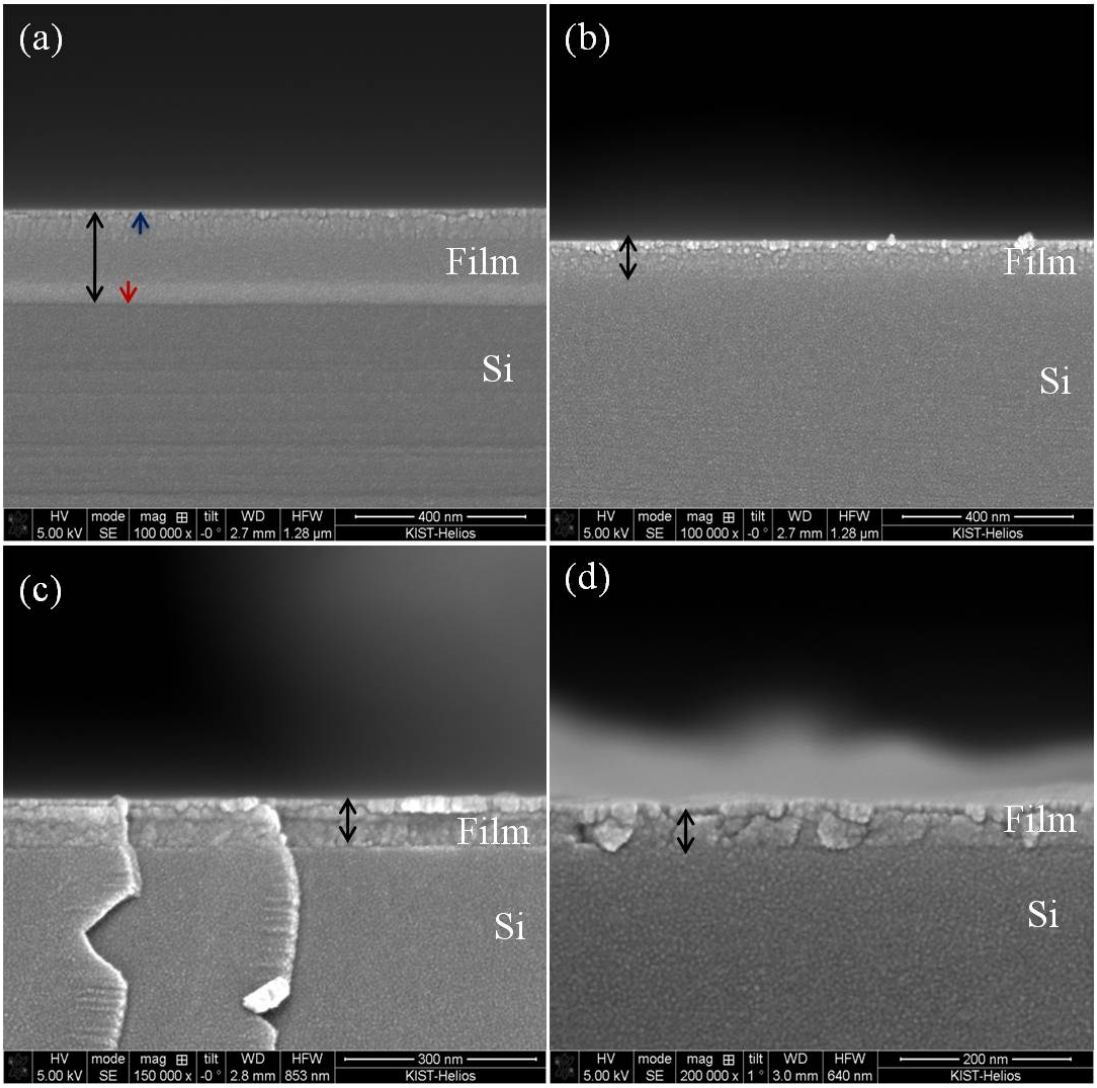

Fig.S2. Cross-sectional SEM images of (a) pristine, (b) 500 °C, (c) 600 °C and (d) 700 °C annealed $SrVO_3$ thin films on Si substrates.

Formation of SiO_2 layer is obvious because of rapid oxidation of Si substrate surface during the deposition process and has been reported in several oxide thin films (see ref. 7-10 and discussion therein). After the SiO_2 layer, $SrVO_3$ thin film is visible with disparate layers. The upper layer thickness is ~21 nm (marked by blue arrow) and the middle layer (between the red and blue arrows) thickness is ~56.3 nm. It is interesting to note that the thickness of $SrVO_3$ gradually decreased with increasing the annealing temperature. Film thickness of 500 °C, 600 °C and 700 °C annealed thin film is 42.4 nm, 36.2 nm and 29.7 nm, respectively. Decrease in the overall film thickness may be due to the densification of film material or eradication of SiO_2 layer and has been evidenced in the XRR studies. It is also visible from the images that some irregular island growth of material is exist in the annealed thin films (especially in 600 °C and 700 °C annealed thin films) which may cause high roughness or degradation in film quality. Our XRD results have shown a little decrease in the peak intensity, suggesting scarcity in the film quality of 600 °C and 700 °C annealed samples, which may be originate by the inter-layer or surface-interface layer diffusion processes. However, our XRD results have not shown formation of Si-$SrVO_3$ kind of mixed phases and strengthen the sustainability of orthorhombic phase, even at high temperature annealing.

(iii) V K-edge EXAFS simulation and structural parameters

Table 1. Structural parameters obtained from the V K-edge EXAFS fittings (coordination number (N), bond distance (R), edge-energy correlation (ΔE) and Debye–Waller factor (ss). The values in the parenthesis represent error therein.

Sample name	Shell	N	R (Å)	ΔE (eV)	ss($Å^{-2}$)
VO_2 reference	V-O1	4	1.56(8)	3.0	0.001(5)
	V-O2	2	1.80(4)	3.0	0.009(1)
	V-V	2	2.25(8)	3.0	0.048(8)
Pristine $SrVO_3$	V-O1	1	1.54(3)	1.0	0.004(2)
	V-O2	2	1.71(8)	1.0	0.006(2)
	V-V	1	2.56(2)	1.0	0.012(5)
500 °C $SrVO_3$	V-O1	1	1.54(1)	1.0	0.007(1)
	V-O2	2	1.71(1)	1.0	0.006(9)
	V-V	1	2.55(1)	1.0	0.003(1)
600 °C $SrVO_3$	V-O1	1	1.54(7)	1.0	0.003(2)
	V-O2	2	1.64(4)	1.0	0.001(3)
	V-V	1	2.48(4)	1.0	0.046(6)
700 °C $SrVO_3$	V-O1	1	1.47(1)	1.0	0.005(9)
	V-O2	2	1.63(2)	1.0	0.001(5)
	V-V	1	2.51(1)	1.0	0.002(3)