

Multitarget Reactive Magnetron Sputtering Towards the Production of Strontium Molybdate Thin Films

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The survey spectra of all samples were found to be similar. The spectrum of sample #260719 (14.8% Mo) in Figure S1 shows a more pronounced Sr 3d peak due to a higher strontium concentration.

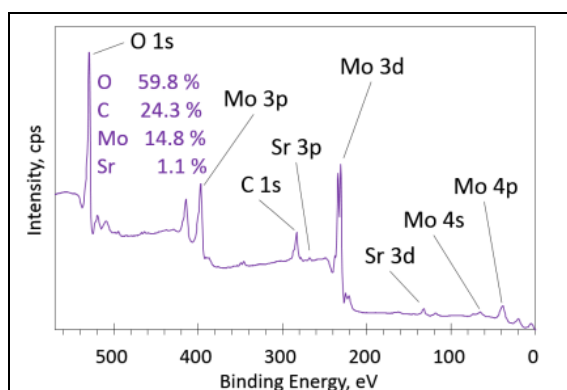


Figure S1. Survey XPS spectrum of the film containing 14.8 at.% Mo.

A comparison of normalized-intensity high-resolution Mo 3d XPS spectra before deconvolution for all Mo concentrations is presented in Figure S2. Differences in the Mo 3d spectra in this picture indicate the presence of lower-valence states of molybdenum for some samples.

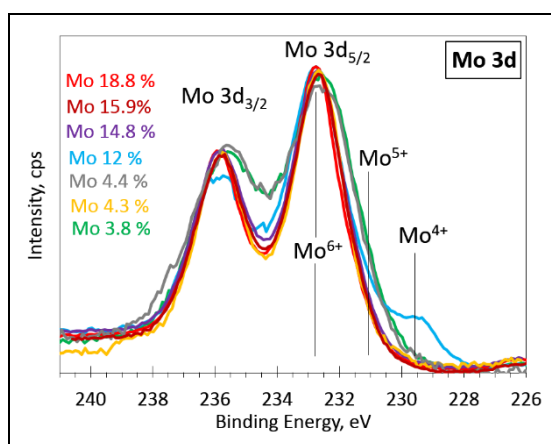
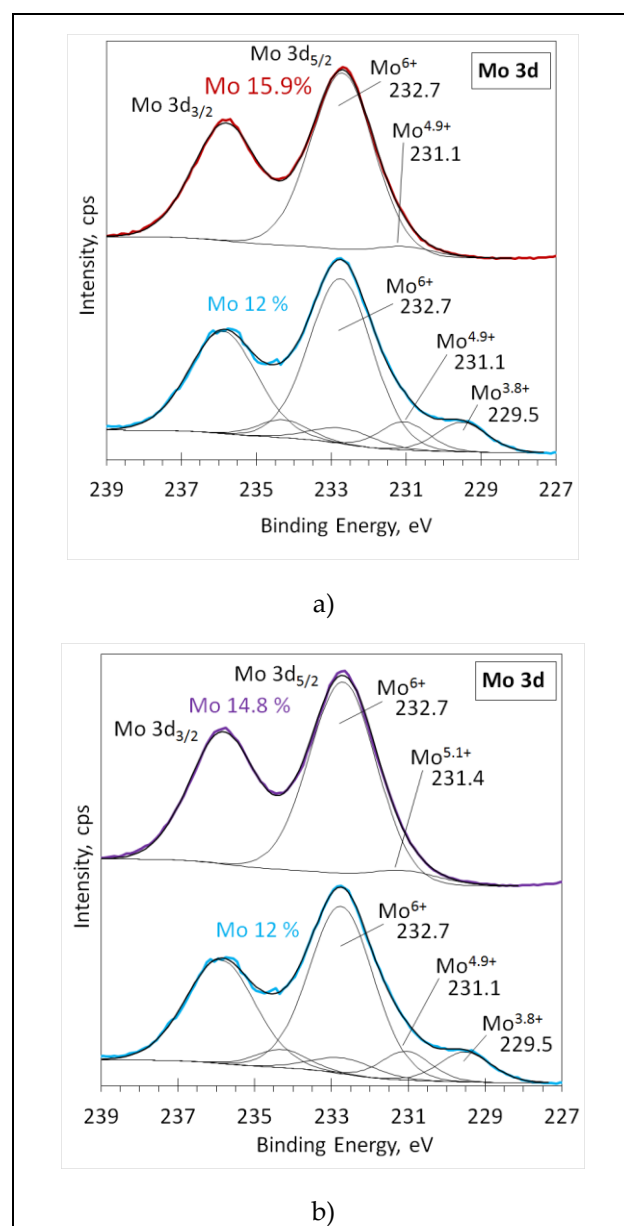
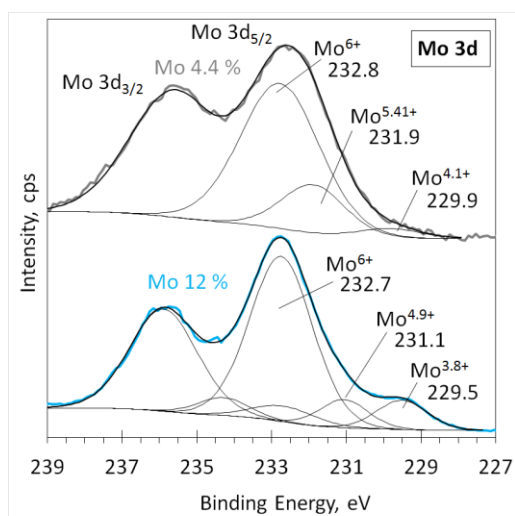


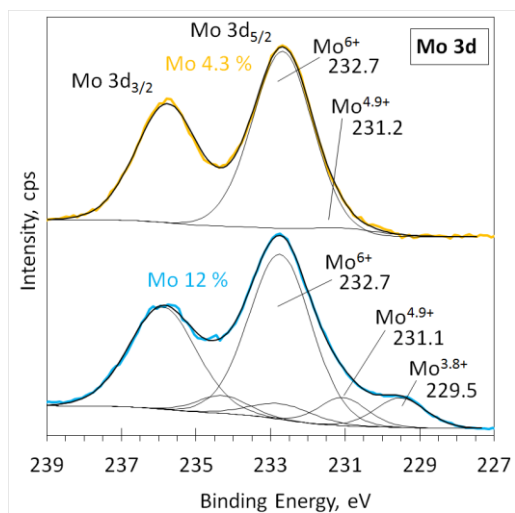
Figure S2. Comparison of normalized-intensity high-resolution Mo 3d XPS spectra for samples with various Mo concentrations.

A comparison of high-resolution Mo 3d XPS spectra for all samples with that of sample #310719 (Mo 12.0%) is presented in Figure S3. The Mo 3d spectrum of sample #310719 was used as a reference since it clearly exhibited the presence of lower-valence peaks of molybdenum oxide. For all samples (except sample #310719), only the Mo 3d_{5/2} peak fitting is shown in this picture for clarity.

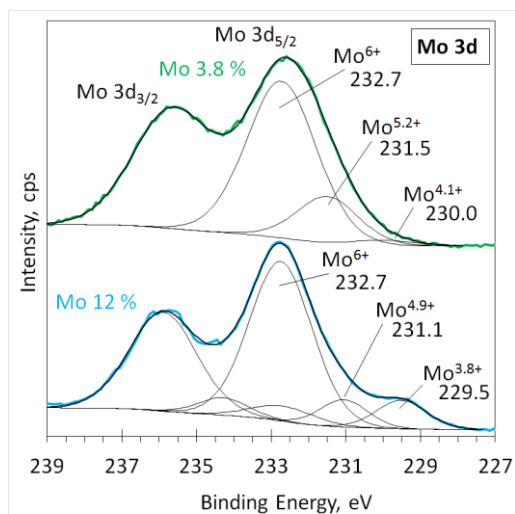




c)



d)



e)

Figure S3. Comparison of high-resolution Mo 3d XPS spectra for all samples with those of sample #310719 (12.0% Mo).

Normalized Sr 3d spectra for samples with different Mo concentrations are presented in Figure S4. From this picture, one can see that the Sr 3d spectra for these samples are very similar. The deconvolution of all spectra resulted in two overlapping peaks of a typical Sr 3d spin-orbit doublet. The peak fitting results are shown only for the sample containing 3.8% Mo (Figure S4, spectrum at the bottom), not to overload the figure.

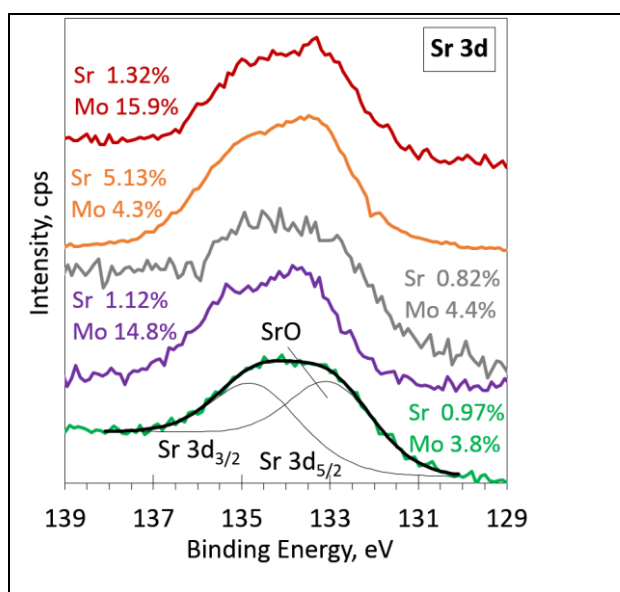


Figure S4. Normalized-intensity high-resolution Sr 3d XPS spectra for samples with different Mo concentrations.

Comparison of the oxygen XPS spectra in the O 1s region (Figure S5) showed negligible differences between samples. Deconvolution of all spectra resulted in two peaks – a high-intensity peak at approximately 530.5 eV and a lower-intensity peak at approximately 532.3 eV. We attributed the main peak at 530.5 eV to oxygen-molybdenum bonds – its position corresponds to the known peak position for different molybdenum oxides: MoO₃ (530.65 eV), MoO (530.5 eV), and MoO₂ (530.45 eV) [11]. It should be considered that the known binding energy values for the O-C=C bonds are very similar (531.0 – 531.4 eV) [11], and the peaks for these bonds could overlap with the main peak. The peak of lower intensity at ca. 532.3 eV may be attributed to the C-O-C bonds (532.8 eV) with a possible overlap of the O-H bonds (533 eV) [11,12] from atmospheric contaminants. The peak fitting is shown only for the sample containing 14.8% Mo for clarity (Figure S5, spectrum at the bottom).

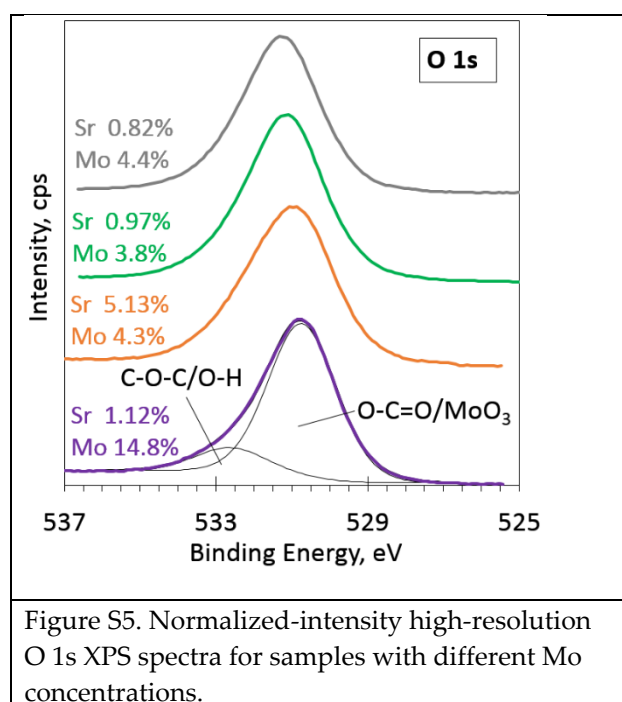


Table S1. Relative concentration of Mo bonds for all samples calculated by means of spectra deconvolution.

Mo bond	#140819	#150819	#260719	#310719	#020819	#120819	#250719
Mo ⁴⁺ , %	0	0	0	11.2	2.4	4.0	0
Mo ⁵⁺ , %	10.1	5.7	11	10.2	20.3	20.3	5.3
Mo ⁶⁺ , %	89.9	94.35	89.0	78.6	77.2	75.7	94.7

The XRD pattern of different samples and the Al₂O₃ substrate are shown in Figure S6. In the XRD patterns of samples #260719, #310719, #020819 and #120819 no visible peaks corresponding to molybdenum oxide were detected, and only substrate-related peaks of Al₂O₃ were identified.

