Supplementary Information

Growth Mechanism of [100]-Oriented TaON Film through an Endotaxial Transformation from a (012)-$LiTaO_3$ Single Crystal Substrate

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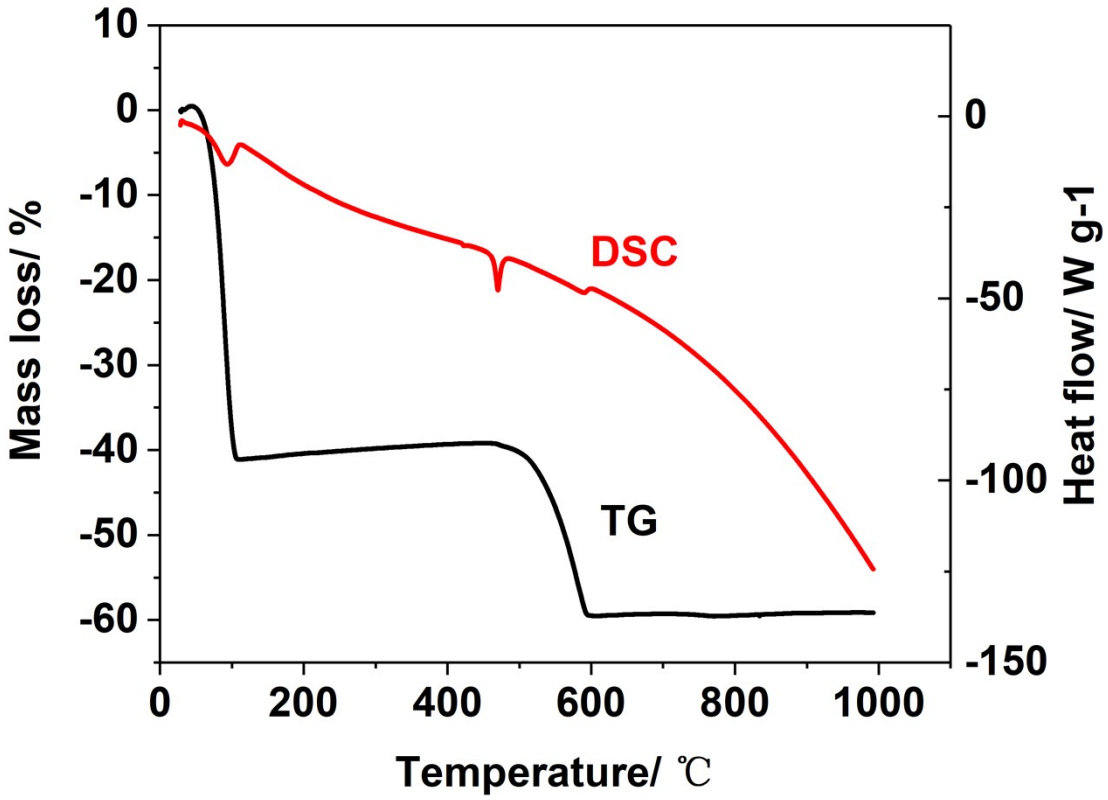

Fig. S1 TG/DSC of the raw materials $LiOH \cdot H_2O$.

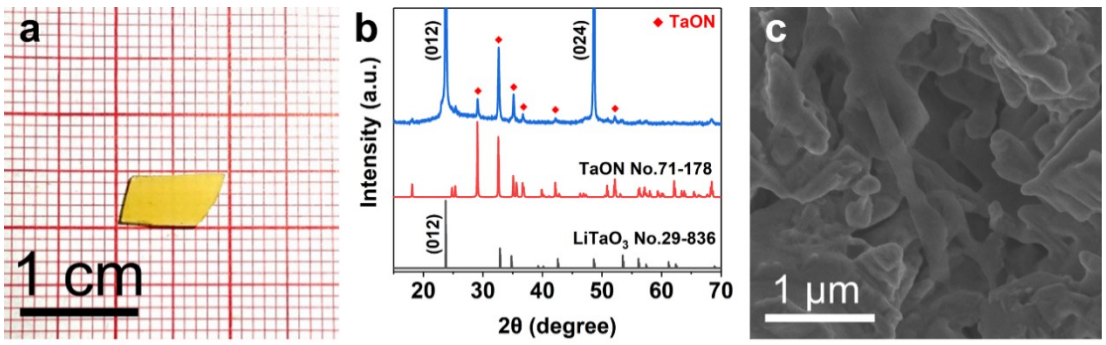

Fig. S2 (a) The photograph, (b) the XRD patterns and (c) the SEM image of the TaON films grown on the (012) surface of $LiTaO_3$ single crystal with only NH_3 gas.

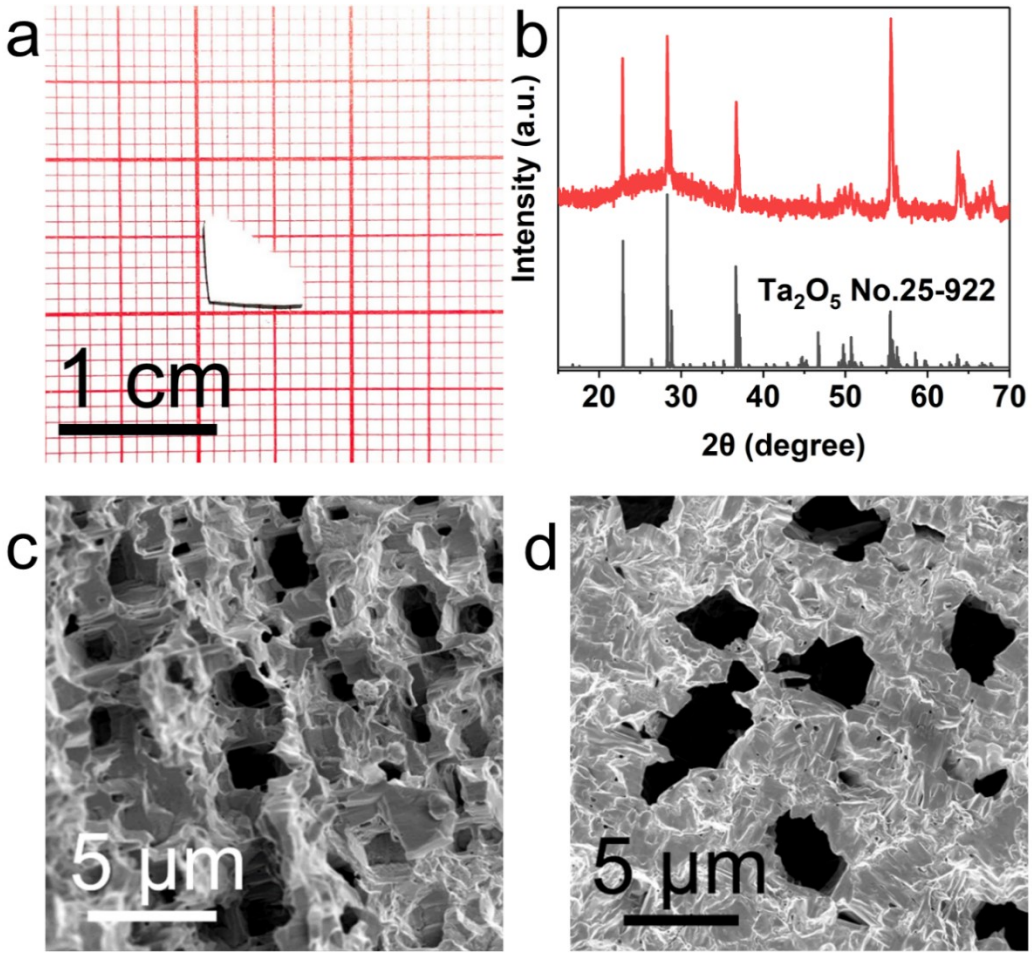

Fig. S3 (a) Photograph, (b) XRD patterns and SEM images of the (c) front and (d) back surface of [012]-$LiTaO_3$ single crystal substrate are treated at high temperature with Ar/CCl_4 flow (without NH_3). The gray pattern in (b) is a reference XRD pattern shown for comparison.

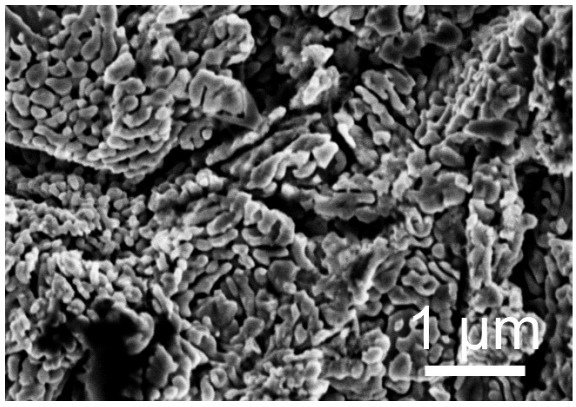

Fig. S4 SEM image of TaON films obtained at 600 °C after cleaning by rinsing in deionized water.

Table S1. ICP was used to measure the content of metal Li in different solutions.

Solution	The elemental concentration (mg/L)
Clean the tube furnace wall (600 ℃)	1.70
Clean the tube furnace wall (700 ℃)	81.17
Clean the tube furnace wall (800 ℃)	110.20
Clean the films and the abstracts (600 ℃)	6.07
Clean the films and the abstracts (700 ℃)	79.50
Clean the films and the abstracts (800 ℃)	95.42
Clean the tube furnace wall (in comparative experiments)	148.90

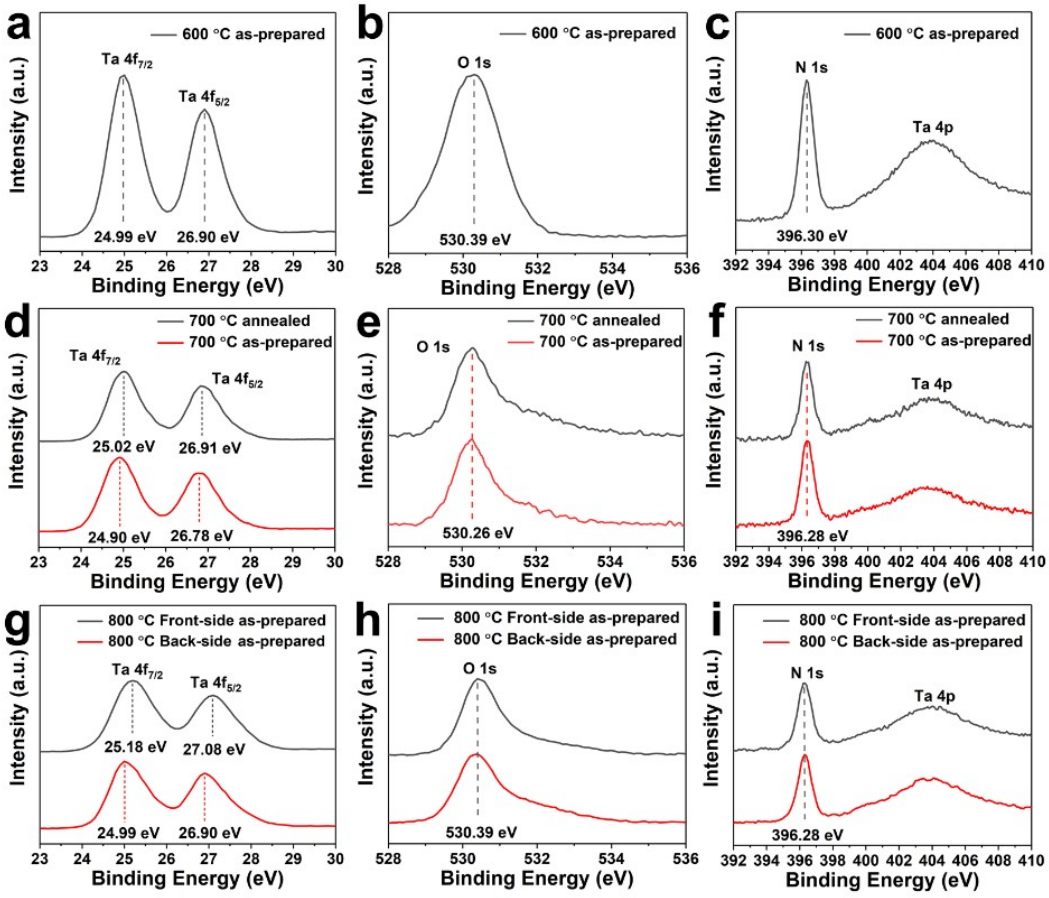

Fig. S5 (a) The Ta 4f, (b) O 1s and (c) N 1s XPS spectra of the as-prepared film obtained at 600 °C. (d) The Ta 4f, (e) O 1s and (f) N 1s XPS spectra of the as-prepared films obtained at 700 °C before and after annealing treatment. (g) The Ta 4f, (h) O 1s and (i) N 1s XPS spectra of the front and back sides of the as-prepared films obtained at 800

°C.

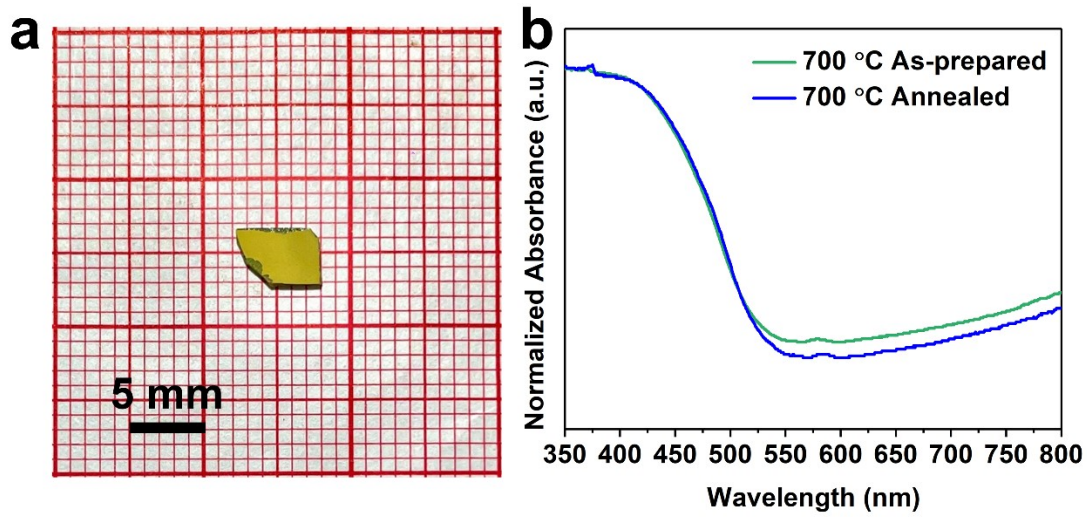

Fig. S6 (a) Photograph of the film obtained at 700 °C after annealing treatment. (b) The UV-Vis absorption spectra of the films obtained at 700 °C before and after annealing treatment.

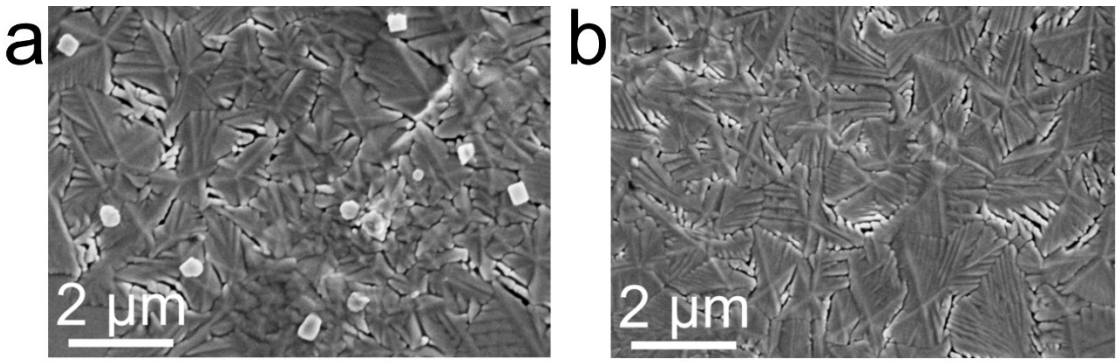

Fig. S7 SEM images of the substrates after 800 °C reaction before (a) and after cleaning (b).

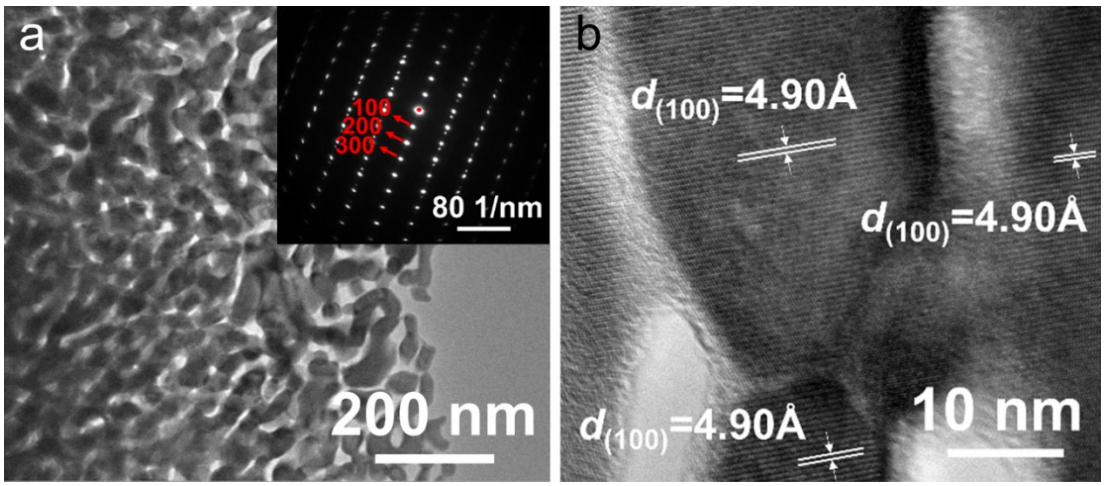

Fig. S8 (a) The TEM and (b) HR-TEM image of the back of the [100]-oriented TaON films after ion thinning. The SEAD of this region is shown in the upper right in (a).

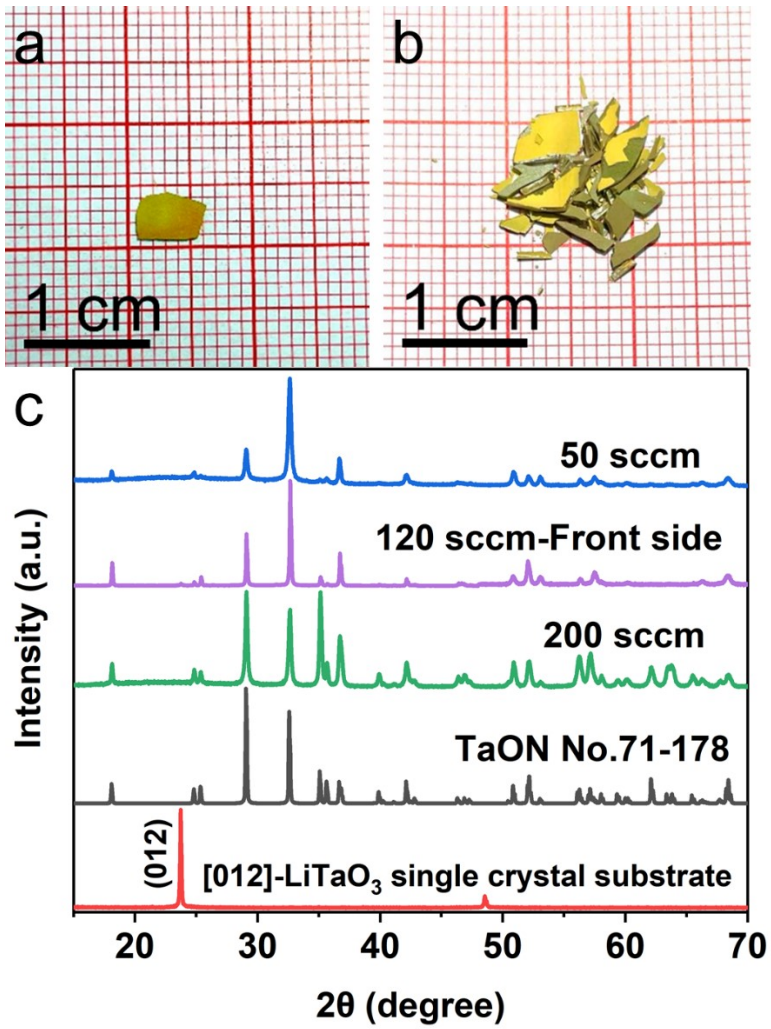

Fig. S9 Photographs of the nitridation products prepared with an (a) 50 sccm and (b) 200 sccm flow of CCl_4 in Ar. XRD patterns of the nitridation products prepared with different CCl_4 flow rates in Ar. For comparison, reference XRD patterns are also shown.

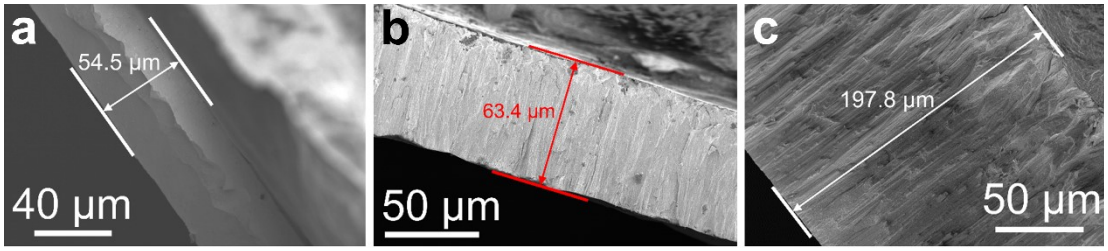

Fig. S10 SEM images of the cross-sections of the TaON films prepared via CCl_4-assisted high temperature nitridation with reaction times of (a) 5 h, (b) 10 h, and (b) 20 h.

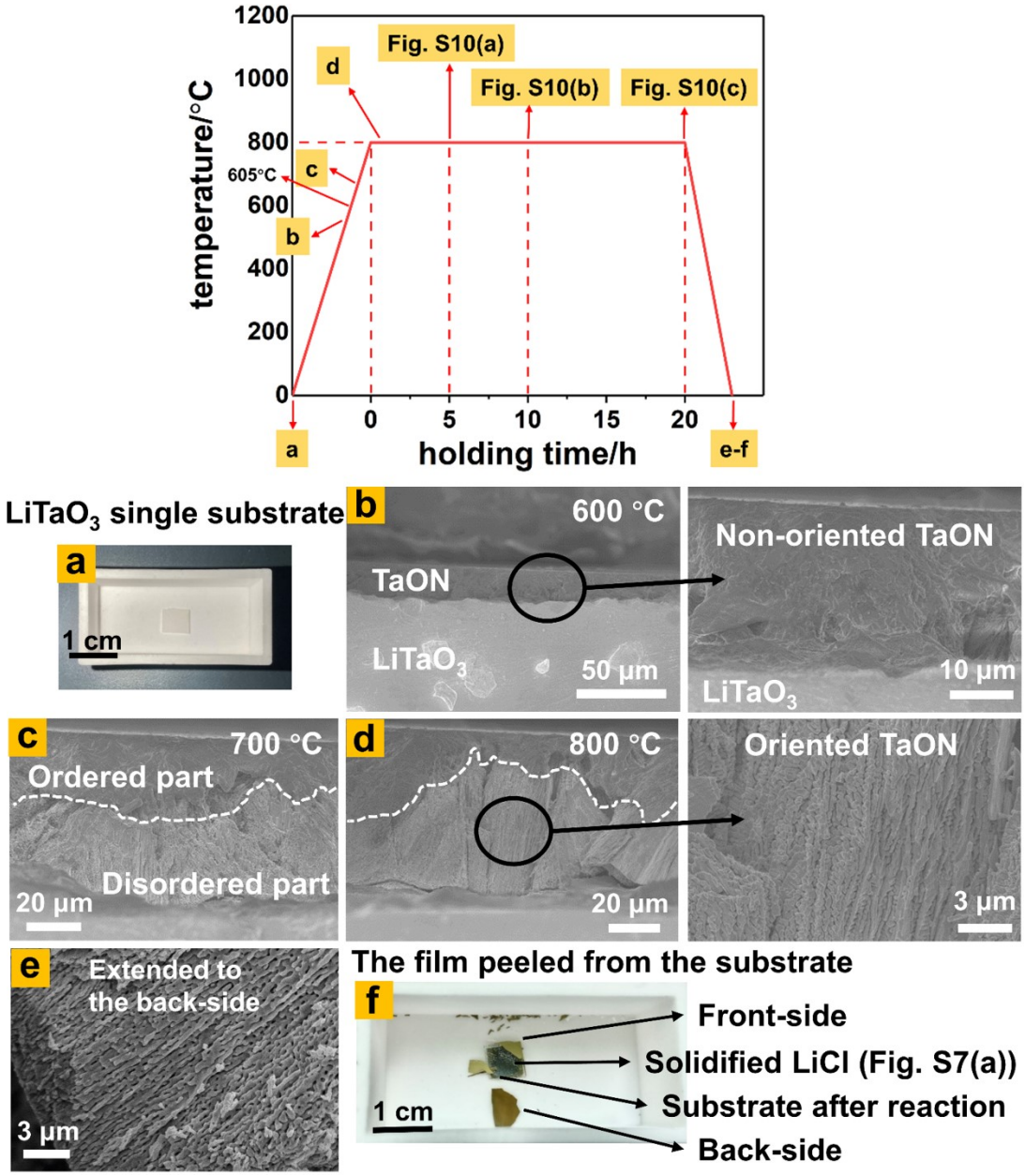

Fig. S11 SEM images of the cross-sections and photographs for TaON films evolving with time.