# Highly reversible Li-ion (de)intercalation to metastable $\beta$-$MoO_3$

**Tokyo Tech., Dept. Chem. Sci. Eng.[1], Material Research Center for Element Strategy[2]**

**°(M1) Shuxin Zhang[1], Takuto Soma[1], Tatsuya Yajima[1], Akira Ohtomo[1,2]**

**E-mail: zhang.s.ai@m.titech.ac.jp**

**[Introduction]** Molybdenum trioxide ($MoO_3$) has received much attention due to its intriguing physical properties and a wide variety of applications including batteries, gas sensors, and catalysts. $MoO_3$ is often found with two polymorphs: orthorhombic $\alpha$-$MoO_3$ with a layered structure and monoclinic $\beta$-$MoO_3$ with a $ReO_3$-derived distorted structure. However, it is difficult to grow metastable $\beta$-$MoO_3$ thin films, especially with both single phase and a single orientation. Here we report on epitaxial stabilization and Li-ion electrochemistry of pure $\alpha$- and $\beta$-$MoO_3$ films, demonstrating perfect phase control by using pulsed laser deposition (PLD) and Li-ion electrochemical cells. We found that $\beta$-$MoO_3$ indicated better reversibility and durability for Li-ion (de)intercalation process compared to $\alpha$-$MoO_3$.

**[Experiment]** Epitaxial $MoO_3$ films were grown on (100) $SrTiO_3$ (STO) and (100) $(LaAlO_3)_{0.3}$-$(SrAl_{0.5}Ta_{0.5}O_3)_{0.7}$ (LSAT) substrates by using PLD. The Li-ion electrochemical reactions were performed using a standard three-electrode system [1].

**[Results and discussion]** Figure 1 shows XRD patterns for the $\alpha$-$MoO_3$ film on STO and the $\beta$-$MoO_3$ film on LSAT. Note that the *a*-axis-oriented and single-phase $\beta$-$MoO_3$ thin film was obtained for the first time. Figure 2 shows room-temperature cyclic voltammetry (CV) curves for the $\alpha/\beta$-$MoO_3$|$LiClO_4$: PC|$LiCoO_2$/Al cells at a scan rate of 200 mV/s. The $\beta$-$MoO_3$ film exhibited high reversibility against repeated Li-ion (de)intercalations. We found another striking difference in the durability. Figure 3 shows XRD patterns for both of $\alpha$- and $\beta$-$MoO_3$ films taken after the Li-ion electrochemical reaction. The $\beta$-$MoO_3$ film showed only peak shift of *h*00 reflections, indicating a $\beta$-$Li_xMoO_3$ phase. On the other hand, the $\alpha$-$MoO_3$ film showed no reflection, indicated an amorphous phase. These results pave a way for further investigations into electrical conductivity control of $d^0$-insulator $MoO_3$.

[1] K. Yoshimatsu *et al.*, *Appl. Phys. Express* **9,** 075802 (2016).

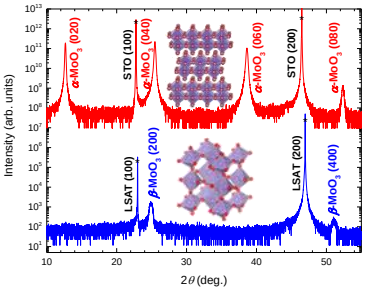


**Fig. 1** XRD patterns of $MoO_3$ films before electrochemical reactions.

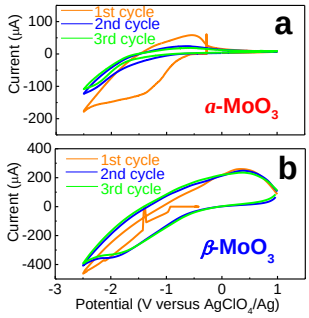


**Fig. 2** CV curves for $MoO_3$ films taken during repeated Li-ion electrochemical reactions.

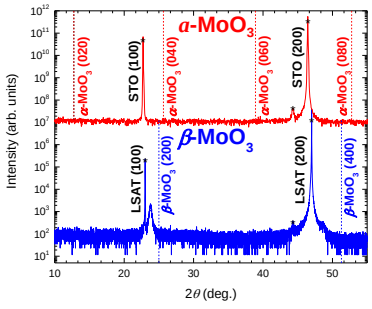


**Fig. 3** XRD patterns of $MoO_3$ films after electrochemical reactions.