

# X-ray photoelectron spectroscopy of partially oxidized ultrathin films of 4d refractory metals deposited by e-beam physical vapor deposition

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The X-ray photoelectron spectroscopy (XPS) spectra of electron-doped 4d transition metal oxides show multiple peaks due to the final-state screening effect of conduction carriers [1, 2]. Occasionally these ‘extra’ peaks get confused as originating from other oxidation states of the cation. The theoretical analysis of the XPS spectra of  $d^1$  and  $n$ -doped  $d^0$  transition metal oxides pointed out that such multiple peaks are not always originating from other ions but are intrinsic to the material [1].

We have grown ultrathin films of partially oxidized 4d refractory elements (Nb and Mo) on  $\text{SrTiO}_3$  (111) substrates by using e-beam physical vapor deposition. The samples were grown by varying the flow of oxygen from 0.00 to 0.30 SCCM (Samples: Nb\_0.00 to Nb\_0.30), which varied the pressure of the growth chamber from  $1 \times 10^{-11}$  to  $1.7 \times 10^{-6}$  mbar, respectively. The films were in contact with air before the XPS measurements to purposefully introduce native oxide  $\text{Nb}_2\text{O}_5$  [3]. The valence band and Nb 3d XPS spectra are shown in Fig. 1 (a) and (b) respectively. We performed a careful fitting of Nb 3d XPS spectra by considering the various  $\text{NbO}_x$  reported. Starting from Nb\_0.00 containing  $\text{Nb}^0$  and  $\text{Nb}^{5+}$  and the seemingly fully oxidized Nb\_0.30 containing  $\text{Nb}^{5+}$ , we estimated the positions of satellite peaks originating from the screening effect of conduction carriers. We also noticed a dependence of this satellite peak upon the carrier density near the Fermi level. A comparison with the Nb 3d XPS spectra of conducting perovskite  $\text{SrNbO}_3$  and insulating perovskite  $\text{AgNbO}_3$  (gathered from other projects) provided further proof for this argument. We observed a similar effect when this experiment was repeated on  $\text{MoO}_x$ . This work provides experimental confirmation of the final-state screening effect in electron-doped all oxides of  $\text{BO}_x$  ( $\text{B}=\text{Nb}$  and  $\text{Mo}$ ).

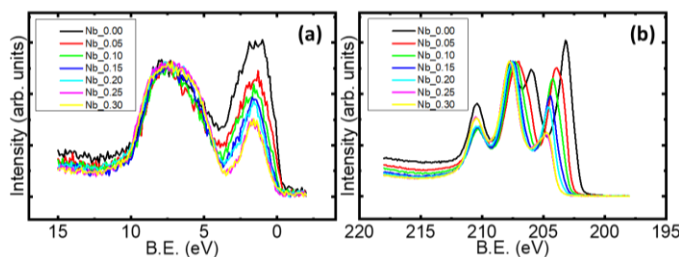


Fig. 1 The XPS spectra of (a) valence band and (b) Nb 3d of  $\text{NbO}_x$  films grown under different flows of oxygen (Sample code Nb\_X implies X SCCM of oxygen)

## References

- [1] Lin, C., et al., Final-state effect on x-ray photoelectron spectrum of nominally  $d^1$  and  $n$ -doped  $d^0$  transition-metal oxides. *Physical Review B*, 2015. 92(3): p. 035110.
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