Depth profile of Nb in anatase $Ti_{1-x}Nb_xO_2$ thin films grown by mist chemical vapor deposition method

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[Introduction] Niobium-doped anatase titanium dioxide ($Ti_{1-x}Nb_xO_2$: TNO) has gained much attention due to its transparent conducting properties.[1] The fabrication of TNO thin films has been mainly studied using vacuum physical vapor deposition (PVD). Recently, mist chemical vapor deposition (mist-CVD), which is a high-throughput, scalable, cost-effective, and environmentally-friendly process,[2] has also been applied to the fabrication of TNO thin films.[3] However, TNO thin films fabricated using mist-CVD show low transparent conducting properties,[3] compared with the ones deposited using PVD. We speculate that Nb doping mechanism plays an important role in the properties. Therefore, in this study, we aimed to reveal the depth profile of Nb atoms in TNO thin films fabricated by mist-CVD to understand the doping mechanism.

[Experiment] Titanium isopropoxide, $Ti(OC_3H_7)_4$, and niobium ethoxide, $Nb(OEt)_5$, were used as Ti and Nb sources, respectively. These two reagents were dissolved in ethanol wherein Nb atomic concentration was set to 0, 5, 10, and 20 atom%. The solution was atomized into mist droplets by 2.4 MHz ultrasonic transducers, and subsequently transferred by N_2 gas to the quartz tube placed in a furnace. A glass substrate was put inside the tube, and TNO thin films were deposited at 400 °C for an hour. Subsequently, the sample was annealed (600 °C) in a vacuum (2×10^{-3} Pa) for 30 minutes. The depth profiles of the amount of Nb and Ti were characterized using auger electron spectroscopy (AES).

[**Results**] We obtained anatase structure for all the films. Figure 1 shows the AES depth profile of the TNO thin films fabricated using sputtering and mist-CVD methods. Although the sputter-deposited TNO thin film shows a constant Nb/(Nb+Ti) atom ratio, the TNO thin films fabricated by mist-CVD show a considerable increase in the concentration of Nb atom toward the TNO surface. The mechanism will be discussed at the conference, along with the analysis of the chemical state and physical properties.

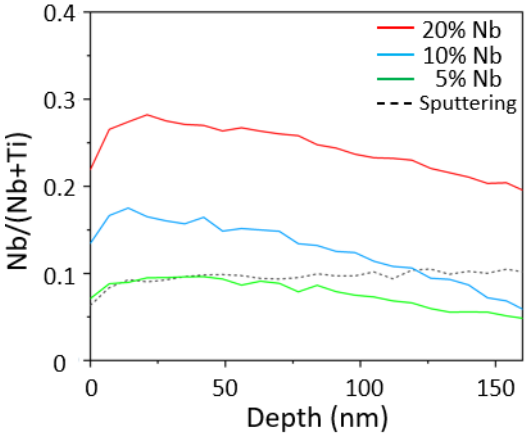

Figure 1. Auger electron spectroscopy depth profiles for the Nb/(Nb+Ti) atom ratio of thin films deposited at the different Nb atomic concentration in ethanol. The depth profile for the sputtered anatase Nb-doped TiO_2 thin films is shown as a reference.

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[3] DS. Bhachu *et al.*, *Adv. Funct. Mater.* 24 5075-5085 (2014).