Pulsed laser deposition and characterization of NbON epitaxial thin films

Univ. of Tokyo [1], KAST[2] ◦Vitchaphol Motaneeyachart[1], Yasushi Hirose[1,2], Atsushi Suzuki[1], Shoichiro Nakao[2], and Tetsuya Hasegawa[1,2]

E-mail: motaneeyachart@chem.s.u-tokyo.ac.jp

Baddeleyite-type tantalum oxynitride (TaON) has been extensively studied as a photocatalyst because of its high photocatalytic activity for water oxidation with maximum quantum yield of 10% under visible light irradiation [1]. However, high cost of Ta is a barrier for its practical uses. NbON is a possible alternative to TaON; Nb is more abundant than Ta and Nb^{5+} and Ta^{5+} have the same electron configuration and similar ionic radii. Furthermore, bandgap (E_g) of NbON is smaller than that of TaON [2] due to higher electronegativity of Nb than Ta [3]. In this study, we fabricated baddeleyite NbON, which is the most stable phase [4], and metastable rutile NbON in epitaxial thin film forms by nitrogen plasma assisted pulsed laser deposition (NPA-PLD) method and investigated their physical properties.

A $Nb_2O_{4.8}$ target was ablated by a KrF excimer laser (λ = 248 nm) under supply of nitrogen gas activated into radicals by a RF plasma source. Figure 1(a) shows θ-2θ XRD patterns of NbO_xN_y thin films deposited at various substrate temperatures (*Ts*) on yittria-stabilized zirconia (YSZ) (100) substrates, of which lattice constants match well with those of baddeleyite NbON [4]. The films grown at *Ts* ≤475 ºC were amorphous whereas the films grown at *Ts* ≥500 ºC showed *h*00 diffraction peaks of baddeleyite structure. Although the diffraction intensity increased with *Ts*, the film fabricated at 600 ºC was black in color due to nitrogen deficiency. More stoichiometric films were obtained by using two-step growth method, where a thin seed layer of NbO_xN_y was firstly grown at 600 ºC and then thick main layer was deposited on it at 500 ºC. The obtained films showed intense diffraction peaks (Fig. 1(a)) as well as yellow color with E_g of 2.3 eV (Fig. 1(b)). The chemical composition of the film was evaluated as $NbO_{0.89}N_{0.99}$.

In the presentation, we will also discuss the transport properties of the baddeleyite NbON thin films and epitaxial growth of metastable rutile NbON thin films. A part of this study was financially supported by CREST, JST.

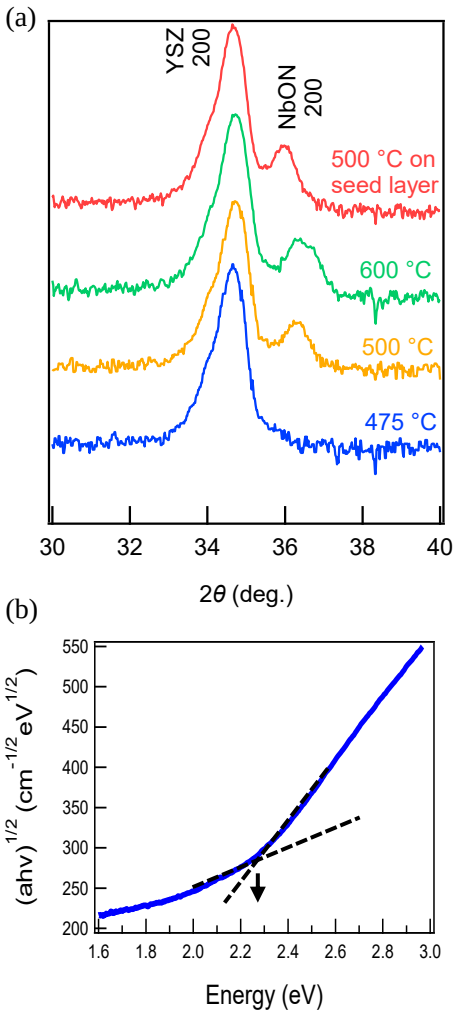

Figure 1. (a) θ-2θ XRD pattern of the baddeleyite NbON film grown on YSZ(100) substrate at various *Ts* = (475 – 600 ˚C). (b) Tauc plot of the baddeleyite NbON thin film assuming indirect band gap.

References

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