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Preparation of a single-phase TaO₂ thin film

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Rutile-type transition metal dioxides with a d^1 configuration such as VO₂ and NbO₂ attract much attention because of their metal-insulator transition at relatively high temperature (340 and 1080 K, respectively). TaO₂ is also a rutile-type metal oxide. Since it has a d^1 configuration (5 d^1 , Ta⁴⁺), one may expect it to show a meta-insulator transition as seen in VO₂ and NbO₂. So far few are reported on the physical property of TaO₂. This is mostly because TaO₂ is a metastable compound in a Ta-O binary system, and is difficult to be obtained as a single phase.

Oxidation and reduction approaches have been presented for preparation of TaO_2 . In the approaches, TaO_2 can be yielded but the product usually contains other Ta oxides such as Ta_6O , Ta_2O and Ta_2O_5 . Multiphase product makes it difficult for us to study the intrinsic transport property of TaO_2 . A main issue for research of this compound is therefore to find a way to stabilize only TaO_2 among Ta-O metastable and stable compounds.

One of the effective ways to obtain a metastable compound is to stabilize the crystal structure of the compound in a form of film by using a template substrate. For instance, a metastable α -Ga₂O₃ with a corundum structure is obtained as a thin film grown on a corundum Al₂O₃ substrate.¹ For TaO₂, it is expected that this metastable compound is stabilized in a thin film grown on a rutile-type substrate.

A rutile-type NbO₂ is a promising substrate from viewpoint of a lattice matching with TaO₂. In addition, NbO₂ thin films are grown epitaxially on Al₂O₃(0001) substrates using a pulsed laser deposition (PLD) technique. NbO₂ thin films can be used as a template layer for the TaO₂ film growth.

We prepared TaO₂ thin films using NbO₂ template layers on Al₂O₃(0001) substrates by a PLD method. Film thickness is 8 nm for NbO₂ template layer and 43 nm for TaO₂. XRD measurements found that the film is a single-phase tetragonal TaO₂ with an (100)-orientation (Fig. 1). Importance of structural stabilization for a single-phase TaO₂, and the structural and electrical properties of the film are presented.

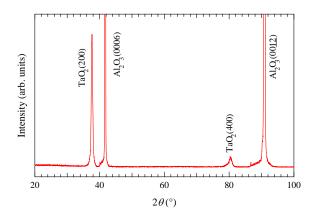


Fig. 1 XRD pattern of a TaO₂ thin film prepared using a NbO₂ template layer on Al₂O₃(0001).

[1] K. Kaneko, H. Kawanowa, H. Ito, and S. Fujita, Jpn. J. Appl. Phys. 51, 020201 (2012).