Epitaxial growth of bismuth oxyhalides thin films with mist CVD at atmospheric pressure

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Bismuth oxyhalides (BiO*X*, *X* = Cl, Br, I) are a series of layered tenary compounds with excellent photo-energy conversion applications, promising for photocatalysis and photovoltaics [1–2]. While the indirect bandgaps of 1.8, 2.6, 3.2 eV for *X* = Cl, Br, I, respectively, enable to harvest light from visible to ultraviolet region, the layered structure prevent effcient recombination of photo-excited electron and hole pairs [1]. In order to extract the full potential of these compounds, it is necessary to investigate quantitatively fundamental properties such as bandgap, optical absorption, and photoconductivity, by using single crystals. However, sufficiently large single crystals of BiO*X* have not been available so far. In this study, we developed facile growth route for epitaxial thin films of BiO*X*.

Bismuth oxyhalide epitaxial thin films were grown with mist chemical vapor deposition under atmospheric pressure, suitable for volatile elements such as bismuth [3]. N, N-dimethylformamide solution of corresponding BiX_3 was nebulized into microscale mists and transferred by N_2 gas onto $SrTiO_3$ (001) single crystal substrates heated at 250 − 450 °C. N_2 and O_2 gases were used for diluting the mist during the deposition of BiOCl and the other BiO*X*, respectively.

X-ray diffraction showed successful growth of BiO*X* (001) epitaxial thin films at optimum temperateure for each composition (Fig.1). Full width at half maximum of rocking curves around 003 peaks was less than 0.1° for all the BiO*X*, indicating good crystallinity (Fig. 2). The film morphology was highly dependent on the growth temperature, and the flat surface with step terrace structure was observed for each film at the optimum growth temperature (Fig. 3). Lower growth temperatures resulted in partial coverage of the films, while higher growth temperatures resulted in rough surface accompanied by degraded crystallinity.

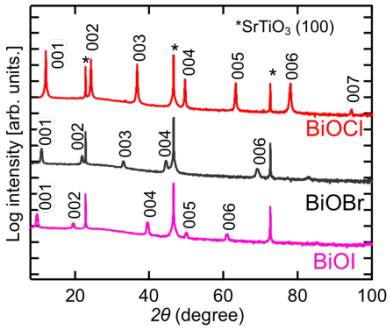

Fig. 1. X-ray diffraction *θ*-*2θ* patterns of BiO*X* thin films.

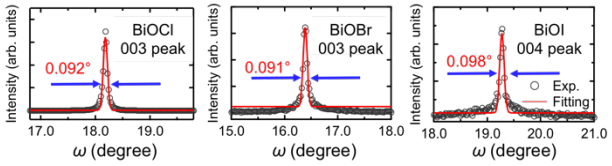

Fig. 2. Rocking curve of BiO*X* thin films.

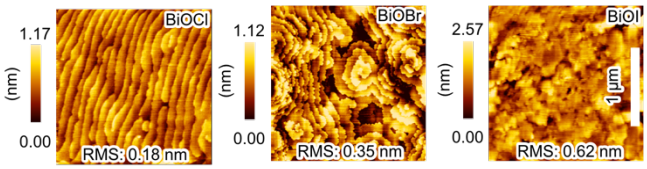

Fig. 3. Atomic force microscopy images of BiO*X* thin films.

Reference: [1] Y. Yang *et al.*, *Adv. Colloid Interface Sci.* **254**, 76 (2018). [2] R. Hoye *et al.*, *Adv. Mater.* **29**, 1702176 (2017). [3] Z. Sun *et al.*, *Cryst. Growth Des.* **19**, 7170 (2019).