Phonon modes of $CH_3NH_3PbBr_3$ hybrid perovskite thin film formed by sequential vacuum evaporation method

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1. Introduction

The exploration of a new physical property for various THz-based applications such as THz-wave sensing, modulation, and imaging devices, is one of the key challenges in the research of organic-inorganic hybrid perovskite materials. Such THz-based applications require a good, sensitive, and stable absorption property in the range of 0.5–2.5 THz. To achieve this property, candidate materials should possess regular and fixed phonon modes without any defect or impurity. For this purpose, $CH_3NH_3PbBr_3$, an organic-inorganic hybrid perovskite thin film produced by a sequential vacuum evaporation method [1] on a flexible PET substrate, was investigated in this study.

2. Experimental method

The $MAPbBr_3$ thin films were formed by the sequential vacuum evaporation (SVE) method. Firstly, $PbBr_2$ layer (100 nm) was evaporated with the deposition rate of 10 Å/s on Si, glass, and PET (Polyethylene terephthalate) substrates. Sequentially, MABr layer (300 nm) was evaporated with the deposition rate of 2.0 Å/s. [2] Finally, the grown films were post-annealed at 110 ℃ for 10 min and protected by ultra-thin PTAA ([poly[bis(4-phenyl)(2,4,6-trimethylphenyl)amine]]) layers (5 nm) spin-casted with 5 mg/4 ml of PTAA/chlorobenzene solution at 4 krpm. All samples were characterized by XRD, XPS, UV-Vis, SEM, and THz-TDS. The phonon-dispersion relation and IR absorption spectrum of $MAPbBr_3$ were also calculated by first-principles calculation based on density functional theory.

3. Results and discussion

Although the thin film contains only molecular defects related to CH_3NH_2 incorporated in the perovskite structure, our THz-wave-absorption measurement and first-principles simulation confirmed that these molecular defects do not influence the three phonon modes originating from the transverse vibration (0.8 THz), longitudinal optical vibrations (1.4 THz) of the Pb-Br-Pb bonds, and the optical vibration of Br anion (2.0 THz). After spin-casting an ultra-thin PTAA polymer protection layer on the hybrid perovskite thin film, there is no significant effect on the phonon modes. Thus, this novel flexible organic-inorganic hybrid perovskite material is a potential candidate for THz-based applications. [3]

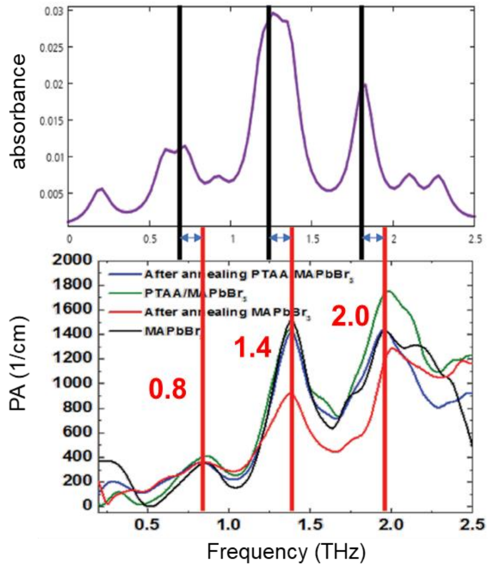

Figure 1. Calculation (upper) and experimental (lower) results of THz absorption spectrum $MAPbBr_3$.

[1] Y.-M. Lee, J.-H. Yun, A. Matsuyama, S. Kobori, M.-C. Jung, *et al. Appl. Phys. Express* **12**, (2019).

[2] S. Kobori, Y. Nakamoto, M.-C. Jung, *et al. The 65th JSAP Spring Meeting* (2018.3.17) 17p-P6-20.

[3] I. Maeng, S. Lee, H. Tanaka, M.-C. Jung, *et al.* (in press) *NPG Asia Materials*.