CH₃NH₃PbCl₃単結晶基板上 CH₃NH₃PbI₃薄膜のエピタキシャル成長 Epitaxial growth of CH₃NH₃PbI₃ thin films on CH₃NH₃PbCl₃ single crystal substrates 東大工¹. 東大先端研² ^O(M2) 劉 子豪¹. 松下 智紀^{1,2}. 近藤 高志^{1,2}

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Metal halide perovskites have attracted significant attention because of the promising scenario of being the next generation photovoltaic materials. The materials exhibit unique properties such as strong absorption and long carrier lifetime. Recently the power conversion efficiencies of perovskite solar cells have reached 25.2%. So far most of these devices have been based on polycrystalline thin films grown by spin coating. To further study the properties of perovskites, single crystals are required, and we believe that single crystalline perovskites will also play an important role in functional devices. We have tried to grow $CH_3NH_3PbI_3$ (MAPbI₃) on $CH_3NH_3PbBr_3$ single crystal substrate, but only obtained $CH_3NH_3Pb(Br_{1-x}I_x)_3$ alloy due to interdiffusion of halogen ions [1]. In order to get heterostructure of pure perovskites, we replaced the substrate with CH₃NH₃PbCl₃ (MAPbCl₃) single crystal, which has a larger mismatch.

MAPbCl₃ single crystal is fabricated by inverse temperature crystallization [2]. Then 200 nm MAPbI₃ thin film is grown by coevaporating CH_3NH_3I and PbI_2 on (001) surface of the substrate at a temperature of 21°C. The rate of PbI₂ is 0.15 Å/s. CH₃NH₃I is controlled by pressure and is kept at 0.0015 Pa. The pattern of $2\theta/\omega$ scan along normal direction of surface after coevaporation is present in Fig. 1, indicating that we have succeeded in growing pure MAPbI₃ on MAPbCl₃ single crystal substrate. This may be the result of the large lattice mismatch which could suppress interdiffusion. The inset of Fig. 1 shows that perovskite alloy still exists. Combining with the reciprocal space map in Fig. 2, we conclude that the alloy thin film formed pseudomorphically, and that the iodine composition is calculated to be about 1.3%. This is much smaller than that of bromide perovskite case. The detail of the thin film will be discussed in the presentation.

[1] K. Kimura, Y. Nakamura, T. Matsushita, T. Kondo, Jpn. J. Appl. Phys., 58, SBBF04, (2019).

[2] G. Maculan et al., J. Phys. Chem. Lett., 6, 3781, (2015).



Fig. 1 XRD patterns of $2\theta/\omega$ scan after evaporation. The Fig.2 Reciprocal space map of the substrate inset shows the detail of the substrate peak around (002). and alloy around the diffraction peak (024).