

MS26-04 | THEORETICAL STUDY OF SINGLE-ELEMENT QUASI-PERIODIC THIN FILMS FORMED ON AG-IN-YB QUASICRYSTAL

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Developments in the preparation and understanding of the surfaces of Quasicrystals (QCs) enable us to use QCs as a template of the epitaxial growth of the quasi-periodic thin films, and we recently reported the first successful fabrication of three-dimensional quasi-periodic Pb thin film using the Ag-In-Yb QC as a template [1]. It was confirmed that Pb film grown on the QC template forms a three-dimensional quasi-periodic structure. But, more surprisingly, the accumulated Pb occupy the absent rhombic triacontahedral sites, which is a structural building unit of the substrate QC, created by the crystal truncation of the substrate QC at the surface. Recent theoretical advances in the structure of the quasi-periodic thin film of Bi [2], Sb and Ag [3] obtained using the first-principles calculations based on the density functional theory will be discussed.

[1] H.R. Sharma, K. Nozawa, J.A. Smerdon, P.J. Nugent, I. McLeod, V.R. Dhanak, M. Shimoda, Y. Ishii, A.P. Tsai, and R. McGrath *Nat. Commun.* **4**, 2715 (2013).

[2] K. Nozawa and Y. Ishii, *J. Phys. Conf. Ser.*, **809**, 012018 (2017).

[3] K. Nozawa, *Proceedings of International Scientific Conference on Engineering and Applied Sciences 2018*, 197 (2018).