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.