Exploration of new quasicrystals and approximants by using machine learning

H. Uryu[1*], T. Yamada[1], H. Takakura[2], Y. Inada[3], K. Kimura[3], R. Tamura[4], L. Chang[5], R. Yoshida[5]

[1]Tokyo University of Sciense, Department of Applied physics, Tokyo, 125-8585, Japan
[2]Hokkaido University, Division of Applied Physics, Sapporo, 060-8628, Japan
[3]The University of Tokyo, Department of Advanced Materials Science, Kashiwa. 277-8561, Japan
[4]Tokyo University of Sciense, Department of Materials Science and Technology, Tokyo, 125-8585, Japan
[5]Research Organization of Information and System, The Institute of Statistical Mathematics, Tachikawa, 190-8562, Japan

[*]1521512@ed.tus.ac.jp

Very recently, Liu et. al. proposed a machine learning (ML) approach to distinguishing quasicrystals (QCs) and related approximants (ACs) from ordinary crystals. [1] They built a supervised ML model that classifies any given chemical composition into three structural classes (QCs, ACs, others), and demonstrated its potential predictive power. In this study, we built models according to the previous study and searched for new QCs and ACs base on the predictive candidate compositions from the given models.

Our models achieved a prediction accuracy of 0.999. With this, we screened 27,220 virtual ternary alloy systems, which resulted in 701 systems predicted to be QCs or ACs. We synthesized 19 Sc-Zn-Ti alloy samples around the candidate compositions of the predicted QC/AC phase and characterized the synthesized materials by using a powder and single-crystal X-ray diffraction (XRD) method. Fig. 1 shows the powder XRD pattern of a sample with the nominal composition of $Sc_{15}Ti_2Zn_{83}$, and the calculated XRD pattern of $ScZn_6$ 1/1 approximant. [2] All the peaks could be assigned to the 1/1 approximant with a lattice parameter equal to 13.81 Å. By performing a single-crystal X-ray structure analysis, this phase was determined to have a body-centred packing structure consisting of the Tsai-type rhombic triacontahedron cluster (space group *Im-3*), as depicted in Fig. 2.

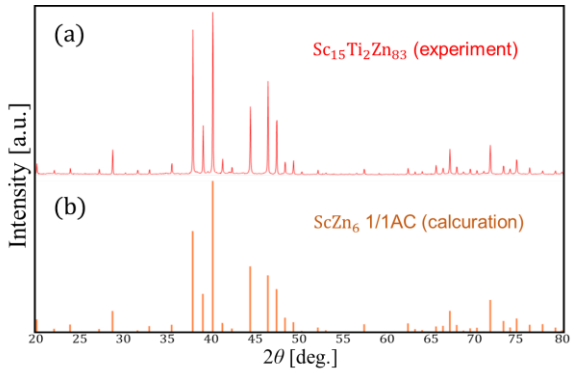

Figure.1 Powder X-ray diffraction patterns of $Sc_{15}Ti_2Zn_{83}$

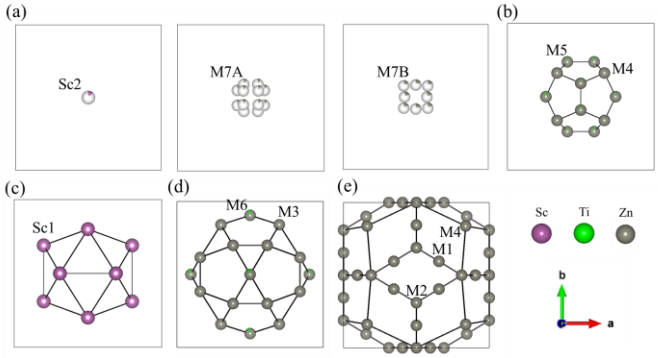

Figure.2 Shell structures of Tsai-type cluster of $Sc_{15}Ti_2Zn_{83}$ 1/1

[1] Chang Liu, Erina Fujita, Yukari Katsura, Yuki Inada, Asuka Ishikawa, Ryuji Tamura, Kaoru Kimura, Ryo Yoshida, DOI:10.21203/rs.3.rs-240290/v1

[2] Qisheng Lin and John D. Corbett , *Inorg. Chem.* 2004, 43, 6, 1912–1919

Keywords: quasicrystal; approximant crystal; machine learning; virtual high-throughput screening