

Development of Quasicrystals Datasets and Applications to Machine LearningErina Fujita,^{1†} Chang Liu,¹ Yukari Katsura,^{2,5,6} Kaoru Kimura,¹ Asuka Ishikawa,³Ryuji Tamura,³ Tomoya Mato,² Koichi Kitahara,⁴ Keiichi Edagawa,⁷ Ryo Yoshida¹¹ *The Institute of Statistical Mathematics (ISM), Tachikawa, Tokyo, Japan*² *National Institute for Materials Science (NIMS), Tsukuba, Ibaraki, Japan*³ *Tokyo University of Science, Katsushika- ku, Tokyo, Japan*⁴ *National Defense Academy, Yokosuka, Kanagawa, Japan*⁵ *Tsukuba University, Tsukuba, Ibaraki, Japan*⁶ *RIKEN, Chuo-ku, Japan*⁷ *The University of Tokyo, Meguro-ku, Tokyo, Japan*

Email: fujita-e@ims.ac.jp

ID: PST07**Poster****Aug. 24, 16.00 - 17.30**

Quasicrystals are solid-state materials with unique symmetry not allowed in ordinary crystals and they were first discovered in 1984. In recent years, machine learning has been employed to explore quasicrystals with unique properties inherent to quasiperiodic systems. However, the lack of open data on quasicrystal composition, structure, and physical properties has hindered the widespread use of machine learning in quasicrystal research. As the quasiperiodic materials exhibit distinct characteristics different from conventional periodic systems, experimentally observed data is considered to play a major role of material informatics in this field.

Comprehensive literature review and manual data extraction were conducted to develop open datasets consisting of compositions, structure types, phase diagrams, sample preparation processes and temperature-dependent thermal, electrical and magnetic properties for a wide range of stable and metastable quasicrystals and approximants [1].

Those datasets were applied to machine learning. Specifically, (1) prediction and validation of quasicrystal forming compositional regions by machine learning [2, 3], (2) prediction of the existence of quasicrystals from experimental XRD pattern images [4], and (3) exploration of thermal diode materials using experimental temperature-dependent properties. Further research utilizing those datasets are expected to accelerate the understanding of QC characteristics.

References

1. HYPOD: <https://doi.org/10.6084/m9.figshare.25650705.v2>
2. C. Liu, E. Fujita, Y. Katsura, Y. Inada, A. Ishikawa, R. Tamura, K. Kimura, and R. Yoshida, "Machine learning to predict quasicrystals from chemical compositions", *Adv. Mater.* **33**, 2102507 (2021).
3. C. Liu, K. Kitahara, A. Ishikawa, T. Hiroto, A. Singh, E. Fujita, Y. Katsura, Y. Inada, R. Tamura, K. Kimura, and R. Yoshida, "Quasicrystals predicted and discovered by machine learning", *Phys. Rev. Mater.* **7**, 093805 (2023).
4. H. Uryu, T. Yamada, K. Kitahara, A. Singh, Y. Iwasaki, K. Kimura, K. Hiroki, N. Miyao, A. Ishikawa, R. Tamura, and S. Ohhashi, "Deep learning enables rapid identification of a new quasicrystal from multiphase powder diffraction patterns", *Adv. Sci.* **11**, 2304546 (2024).

Keywords: Materials Informatics, Open Data, Experimental Data, Quasicrystal, Physical Properties