Advancement of the experimental data analysis for 2D material structure

Takeo Hoshi

Department of Applied Mathematics and Physics, Tottori University,

4-101 Koyama-Minami, Tottori 680-8550, Japan.

The open source software 2DMAT, a data-analysis software of total-reflection high-energy positron diffraction (TRHEPD) experiment, was developed in Project for Advancement of Software Usability in materials science (PASUMS) at FY2020 [1]. TRHEPD is a novel experimental technique of structure determination of two-dimensional materials and is being conducted intensively at the Slow Positron Facility of High Energy Accelerator Research Organization (KEK) [2]. We developed a python-based data analysis software of TRHEPD at 2018 and 2019 [3]. The software uses an iterative optimization (Nelder-Mead) algorithm and the grid-base search algorithm. The software was used in several application studies [4, 5] in the collaboration with experimentalists, I. Mochizuki (KEK), A. Takayama (Waseda U) and their co-workers.

In the PASUMS project at FY2020, we reorganized the software and added the Bayesian optimization algorithm, realized by the PHYSBO library [6], and the replica-exchange Monte-Carlo algorithm. The software was called 2DMAT v.1 and was published at Feb. 2021 [1]. A hands-on seminar was held at 20. April 2021 and was filled to capacity with 30 participants (https://ccms.issp.u-tokyo.ac.jp/event/4570). Several application studies with 2DMAT are currently underway.

Our successor PASUMS project started in April 2021, so as to add several parallelized algorithms and support other experimental techniques of the structure determination of two-dimensional materials, such as surface X-ray diffraction experiment and low energy electron diffraction experiment.

References

[1] https://www.pasums.issp.utokyo.ac.jp/2DMAT

[2] (Review) Y. Fukaya, *et al*, J. Phys. D: Appl. Phys. 52, 013002 (2019).

[3] K. Tanaka, *et al*, Acta. Phys. Pol. A 137, 188 (2020); JJAP Conf. Series, in press; https://arxiv.org/abs/2002.12165

[4] T. Hoshi, *et al*, Submitted; Preprint: https://arxiv.org/abs/2103.04875

[5] M. Hamada , *et al*, Poster presentation, JPS meeting, online, Mar. 2021.

[6] T. Ueno, *et al*, Materials Discovery 4, 18 (2016); https://www.pasums.issp.u-tokyo.ac.jp/physbo