Unified platform of experiment-data analysis for 2D material structure

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In a PASUMS project at FY2021, an open-source data-analysis framework 2DMAT [1-4] has been developed for experimental measurements of two-dimensional material structures. The present project is the successor of one at FY2020. The current version of 2DMAT is an unified platform for the analysis of different experimental measurement techniques, total-reflection high-energy positron diffraction (TRHEPD) [5], surface X-ray diffraction (SXRD), and low-energy electron diffraction (LEED) experiments by installing corresponding forward problem solvers that generate diffraction intensity data from a given dataset of the atomic positions. Among them, SXRD and LEED were supported as a result of the present project. The current version of 2DMAT offers five analysis methods: (i) Nelder-Mead optimization, (ii) grid search, (iii) Bayesian optimization, (iv) replica exchange Monte Carlo (REMC) method, and (v) population-annealing Monte Carlo (PAMC) method. Methods (ii) through (v) are implemented by parallel computation, which is efficient not only for personal computers but also for supercomputers. Among the above five methods, the PAMC method was implemented in the present project. In addition, the forward problem solver of TRHEPD was also published as an open-source software package by the present project [6,7].

2DMAT was applied to the structure analysis of $Si_4O_5N_3$ / 6H-SiC(0001)-($\sqrt{3} \times \sqrt{3}$)R30° surface, a novel two-dimensional semiconductor, by TRHEPD experiment [2]. A data-driven sensitivity analysis was proposed for the quantitative analysis of experimental uncertainties. The variation over individual fitting parameters was analyzed by solving the eigenvalue problem of the variance-covariance matrix. 2DMAT was used also in other application studies by TRHEPD experiment and the study by T. Takeda (Waseda U.) *et al*. won a poster-session prize [8]. The analysis methods in 2DMAT are general and can be applied also to other problems and was applied to a performance prediction of massively parallel computation by Bayesian inference [4].

As activities to promote 2DMAT, hands-on workshops were held in April 2021 and April

2022, and a study group was held in September 2021. Test calculations in massively parallel computations by the Fugaku supercomputer are underway (hp210228, hp210267).

References

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

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[6] https://github.com/sim-trhepd-rheed/

[7] T. Hanada, *et al*., Comp. Phys. Commun., in press; Preprint: arXiv: 2110.09477

[8] T. Takeda *et al*., the Best Poster Presentation Award at the 2022 Kanto Chapter Conference of the Surface and Vacuum Society of Japan.