Data-scientific software for the surface structure analysis by total-reflection high-energy positron diffraction (TRHEPD)

K.Tanaka,[1*] T.Hoshi[1] , I. Mochizuki[2], and A. ichimiya[2], and T. Hyodo[2]

[1]Department of Applied Mathematics and Physics, Tottori University, Tottori, 680-8552, Japan
[2]Institute of Materials Structure Science (IMSS),
High Energy Accelerator Research Organization (KEK), Tsukuba, 305-0801, Japan

The data scientific software was developed for the surface structure analysis by the total-reflection high-energy positron diffraction (TRHEPD). The experiment has been intensively conducted at the Slow Positron Facility (SPF), Institute of Materials Structure Science (IMSS), High Energy Accelerator Research Organization (KEK) and revealed the structure of the surfaces of interest [1].

The present paper reports the recent activity of the software development for the data analysis of TRHEPD. It is based on the inverse problem in which the atomic positions $X = (X_1, X_2, \dots, X_N)$ of a surface structure are determined from the experimental diffraction data (rocking curve) D_{exp} ($D_{\mathrm{exp}} \Longrightarrow X$). The forward problem ($X \Longrightarrow D_{\mathrm{cal}}(X)$) is solved, for many trial atomic positions X, by the numerical solution of the partial differential equation in quantum scattering problem [2]. The R-factor $R(X) = \left|D_{\mathrm{cal}}(X) - D_{\mathrm{exp}}\right|$, the residual error between the experimental and calculated diffraction data, is minimized as a function of the atomic position. Two possible methods are considered; one is the local search procedure by the gradient-free optimization (Nelder–Mead) method and the other is the global search procedure by the grid or stochastic sampling (Monte Carlo) method. The global search procedure requires a large computational cost and is realized on supercomputers with parallel computation.

This presentation demonstrates the application of the method to several known surface structures, as preliminary attempts. Our data-scientific approach is general and applicable to other experiments also, like Low Energy Electron Diffraction (LEED), when one replaces the forward problem solver. The program code is written mainly in the Python language and will be available online in near future.

Acknowledgement: The present research is supported by Japanese government in the post-K project and KAKENHI funds (19H04125, 17H02828). Several numerical computations were carried out by the supercomputer Oakforest-PACS for Initiative on Promotion of Supercomputing for Young or Women Researchers, Information Technology Center, The University of Tokyo, the HPCI project (hp190066) and Interdisciplinary Computational Science Program in Center for Computational Sciences, University of Tsukuba. Several computations were carried out also on the facilities of the Supercomputer Center, the Institute for Solid State Physics, the University of Tokyo and the Academic Center for Computing and Media Studies, Kyoto University.

References

[1] For review, Y. Fukaya, A. Kawasuso, A. Ichimiya and T. Hyodo, Total-reflection high-energy positron diffraction (TRHEPD) for structure determination of the topmost and immediate subsurface atomic layers, J. Phys. D 52, 013002 (2018).

[2] A. Ichimiya, Many-beam calculation of reflection high energy electron diffraction (RHEED) Intensities by the multi-slice method, Jpn. J. Appl. Phys. 22, 176 (1983).

*Corresponding author, Email: M18J3027Y@edu.tottori-u.ac.jp