Fusion of computational material science and data-driven science with massively parallel computation

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The present project was carried out for several topics in the fusion of computational material science and data-driven science on the ISSP supercomputer. The main collaborators are I. Mochizuki, T. Hyodo (KEK-IMSS-SPF), T. Hanada (Tohoku U), K. Hukushima (U Tokyo), K. Yoshimi, Y. Motoyama (ISSP), T. Fujita (IMS), Y. Yamamoto (UEC), Y. Miyatake (U. Tokyo).

The first topic is the development of the data analysis software of total-reflection high-energy positron diffraction (TRHEPD), a novel experimental technique for surface structure determination [1-6]. Experiments are being conducted intensively at the Slow Positron Facility, Institute of Materials Structure Science, High Energy Accelerator Research Organization. Figure 1 shows the structure determination of the $Si_4O_5N_3$ / 6H-SiC (0001)-($\sqrt{3}\times\sqrt{3}$) R30° (SiON) surface structure [3]. The software development activity was promoted to Project for Advancement of Software Usability in Materials Science in ISSP (https://www.pasums.issp.u-tokyo.ac.jp) in FY2020 and FY2021. Our software was called '2DMAT' and was published as an open-source software [4,5]. A TRHEPD simulator was required for the data analysis by 2DMAT and we used the simulator program 'sim-trhepd-rheed' originally developed by T. Hanada. [4,6].
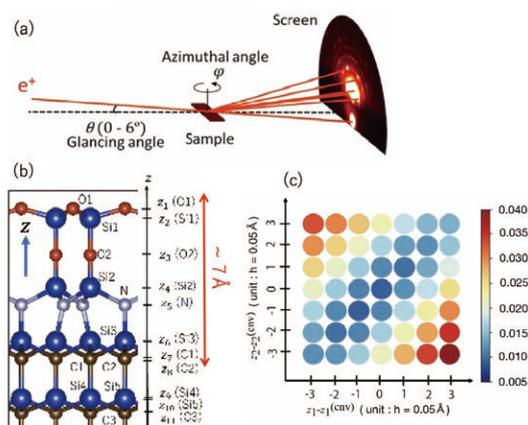

Fig.1 (a) Schematic figure of TRHEPD experiment. (b) The side view of $Si_4O_5N_3$ / 6H-SiC (0001)-($\sqrt{3}\times\sqrt{3}$) R30° (SiON) surface structure. (c) TRHEPD data analysis of the SiON surface structure [3]. The z-coordinate of the surface atom layers is denoted as $z_1, z_2, \ldots, z_7$. The color-coded isovalue plots of the R-factor, the residual function between the experimental and calculated data, on the local grid of the $z_1 - z_2$ plane [3].

The second topic is the method and application of large-scale electronic structure calculations for organic and other materials [7-10]. The study was carried out by our original code ELSES (http://www.elses.jp/), an order-N electronic state calculation code with an *ab-initio*-based tight-binding method and a fragment-molecular-orbital-based method. In

particular, an excited-state theory was constructed for disordered Pentacene/C60 Interfaces [9-10]. The third topic is the development of several fundamental numerical algorithms [11-12].

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