Two-stage data-analysis method for total-reflection high-energy positron diffraction (TRHEPD)

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A two-stage data-analysis method is proposed for total-reflection high-energy positron diffraction (TRHEPD). TRHEPD is a novel experimental method for the determination of surface structure, which has been extensively developed at the Slow Positron Facility, Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK). The data analysis is based on an inverse problem in which the atomic positions of a surface structure are determined from the experimental diffraction data (rocking curves). The relevant forward problem is solved by the numerical solution of the partial differential equation for quantum scattering of the positron. In the present two-stage method, the first stage is a grid-based global search and the second stage is a local search for the unique candidate for the atomic arrangement. The numerical problem is solved on a supercomputer.

1. Introduction

Fast, reliable computational methods used in the analysis of observed data can lead to innovative improvements in experimental measurement techniques. An example is found in the development of cryo-electron microscopy, which won the Nobel Prize in Chemistry 2017.

The present paper focuses on a computational analysis method for total-reflection high-energy positron diffraction (TRHEPD), a novel measurement technique for atomic scale surface structure. At the Slow Positron Facility (SPF), Institute of Materials Structure Science (IMSS), High Energy Accelerator Research Organization (KEK), much work has been conducted to successfully reveal surface structures of interest (see reviews [1, 2] and papers [3–5]). A previous paper [6] reports the recent activity of the software development for TRHEPD data analysis. The software developed was based on a local search algorithm starting with an initial guess of the atom positions.

The present paper proposes, as a following advancement, a two-stage analysis method in which we first use a global search algorithm and then a local search algorithm for a final solution. The method does not require any initial guess, unlike the previous one [6]. Since the computational time cost of a global search would be too large for a personal computer, the present software was developed to use a supercomputer in a modern massively parallel architecture.

The present paper is organized as follows: the experiment and theory of TRHEPD is explained briefly in Section 2; Section 3 details a technical demonstration of the software and several discussions. Summary and a future aspect are described in Section 4.
Fig. 1 Schematic figures of (a) experiment and (b) theory of TRHEPD. In (b), the diffracted beams are schematically depicted both for the positron (THREPD) and electron (RHEED) cases.

2. METHOD

The TRHEPD method is illustrated schematically in Figure 1 and will be briefly explained in this section. The basis of TRHEPD is the same as in reflection high-energy electron diffraction (RHEED) experiments.

The problem is to determine the positions of the atoms at the top-most surface layer and a few subsurface layers. Hereafter, the $z$ axis is chosen to be perpendicular to the sample surface and the position of the $i$-th atom is denoted as $r_i = (x_i, y_i, z_i)$. We denote $N_a$ as the number of the atoms whose positions ($(x_i, y_i, z_i), i = 1, 2, ..., N_a$) are to be determined.

The data analysis is based on the inverse problem in which the surface structure $X$ is determined from the experimental diffraction data, $D_{\text{exp}}(D_{\text{exp}} \Rightarrow X)$. The calculated diffraction data, $D_{\text{cal}}$, can be obtained for the assumed structure $X$; this process is called the forward problem ($X \Rightarrow D_{\text{cal}}(X)$).

2.1 Experiment of TRHEPD

The TRHEPD experiment is shown schematically in Figure 1(a). The incident wave direction is characterized by the glancing angle $\theta$ and the azimuthal angle $\varphi$. We also define the incident wave vector $K^{(\text{in})} = (K \cos \theta \cos \varphi, K \cos \theta \sin \varphi, 0)$ projected on the $x$-$y$ plane.

Diffraction spots on the screen in Figure 1(a) are characterized by the two-dimensional indices $(p, q)$ of reciprocal lattice rods. The intensity of a particular spot, $D_{pq}$, is observed as a function of the incident glancing angle, $\theta (D_{pq} = D_{pq}(\theta))$, and called the rocking curve.

The rocking curve, $D_{pq}(\theta)$, depends also on the azimuthal angle $\varphi$, which is fixed during a rocking curve measurement. The spot with the indices of $(p, q) = (0, 0)$ is usually the brightest and called 00 spot. This paper focuses on the intensity of the 00 spot and we drop the indices for simplicity ($D = D_{00}$). The observed data for discrete glancing angles is denoted as $D \equiv (D(\theta_1), D(\theta_2), ..., D(\theta_\nu))$, where a typical number of the glancing angles is $\nu = 50 - 100$. The present data analysis is carried out on the normalized vector data $D$ ($|D| = 1$) and similarly normalized calculated values. TRHEPD patterns, and hence the rocking curves extracted from them, are hardly affected by the atomic coordinate parallel to the vector $K^{(\text{in})}$, because the energy of the incident beam is typically 10 keV with wave length much shorter than the lattice constants of materials. Thus if the vector $K^{(\text{in})}$ is parallel to the $y$-axis, for example, the rocking curve depends only on the $x$ and $z$ components of the atomic position ($D = D(x_1, x_2, ..., x_N, z_1, z_2, ..., z_N)$). In addition, one can choose the azimuthal angle intentionally shifted from any low-index zone axis so that practically the rocking curve depends almost only on the $z$ components of the atom position ($D = D(z_1, z_2, ..., z_N)$). This is called the one-beam condition [8]. Other choices of the azimuthal angle are called the many-beam condition, where the azimuthal angle is set so that the beam is incident along a low-index zone axis. Then the rocking curve depends only on the $y$ component, since the $z$ component already known by the analysis of the data in the one-beam condition could be fixed. These properties allow us to reduce the number of variables in the analysis of each data set from $3N_a$ to $N_a$. Such dimensional reduction is of great advantage in realizing fast and reliable data analysis.
Therefore, the measurement procedure, typically, consists of three diffraction data sets for different azimuthal angles. One data set is for the one-beam condition, which is denoted as $D^{(OB)}$. The other two sets are for the many-beam condition, which are denoted as $D^{(MB1)}$ and $D^{(MB2)}$. The incident wave vectors $K^{(m)}$ are orthogonal between the two data sets in the many-beam condition. The first procedure in data analysis determines the $z$ component of the atomic position $(z_1, z_2, ..., z_N)$ from the data set in the one-beam condition $(D^{(OB)})$. The second procedure with the already determined $z$ components $(z_1, z_2, ..., z_N)$ fixed determines each component on the $x$-$y$ plane from each set of the two data sets in the many-beam condition $(D^{(MB1)}, D^{(MB2)})$.

2.2 Theory of TRHEPD

The theory of the forward problem ($X \Rightarrow D_{\text{cal}}(X)$) of TRHEPD [7] is based on the full-dynamical quantum scattering problem of the positron wavefunction $\Psi(r)$, which is shown schematically in Figure 1(b). The calculation method [7] was originally developed for electron diffraction (RHEED) but is applicable here, since the TRHEPD method is different from RHEED only in the sign of the charge of the incident particle. As the electron beam penetrates into deeper layers than the positron, owing to refraction off the surface, as schematically shown in Figure 1(b), electron diffraction has added complexities compared to positron diffraction.

The calculation method solves numerically the partial differential equation with a given glancing angle and an azimuthal angle

$$(\Delta + U(r) + E)\Psi(r) = 0,$$  \hspace{1cm} (1)

so as to obtain the rocking curve data $D = D_{\text{cal}}(X)$. Here $U(r)$ is the crystal potential determined by the atomic positions $X$. The crystal potential $U(r)$ is periodic on the $x$-$y$ plane and can be written by the two-dimensional Fourier series

$$U(x, y, z) = \sum_m U_m(z) \exp \left( i(k_x^{(m)} x + k_y^{(m)} y) \right),$$  \hspace{1cm} (2)

where $(k_x^{(m)}, k_y^{(m)})$ is the surface reciprocal lattice vector of the $m$-th rod.

The calculation under the one-beam condition [8] is much faster than that under the many-beam condition, since only one Fourier component $(k_x^{(m)}, k_y^{(m)}) = (0, 0)$ is assumed to be non-zero in Equation (2)

$$U(x, y, z) = U_0(z).$$  \hspace{1cm} (3)

under the one-beam condition. Consequently, the wavefunction can also be written as $\Psi \equiv \Psi(z)$ and Equation (1) is reduced to a one-dimensional scattering problem

$$\left( \frac{d^2}{dz^2} + K^2 \sin^2 \theta + U_0(z) \right) \Psi(z) = 0.$$  \hspace{1cm} (4)

Several codes in Fortran have been developed to solve the forward problem [7–9] and we use the code in Reference [9] in the calculations of the present paper.

2.3 Data analysis algorithm

This subsection details the two-stage method for the data analysis of the TRHEPD data. The method is based on the inverse problem ($D_{\text{exp}} \Rightarrow X$) and the solution $X$ is determined by minimizing the residual function between the calculated and experimental diffraction data

$$R(X) \equiv |D_{\text{cal}}(X) - D_{\text{exp}}|$$  \hspace{1cm} (5)
with a given experimental diffraction data $D_{\text{exp}}$. The function $R(X)$ is called the reliability factor or R-factor.

The two-stage analysis method in the present paper is illustrated in Figure 2. Figure 2(a) shows schematically the first stage in a grid-based global search algorithm. A set of equi-interval grid points $\{X_1^{(g)}, X_2^{(g)}, \ldots, X_M^{(g)}\}$ is shown, where $M$ is the number of the grid points. Then the R-factor is calculated at each grid point, $\{R(X_1^{(g)}), R(X_2^{(g)}), \ldots, R(X_M^{(g)})\}$, and local minimum points $X^{(0)}$ are found that give minimum R-factor values relative to the points around. Since the calculations of the R-factor at the prepared grid points are independent, the procedure is ideal for processing with a supercomputer in the modern massively parallel architecture. Figure 2(b) shows schematically the second stage in the local search algorithm. The atomic position $X$ is updated so as to decrease $R(X)$ from the initial guess $X^{(0)}$, until the position satisfies a convergence criteria ($X^{(0)} \Rightarrow X^{(1)} \Rightarrow X^{(2)} \Rightarrow \cdots \Rightarrow X^{(k)} \Rightarrow \cdots \Rightarrow X^{(\text{sol})}$). The local search algorithm employs Nelder-Mead algorithm [6, 10, 11]. We developed a Python-based data analysis code. The parallelism in the global search is realized by the Message Passing Interface (MPI) technique, a standard technique for parallelism, in the mpi4py library (https://bitbucket.org/mpi4py/mpi4py). The Nelder-Mead algorithm in the local search is realized by the module in the scipy library (scipy.optimize.fmin). The method is standard and the use of the scipy library is not essential.

3. Test problem and the result

3.1 Test problem

The two-stage algorithm was applied in a numerical test problem in the one-beam condition for the Ge(001)-c(4×2) surface structure. The structure is found in many papers, such as Reference [12] and a side is shown in Figure 3(a). The first and second surface atoms are denoted by $S_1$ and $S_2$, respectively, and form an asymmetric dimer. The third surface atoms are denoted by $S_{3a}$ and $S_{3b}$. A top view is shown in Figure 3(b). The asymmetric surface dimers, such as ($S_1$, $S_2$) and ($S_1^\prime$, $S_2^\prime$), form a row in the [1, 10] direction. The upper (vacuum side) atoms align alternatively, like $S_1$ and $S_1^\prime$, with the same height, and the lower (bulk side) atoms align alternatively, like $S_2$ and $S_2^\prime$, with the same height. The $z$ coordinates of $S_1$ ($S_1^\prime$) and $S_2$ ($S_2^\prime$) are denoted by $z_1$ and $z_2$, respectively. The atoms of $S_{3a}$ and $S_{3b}$ are located at the same height with a $z$ coordinate denoted by $z_3$.

The present test problem is to determine the $N = 3$ valuables $z_1$, $z_2$ and $z_3$. In other words, the structure data $X$ lies in the three-dimensional data space ($X \equiv (z_1, z_2, z_3)$). Here a numerically generated ‘reference’ data $D_{\text{ref}}$ is used, instead of the real experimental data $D_{\text{exp}}$. The reference data $D_{\text{ref}}$ is generated numerically corresponding to the known structure $(z_1, z_2, z_3) = (z_1^{\text{ref}}, z_2^{\text{ref}}, z_3^{\text{ref}})$. 

Fig. 2 Schematic figure of the present two-stage search algorithm for finding the minimum point of a given function $R = R(X)$. A grid-based global search is carried out in the first stage (a) and then the local search is in the second stage (b). The initial points in the second stage are obtained in the first stage. The function $R(X)$ is called the reliability factor or R-factor.
Fig. 3 (a) A side view of a part of the Ge(001) surface, in which only an asymmetric surface dimer of (S₁, S₂) and several subsurface layers are depicted. The vertical axis is the z axis or indicates the [001] direction, while the horizontal axis indicates the [110] direction. The upper (vacuum side) and lower (bulk side) atoms in the asymmetric dimer are denoted by S₁ and S₂, respectively. The z coordinates of S₁ and S₂ are denoted by z₁, z₂, respectively. The atoms in the subsurface layer are denoted by S₃a and S₃b and their z coordinate is denoted by z₃. (b) A top view: a pair of the asymmetric surface dimers, such as (S₁, S₂) and (S₁', S₂), form a part of the c(4×2) super structure. The upper (vacuum side) atoms align alternatively, like S₁ and S₁', on the row structure. (c) The real part of the scattering potential (Re[U₀(z)]) averaged over the x-y plane is drawn for the structure in (a) and (b).

\[ D_{\text{ref}} \equiv D_{\text{cal}}(z_1^{(\text{ref})}, z_2^{(\text{ref})}, z_3^{(\text{ref})}) \] [13]. The R-factor is defined as

\[ R(z_1, z_2, z_3) \equiv \left| D_{\text{cal}}(z_1, z_2, z_3) - D_{\text{cal}}(z_1^{(\text{ref})}, z_2^{(\text{ref})}, z_3^{(\text{ref})}) \right|. \] (6)

The reference data is set to be \((z_1^{(\text{ref})}, z_2^{(\text{ref})}, z_3^{(\text{ref})}) \approx (5.231\text{Å}, 4.371\text{Å}, 3.596\text{Å})\). The precision on the order of 10^{-3} Å is beyond experimental spatial resolution but is left here, because the present numerical test is carried out to demonstrate that the present two-stage analysis method can reach the minimum point with a numerical precision finer than experimental spatial resolution.

Figure 3(c) shows the real part of the scattering potential (Re[U₀(z)]) in the case of the reference structure averaged over the x-y plane. The peaks of the function (Re[U₀(z)]) are located at the atomic positions, such as \(z = z_1^{(\text{ref})}, z_2^{(\text{ref})}, z_3^{(\text{ref})}\).

The present numerical computation was carried out on the supercomputer ‘Sekirei’ at the Institute for Solid State Physics, the University of Tokyo. One processor node consists of two Intel Xeon 2.5 GHz (12 core) processors.

3.2 Result

In the first stage, the grid points are generated with an equi-interval of \(h = 0.25\text{Å}\) in the region of \(z_{\text{min}} \equiv 1.00\text{Å} \leq z \leq z_{\text{max}} \equiv 6.00\text{Å}\). The number of the prepared grid points for \((z_1, z_2, z_3)\) is
Fig. 4 Partial regions of the global search. The calculated value of the R-factor \( R = R(z_1, z_2, z_3) \) is plotted at each grid point as colored circles, on (a) the plane of \( z_3 = 3.50 \text{Å} \) and (b) the plane of \( z_1 = 5.25 \text{Å} \). The grid points lie under the constraints of \( 1 \text{Å} \leq z_3 \leq z_2 \leq z_1 \leq 6 \text{Å} \).

\[
M' = \left( \frac{(z_{\text{max}} - z_{\text{min}})}{h} + 1 \right)^3 = 21^3 = 9,261.
\]

In addition, the constraint of \( z_3 \leq z_2 \leq z_1 \) is imposed on the grid points and the number of grid points is reduced to \( M = 1,771 \). The global search is carried out with \( P_{\text{node}} = 8 \) processor nodes or \( P_{\text{core}} = 8 \times 2 \times 12 = 192 \) processor cores. Each processor core performs one MPI process and is responsible for the computation on \( M/P_{\text{core}} = 1,771/192 \approx 9 \) grid points. The total elapsed time for the global search is \( T_{\text{global}} \equiv 13 \text{ s} \), where the elapsed time includes the computational time and the file I/O time. As results, the first, second and third optimal grid points are found at \( X^{(g1)} \equiv (z_1^{(g1)}, z_2^{(g1)}, z_3^{(g1)}) = (5.50 \text{Å}, 4.75 \text{Å}, 3.75 \text{Å}) \), \( X^{(g2)} \equiv (z_1^{(g2)}, z_2^{(g2)}, z_3^{(g2)}) = (5.25 \text{Å}, 4.25 \text{Å}, 3.50 \text{Å}) \), and \( X^{(g3)} \equiv (z_1^{(g3)}, z_2^{(g3)}, z_3^{(g3)}) = (5.25 \text{Å}, 4.75 \text{Å}, 3.75 \text{Å}) \), respectively. Their
R-factor values are $R(X^{(g_1)}) \approx 0.0150$, $R(X^{(g_2)}) \approx 0.0152$, $R(X^{(g_3)}) \approx 0.0193$.

In the second stage, the local search algorithm was carried out with a single node. The methodological details are described in the previous paper [6]. The local search algorithm is an iterative refinement procedure and the first, second and third optimal grid points, $X^{(g_1)}$, $X^{(g_2)}$ and $X^{(g_3)}$, are chosen to be the initial points. (i) When the initial point is chosen to be $X^{(0)} = X^{(g_1)}$, the iterative refinement of the R-factor was converged to $R \approx 0.0058$ after $k = 50$ iterative steps and the converged point is $X^{(sol,1)} = (z_1^{(sol,1)}, z_2^{(sol,1)}, z_3^{(sol,1)}) \approx (5.340\AA, 4.646\AA, 3.685\AA)$. The difference of the converged point and the reference point is $\delta X^{(sol,1)} \equiv X^{(sol,1)} - X^{(ref)} \approx (0.11\AA, 0.27\AA, 0.09\AA)$. The total elapsed time for the local search is $T_{local} \equiv 48$ s. (ii) When the initial point is chosen as $X^{(0)} = X^{(g_2)}$, the iterative refinement of the R-factor was converged to $R = 7 \times 10^{-6}$ after $k = 61$ iterative steps and the converged point is $X^{(sol,2)} = (z_1^{(sol,2)}, z_2^{(sol,2)}, z_3^{(sol,2)}) \approx (5.231\AA, 4.371\AA, 3.596\AA)$. The difference between the converged and reference points, $\delta X^{(sol,2)} \equiv X^{(sol,2)} - X^{(ref)}$, is of the order of $10^{-5}$ Å. The total elapsed time for the local search is $T_{local} \equiv 15$ s. (iii) When the initial point is chosen to be $X^{(0)} = X^{(g_3)}$, the iterative refinement of the R-factor was converged to $R \approx 0.0058$ after $k = 47$ iterative steps and the converged point is $X^{(sol,3)} = (z_1^{(sol,3)}, z_2^{(sol,3)}, z_3^{(sol,1)}) \approx (5.340\AA, 4.645\AA, 3.684\AA)$. The difference between $X^{(sol,3)}$ and $X^{(sol,1)}$ is of the order of $10^{-3}$ Å. In conclusion, we obtained the true minimum $X^{(sol,2)}$ and a local minimum $X^{(sol,1)}(\approx X^{(sol,3)})$.

Figure 4 shows partial regions of the global search. The calculated value of the R-factor $R = R(z_1, z_2, z_3)$ is plotted at each grid point as colored circles on the plane of $z_3 = z_3^{(g_2)} = 3.50\AA$ in Figure 4(a) and on the plane of $z_1 = z_1^{(g_2)} = 5.25\AA$ in Figure 4(b). One can find that the R-factor is sensitive not only to the top-most surface atoms $(z_1, z_2)$ but also to the atoms below $(z_3)$. Figure 5 shows the iterative refinement of the R-factor with the initial point of $X^{(0)} = X^{(g_2)}$. Figure 6 shows the rocking curves for $X = X^{(g_2)}$ obtained in the first stage and for $X = X^{(sol,2)}$ obtained in the second stage. The rocking curve is plotted also for the reference point $X = X^{(ref)}$.

Here several points are noted: (i) the present computation demonstrates that the two-stage algorithm reaches the exact solution ($R \rightarrow 0$) for a numerically generated reference data. When one analyzes real experimental data, an optimized value of $R \leq 10^{-2}$ is usually acceptable, owing to the uncertainties involved in the experimental data; (ii) the second stage can be parallelized, as well as the first one, since one can run multiple local search processes with different initial points, $X^{(0)}$. Possible
candidates of the initial points are (local) minima or saddle points on grid.

Finally, we should comment on the potential limitation of the grid-based global search. The number of grid points $M$ is usually proportional to $m^N$ ($M \propto m^N$), where $N$ is the number of the variables and $m$ is the number of grid points on one axis. Consequently, the grid-based global search will incur a huge computational cost, when the number of variables $N$ is larger ($N \gg 3$). Such a case should be analyzed by Bayesian inference with a Monte Carlo algorithm. The Monte Carlo algorithm is known as a reliable and efficient sampling method. The method provides the posterior probability of atomic positions through Bayes’ theorem and enables us to evaluate the uncertainty of estimated atomic positions. This method has been applied to surface structure analysis by X-ray diffraction investigations [14, 15]. We are now developing another global search method with a massively parallel Monte Carlo algorithm [16].

4. Summary

The present paper proposes a two-stage analysis method for the surface structure determination by total-reflection high-energy positron diffraction (TRHEPD) experiments. The algorithm realizes a global search that does not requires any initial guess. A test problem is solved with a numerically generated reference data. The software is based on the inverse problem, where the forward problem is a quantum scattering problem or partial differential equation. Analysis of real experimental data is ongoing. The program code will be available online in the near future.

A future aspect of this research will be the extension of this method into a more general data analysis software on surface structure, not only for positron diffraction but also for X-ray and electron diffraction by substitution of the forward problem solver.

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