Fully performed constant-momentum-transfer-averaging in low-energy electron diffraction demonstrated for a single-domain Si(111)4×1-In surface

Tadashi Abukawa,* Tomoyuki Yamazaki, and Shozo Kono
Institute of Multidisciplinary Research for Advanced Material, Tohoku University, Sendai 980-8577, Japan
(Received 30 November 2006; Accepted 18 December 2006; Published 23 December 2006)

The usefulness of fully performed constant-momentum-transfer-averaging (CMTA) in low-energy electron diffraction (LEED) has been demonstrated for a single-domain Si(111)4×1-In surface. In the fully performed CMTA, thousands of I(V) curves were measured for the single-domain Si(111)4×1-In surface and CMTA intensity profiles were obtained for more than three hundred reciprocal rods in order to directly reconstruct three dimensional (3D) atomic positions of the surface. In the direct reconstruction, the minimum function method, a standard method in X-ray crystallography of the Patterson function analysis, was used. The 3D Si positions so obtained were in excellent agreement with the known heavily-reconstructed surface Si positions of 4×1. Indium atoms were not ‘visible’ in the present case due to large thermal vibration amplitude of indium atoms for the room-temperature sample, which is not an inherent shortcoming of the fully performed CMTA method. [DOI: 10.1380/ejssnt.2006.661]

Keywords: Low energy electron diffraction (LEED); Surface structure; Indium; Si(111)

I. INTRODUCTION

Low-energy electron diffraction (LEED) is the most common technique for the surface crystallography [1–3]. Strong interactions between the low-energy electrons and surface atoms cause the high sensitivity for the surface atomic structure. As a result, strong dynamical diffraction is inherent in LEED, thus the simple kinematical theory is hardly applicable to the LEED analysis. For the last several decades, we witnessed the development of sophisticated LEED dynamical theories to reproduce I(V) curves in surface crystallography [1–3]. LEED dynamical analysis has become rather a handy tool for surface structural analysis nowadays. However, the complicated dynamical effect prevents direct extract of structural information from the experimental data, and several arbitrary processes in the analysis greatly reduce the reliability of the result. Thus, LEED dynamical analysis still has rather large disadvantages over a method based on kinematical diffraction, such as surface x-ray diffraction (SXRD) [4]. If a kinematical analysis becomes applicable by some additional means, LEED will become a comprehensvive method for the surface crystallography.

More than 30 years ago, Lagally et al. [5, 6] proposed a promising kinematical mean, called later constant momentum transfer averaging (CMTA), to eliminate the dynamical effect by experimental efforts. In CMTA, LEED I(V) curves were measured at several incident angles and averaged as a function of the momentum transfer (scattering vector). In principle, dynamical components of I(V) curves strongly depend on both of the incident angle and the momentum transfer while the kinematical components mainly depend on the latter. Thus, it is expected that the averaging of several I(V) curves over different incident angles eliminates the dynamical component of LEED I(V) curves. Although CMTA was partially successful until 1980’s [7], its usage gradually decayed in accordance with the progress of dynamical theory for the LEED analysis.

It might have been possible that the insufficient performance of classical LEED acquisition systems limited the usefulness of CMTA since it required a large amount of LEED data sets for effective structure analysis. Computational power was not at close hand for such large data sets either.

The recent progress in image detection devices and computer hardware enables us to acquire large data sets required for a full performance of CMTA. Indeed, CMTA was revived rather recently by Wu et al. [8] as Patterson function analysis of multi-incidence LEED. They found the importance of the symmetrical averaging about incident azimuth, in addition to the original CMTA method.

Very recently, Wang et al. [9] applied this method to a triple domain Si(111)4×1-In surface (abbreviated as 4×1-In), and successfully obtained a correct structure from their Patterson function. They practically proved the ability of CMTA for the surface structure analysis with help of kinematical and dynamical simulations. Unfortunately, they treated the substrate as known to solve the Patterson function, and did not derive structure image directly from their Patterson function. This might be caused by an imperfection of the Patterson function originated from the triple-domain sample they used. Since fundamental spots overlap each other for a triple-domain sample, the fundamental spots can not be used, thus only surface super-structure spots were used in the previous study [9]. It may be possible to derive a three dimensional structure in straightforward manner for a full Patterson function in which both the fundamental and the superstructure spots are included.

The purpose of the present study is, therefore, to demonstrate the true power of fully performed CMTA, i.e. the capability of the direct structure reconstruction from a full Patterson function obtained by CMTA for a single-domain 4×1-In surface avoiding the the triple-domain problem. Since the Si(111) substrate has a three-fold symmetry, one-fold 4×1-In structure can takes triple orientations with an equal probability on the Si(111) surface. A single-domain 4×1-In was reported for a slightly vicinal substrate [10], where one of the triple orientation was dominantly grown on terraces between regularly ar-
The 4×1-In surface is known to have a unique electronic structure; one dimensional metallic character of the surface states at room temperature (RT) [10, 11]. Thus this surface has attracted much attention as a prototype of one-dimensional metallic system realized on a surface. Indeed, a phase transition, which should be related to the one-dimensional metallic character, was reported to occur from the RT phase of 4×1 to a low-temperature (LT) phase of 8×2 [12]. A variety of models for the 4×1-In surface had been proposed by a number of techniques [13] until Bunk et al. [14] proposed a plausible model by SXRD in 1999. The ball-and-stick model of the SXRD model is shown in Fig. 1. A rectangular unit cell is shown on the top view of the model. The LT 8×2 phase was also investigated by SXRD [15], and rather small atomic displacements were concluded for the 4×1 to 8×2 phase transition. Very recently, a new structural model and a dynamical fluctuation model for this transition were proposed by SXRD [14]. (a) top view, (b) side view from [110]. Large grey circles represent In atoms, and open and solid circles are Si atoms. Shaded rectangle represents the 4×1 unit cell.

In the present study, we prepared the single-domain 4×1-In surface according to the recipe in ref. 10, and measured thousands of \( I(V) \) curves at 21 different incident angles. CMTA intensity profiles for more than three hundreds reciprocal rods were obtained by CMTA methods from the measured \( I(V) \) curves. Then, a 3D Patterson function was calculated by the Fourier transformation from the CMTA profiles. 3D arrangements of surface Si atoms have directly been reproduced from the Patterson function by the minimum function method, a standard technique in x-ray crystallography. The positions of surface Si so obtained were in excellent agreement with the known atomic structure of the surface.

FIG. 1: Ball-and-stick model of Si(111)4×1-In surface structure as proposed by SXRD [14]. (a) top view, (b) side view from [110]. Large grey circles represent In atoms, and open and solid circles are Si atoms. Shaded rectangle represents the 4×1 unit cell.

II. EXPERIMENTAL

We used standard four-grid LEED optics (OCI, BDL5000R) and a sample manipulator with xyz-translations and \( \theta \)- and \( \phi \)-rotation axes in an ultra-high vacuum chamber at a base pressure of \( 1 \times 10^{-8} \) Pa. Since the quick and effective acquisition is the key to realize the full-performance CMTA LEED, we used a high sensitive CCD video camera to measure LEED patterns, and the whole screen images were stored in a personal computer (PC) by a frame grabber card. Then, every spot on the screen images could be used to make \( I(V) \) curves by an off-line analysis. The incident electron energy and the image acquisition were controlled by the PC, and the \( I(V) \) measurement was fully automated except for changing the incident angle by a sample rotation.

We followed the recipe described in ref. 10 to make a single domain 4×1-In. Briefly, we used a 1.1°-off-normal Si(111) wafer. Indium of 1.4ML was deposited by a Knudsen-cell on the Si(111)7x7 clean surface at RT. Then the surface was annealed at 500°C for 2 min. A typical single-domain 4×1-In LEED pattern as obtained is shown in Fig. 2, where a 1×1 unit and a rectangular 4×1 unit are superimposed. We could repeatedly obtain the single-domain 4×1-In surface with an ignorable minor-domain ratio as shown in Fig. 2. As marked in Fig. 1, we chose \( x \) and \( y \) axes as parallel to [112] and [110] directions, respectively. Therefore, the mirror index \( h \) and \( k \) are the indexes of [112] and [110] directions, respectively.

For each \( I(V) \) measurement, the incident energy was scanned from 30 to 400 eV with constant interval of 0.05 Å\(^{-1}\) in a wave number. Since all the spots of the stored patterns were used to form \( I(V) \) curves, more than 150 curves were obtained from each \( I(V) \) measurement for the 4×1-In surface at a certain incident angle. CMTA was performed with 21 sets of LEED \( I(V) \) measurements in the present study. The 21 sets consist of one \( I(V) \)
FIG. 3: (a) (Upper seven curves) LEED intensity curves of (1,0)-rod at seven different incident angles for the 4×1-In surface. (Bottom curve) CMTA curve of (1,0) rod obtained by the averaging of all (1,0)-rods measured at different incident angles. (b) Example of the CMTA curves resulted from 21 measurements at different incident angle. \((h,k)\)-indexes are shown on the left side of curves.

measurement at the incident angle of \(\theta = 0^\circ\), seven measurements at \(\theta = 10^\circ\) with every 30\(^\circ\) in azimuth from \(\phi = 0^\circ\) to 180\(^\circ\) and thirteen measurements at \(\theta = 20^\circ\) with every 15\(^\circ\) in azimuth from \(\phi = 0^\circ\) to 180\(^\circ\). Taking advantage of the mirror symmetry of the single-domain 4×1-In surface, we expanded these data sets to the other azimuth range, i.e. incident azimuth of \(\phi = 180^\circ\) to 360\(^\circ\).

After the \(I(V)\) acquisition, each \(I(V)\) curve was transformed into an intensity profile as a function of momentum transfer, and consequently the intensity along the reciprocal rod \(I_{h,k}(L)\) is obtained, where \(h\) and \(k\) are the mirror indexes and \(L\) the momentum transfer along the rod, and \(i\) an index of the incident angle. We assumed an inner-potential of 10 eV to calculate \(L\) value inside the crystal. Finally, CMTA intensity for each reciprocal rod was obtained as

\[
\tilde{I}_{h,k}(L) = \frac{1}{N_{h,k}(L)} \sum_i I_{h,k}^i(L) w(L)
\]

(1)

which is the average of \(I_{h,k}^i(L)\) over \(i\)'s, where \(N_{h,k}(L)\) and \(w(L)\) are the number of the measurements at \(h, k\) and \(L\), and a Welch window function to suppress termination errors in the following Fast Fourier transformation (FFT), respectively.

III. EXPERIMENTAL RESULTS AND PATTERSON FUNCTION EVALUATION

Typical \(I_{h,k}^i(L) w(L)\) curves are shown in Fig. 3(a), where the window function is already multiplied. Upper seven curves are for (1, 0)-rods at different incident angles. The incident angles are shown on the right hand side of curves. The bottom curve in Fig. 3 (a) is the resulting CMTA curve for (1, 0)-rod \(\tilde{I}_{1,0}(L)\), as evaluated by Eq.(1) with all 21 measurements. (Other resulting CMTA curves are evaluated with all 21 measurements unless otherwise stated.) Distinct peaks at nearly a constant interval (\(\Delta L \approx 2\,\text{Å}^{-1}\)) correspond to the bulk reflections. We can see how the incident angles affect the LEED \(I_{h,k}(L)\) curves in Fig. 3 (a). The multiple-scattering, which strongly depend on the incident angle, causes the intensity variation of these peaks and position shift, and creates some satellite peaks and shoulders. However, one might always find certain common features among the same \((h,k)\)-rods at different incident angles. These common features would represent the kinematical diffraction components which we desire. We expect the enhancement of these kinematical features and the reduction of the multiple-scattering features in the averaged curve, i.e. CMTA curve, shown at the bottom of Fig. 3(a). A few examples of obtained CMTA curves are shown in Fig. 3 (b). We can see some distinct peaks and structures in the fractional order curves and bulk peaks in the integral order curves.

We have obtained CMTA curves for more than three hundreds of \((h,k)\)-rods from the 21 measurements at different incident angles. From these CMTA curves, a 3D CMTA intensity \(\tilde{I}(h, k, L)\) was constructed. This is considered as an absolute square of the structural factor \(|F(h, k, L)|^2\) of the 4×1-In surface if CMTA works. A section of \(\tilde{I}(h, k, L)\) are presented as a color scale image in Fig. 4, where the rod width was artificially enlarged for the sake of visibility. One can overview the shape and the size of the probed area in reciprocal space from Fig. 4. The shape is an upside-down cone with diameters in \(h\) and \(k\) directions of 20 Å\(^{-1}\) and the height in \(L\) direction of 13 Å\(^{-1}\). These sizes determine the real space resolution for the kinematical analysis.

The Patterson function was obtained by a Fourier transformation of \(\tilde{I}(h, k, L)\), and should correspond to the self-correlation function of the atomic structure. Although the complete structure is not immediately solved from the Patterson function, many hints for the structure...
are directly extracted from it. As shown later, several
techniques have already been developed to solve the Pat-
terson function in x-ray crystallography [21]. Here, we use
the magnitude of the Fourier transformation as a Patter-
son function

$$P(r) = \sum_{h} \sum_{k} \sum_{L} \tilde{i}(h, k, L)e^{i\mathbf{s} \cdot \mathbf{r}}$$

where s is the momentum transfer corresponding to the
indexes of (h, k, L). P(r) was calculated by a FFT code
in the space of $13.3 \times 3.84 \times 40$ Å³ with 0.1Å resolutions
for all dimensions.

IV. STRUCTURE ANALYSIS

A. Bond orientation

A spherical section, at $r = 2.35$ Å, of the obtained $P(r)$
for the 4x1-In surface is shown in Fig. 5, and four hor-
izontal sections at different heights of $P(r)$ are shown
in Figs. 6 (a)-(d). These sections are represented by the
color-scaled contour plots, and their intensity was nor-
malized by a maximum value of $P(r)$ at the origin. There
are several distinct spots in these sections, which should
correspond to inter-atomic vectors of the 4x1-In surface.

At the first step, we consider the spots relating to the
nearest neighbor atoms of the surface structure. Since
2.35 Å is a bond length of bulk Si, the nearest neighbor
vectors of Si, i.e., the Si-Si bond orientations, should
appear on the sphere in Fig. 5. It is worth noting that the
Patterson function always has an inversion symmetry and
4x1-In surface has a mirror symmetry about the $xz$ plane.
Thus, most of the spots on the full sphere can be judged
from the hemisphere in Fig. 5.

The spots labeled B1, B2, B3, and B4 are all pointing
along one of the (111) directions, and should correspond
to the Si-Si bonds forming the bulk diamond structure.
All Si-Si bonds pointing along the (111) directions were
observed on the full sphere. The spots labeled S1, S2, S3
and S4 do not follow the three-fold symmetry of the bulk
silicon, but follow the one-fold symmetry of the surface.
S1 on the equator indicates the existence of in-surface-
plane Si-Si bond at the surface. This in-plane bond agrees
well with the in-plane zigzag chain of Si atoms in the
SXRD model. Thus, S1 corresponds to the inter-atomic
vector between the Si atoms labeled 1 and 2 in the model
of Fig.1. S2 (S3) agrees with the back bond between the
Si atoms labeled 2 and 4 (1 and 3) in Fig.1. Thus, all
observed spots on the sphere, except for a faint spot S4,
perfectly fit the Si framework of the SXRD model. The
faint S4 would indicate a direction of the In-In bonds.
Since a large thermal vibration is expected for indium
atoms at RT [22], In-In bonds as well as In-In bonds are
expected to be weak in the present Patterson function.

As far as we see in the spherical section of $P(r)$, there
are no serious artifacts that might be induced by the dy-
namical effect in LEED. It is very important for the re-
liable structural analysis to have an artifact-free $P(r)$.
Although we notice some dynamical effects still exist
as slight modification of peak intensity or smooth back-
ground in $P(r)$, the present effective artifact-free $P(r)$
proves the validity of the CMTA method.

We have also calculated $P(r)$ excluding the fundamen-
tal rods, as it had been done in ref. 9 for the triple-domain
surface. Although there were no serious artifact in the
$P(r)$, some important structures, which related to sub-
strate, were smeared or vanished in the $P(r)$. Effect of
the fundamentals rod for the structure determination will
be discussed further in the next section.

B. Solving surface structure

The nearest neighbors are only parts of the information
included in $P(r)$. Here we attempt to derive the whole
surface structure from $P(r)$ using a standard procedure in
x-ray crystallography. As mentioned above, a number of
techniques and procedures to solve the Patterson function
are known in x-ray crystallography [21]. The minimum
function method, which we use here, is known as one of
the most fundamental and successful methods of solving
a Patterson function.

In general, the first step is to find a small cluster of
spots that repeatedly appears in $P(r)$. Such repeated
clusters are probably replicates of atomic clusters truly
existing in the surface structure. The minimum function
is a special method to estimate a correlation between the
cluster and the $P(r)$. When the $i$-th position of a
repeated cluster is expressed by $r_i$, the minimum function
$M(r)$ is defined as

$$M(r) = \text{Min} \{ P(r - r_1), P(r - r_2), \ldots, P(r - r_n) \}$$

where the function $\text{Min} \{ \}$ gives a minimum value from
the listed functions in the braces, and $n$ is the number of
atoms composing the cluster. Thus, $M(r)$ takes a mini-
um of the Patterson functions shifted by $r_i$. If one
choose a suitable cluster, the atomic structure, which we
want to know, may directly appear in $M(r)$.

When we survey the Patterson maps in Figs. 6(a)-(d),
we find that a cluster consisting of four spots in a dia-
mond shape repeatedly appears in the horizontal slices.
FIG. 6: (a)-(d) Horizontal sections of $P(r)$ at, (a) $z = 0.0$ Å, (b) $z = -2.25$ Å, (c) $z = -3.10$ Å, and (d) $z = -6.30$ Å. The intensity is normalized to the maximum value of whole $P(r)$, and shown by color scale and contour. (e) Ball-and stick models of $1 \times 1$- and b-clusters (see text). (f)-(i) Horizontal sections of $M(r)$ by b-cluster at, (f) $z = 0.0$ Å, (g) $z = -2.25$ Å, (h) $z = -3.10$ Å, and (i) $z = -6.30$ Å. (j) Top view of the SXRD model. Large shaded circles, medium open circles, medium solid circles, small solid circles and small open circles represent In atoms, zigzag chain Si, first-layer Si, second layer Si, 4th-layer Si, respectively.

Some of them are marked in Fig. 6(a)-(d) by solid lines. We call it a $1 \times 1$-cluster as shown in Fig.6(e). Since every side-length of the $1 \times 1$-cluster is 3.84 Å, it is immediately conjectured that they are the replicates of the substrate $1 \times 1$ unit in the $4 \times 1$-In surface. This $1 \times 1$-cluster is not suitable for the minimum function analysis, because several equivalent clusters exist in the $4 \times 1$ unit cell as the substrate.

Next, we consider a boomerang shaped clusters shown by broken lines in Figs. 6(a)-(c). We call it as a b-cluster as shown in the Fig.6(e). A distance between neighbor spots in the b-cluster is 2.35 Å, which corresponds to the bond length of Si. This strongly suggests that it is a footprint of Si-Si bonds existing on the surface. Although we already know the structural model, we believe that it is not difficult to identify the b-cluster from the present $P(r)$ without knowing the structural model beforehand.

Since the b-cluster consists of two spots in the $4 \times 1$ unit cell, $M(r)$ by b-cluster is just a minimum function between two shifted $P(r)$. The spots coordinates of the cluster are $(0, 0, 0)$ and $(1.34, 1.92, 0.08)(\text{Å})$. The latter was precisely determined as a three-dimensional peak position of the $S_1$ spot in Fig.5. Horizontal sections of a calculated $M(r)$ by b-cluster are shown in Figs. 6(f)-(i). The height ($z$-value) of the each section of Figs. 6(f)-(i) is the same as that of a corresponding section of $P(r)$ on the left side. Since the spots in the b-cluster are positioned almost at the same height, $M(r)$ section at certain
height can be roughly estimated from a horizontal section of $P(r)$ at the same height. For example, one could approximately obtain $M(r)$ section in Fig. 6(f) when one takes a minimum of $P(r)$ section in Fig. 6(a) and its copy shifted by $(1.34, 1.92, 0)$. Please note the color scale bar at Fig. 6(f) for all $M(r)$ sections, where the intensity was normalized by the maximum value of $P(r)$, and the intensity below 4% is ignored. In order to compensate an intensity dumping by the surface sensitivity, the intensity was multiplied by a factor 2 in Fig. 6(g) and 6(h), and 4 in Fig. 6(i).

The structure at the same height with the b-cluster should appear in the section at $z = 0.0$. Indeed, a self image of the b-cluster appears in the center of Fig. 6(f), which correspond to the zigzag chain Si of the SXRD model. The corresponding top view of the SXRD model is illustrated in Fig. 6(j), where medium open circles indicate the zigzag chain of Si. In addition to the zigzag Si, there are faint spots, which might correspond to the half of the In atoms of the SXRD model that locate at the almost same height with the zigzag Si.

Spots arranged in a 1x1 lattice are observed in Fig. 6(g), where the structure at 2.25 Å below the b-cluster should be imaged. This 1x1 structure corresponds to the first-layer of the substrate as shown in Fig. 6(j) by medium solid circles. Similar 1x1 structures in Fig. 6(h) and (i) are explained by the second-layer (small solid circles in Fig. 6(j)) and the 4th layer of the substrate (small open circles), respectively. Most of the Si frameworks of the 4x1 structure, including the zigzag chain and its back bonding structure, are correctly reproduced in the $M(r)$ by the b-cluster.

There are, however, twin structures existing above the zigzag Si layer in the $M(r)$, i.e. we see the same structure both at $\pm z$, when we look over the whole $M(r)$. This is because the b-cluster is too simple, and has an inversion symmetry. In order to eliminate the twin structure, a few more atoms, which destroy the inversion symmetry, should be added to the cluster. In the analysis, we have put two more back-bonding atoms to the b-cluster, which could be obtained from Fig. 6(f) and (g) without the knowledge of the structure model. Thus the new cluster (called b4-cluster hereafter) consists of the four atoms, which are labeled 1, 2, 3, and 4 in Fig. 1, and in Fig. 6(f) and (g). The atomic positions of the b4-cluster were obtained from the nearest neighbors inter-atomic vectors, and they were $(0, 0, 0)$, $(1.34, 1.92, 0.08)$, $(-0.96, 0, -2.15)$ and $(2.30, 1.92, -2.07)$ (Å).

A side view from [110] direction of 3D iso-surface plot of $M(r)$ by the b4-cluster is shown in Fig. 7(a), where the dumping by the depth $z$ was compensated, and the threshold of the iso-surface was set to be 4.2% of the maximum value of $P(r)$. In the figure, the ball-and-stick of the SXRD model is overlaid, where Si atoms are represented by small circles with diameter of 1 Å. In atoms are missing due to expected their large thermal vibration.

V. DISCUSSION

We have examined a effect of the fundamental rods for the structural analysis. Another $M(r)$ was calculated excluding the fundamental rods from the present data. The same view of the $M(r)$ by the b4-cluster with only the superstructure rods is shown in Fig. 7(b). Although some structures fit expected positions, many structures shift was within an error bar which was about 0.1Å for all directions. Although some artifacts are seen in Fig. 7(a) above the surface, they are rather weak and scatter in space so that they can be discriminated from the correct structure. Thus, the structure of Si atoms of 4x1-In surface, which are heavily reconstructed, has been directly reproduced in the present minimum function, although In atoms are missing due to expected their large thermal vibration.
are missing there. Furthermore, there are artifacts, which could not be discriminated from the meaningful structures, especially near and above the zigzag Si. These artifacts must originate from the lacked substrate structure information in $P(r)$ without the fundamental rods. A comparison between Fig.7(a) and (b) demonstrates an importance of the inclusion of the fundamental rods for a direct 3D reconstruction of a surface structure.

One of the problems of the present study is the missing of In atoms in the structural analysis. As mentioned already, the large thermal vibration of indium atoms make the identification of indium position difficult where the diffraction by In atoms is negligible above 100 eV of the primary energy with the back-scattering regime. Although positions of In atoms could be determined by LEED dynamical analysis, as reported in ref. 9 and 17, the contribution of In atoms are diluted in the present data analysis using the whole energy range. In addition, since the dynamical fluctuation model was expected for the $8 \times 2$ to $4 \times 1$ transition [16], large In fluctuations at $4 \times 1$ phase may also contribute to the missing. However, one may see indium atoms both in $P(r)$ and in $M(r)$ with the present method when one cools the sample below the phase transition temperature. Therefore, this problem may not be a serious drawback of the present method.

The obtained Patterson function, or the minimum function, is surprisingly consistent with the known surface structure of $4 \times 1$-In, although In atoms are missing. One obvious reason is the effect of full-performance CMTA method, i.e. the CMTA intensity $I(h,k,L)$ sufficiently approximates the kinematical structure factor. We show how the calculated $P(r)$ is improved by the increasing of averaging number of data sets in Fig.8, where line sections of $P(r)$ calculated from single, 5, 13 and full data sets are compared. As shown by arrows in the figure, three significant artifacts are observed in the curve by the single data set. These features are suppressed with increasing the number of averaging data sets. Data sets required for a reliable $P(r)$ should be case dependent, but 13 data sets may be required for the present case at least.

Another reason of the good $P(r)$ is a filtering action of the Fourier transformation. The kinematical components are effectively picked up from $I(h,k,L)$ into $P(r)$ by the Fourier transformation, while the dynamical components become some meaningless background in $P(r)$. Since the filtering action exists, the CMTA intensity profiles may not be compared directly with the kinematical structure factor. It may be impractical to perform a R-factor type analysis using a direct comparison of intensity profiles on the kinematical basis. We should use the ordinal dynamical analysis of LEED for this purpose, if needed. Since most of the structural framework will be determined by the CMTA Patterson function analysis, the dynamical analysis can be used to optimize detailed parameters at the last stage of the structural analysis.

VI. CONCLUSION

The constant momentum transfer averaging (CMTA) method of LEED was tested for the structural analysis of the Si(111)$4 \times 1$-In surface using a modern data-acquisition technology. The single-domain Si(111)$4 \times 1$-In surface was prepared to avoid a difficulty arising from the otherwise triple-domain structure. Thousands of $I(V)$ curves were measured by the automated LEED system, and the intensity of more than three hundreds of the reciprocal rods was obtained according to the CMTA procedure. The resulting Patterson function was excellently consistent with the known atomic structure of the $4 \times 1$-In surface, although In atoms were missing due to their large thermal vibration. The 3D surface structure has been directly solved from the Patterson function by the minimum function method. It is important to include the fundamental rods for the 3D structural reconstruction.

Acknowledgments

This work was supported in part by the Grants-in-Aid for Scientific Research (A) 12354003, Encouragement of Young Scientist (A) 14702007 and Scientific Research (B) 17360016 of the Ministry of Education, Culture, Sports, Science and Technology of Japan. One (S.K.) of the author acknowledges a partial support from CREST, JST.


http://www.sssj.org/ejssnt (J-Stage: http://ejssnt.jstage.jst.go.jp)
[22] The mean square displacement for In atom is nine times of that of Si at RT, when one estimates the displacement from a very low Debye temperature of In.