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*Daisuke Fujita Standardization of Data Transfer Format for Scanning Probe Microscopy*

*Review*

# Standardization of Data Transfer Format for Scanning Probe Microscopy

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Scanning probe microscopy (SPM) is the most versatile surface chemical analysis method both in the measurement functions and the operational environments. Recent activities and future outlook for SPM standardization through the International Organization for Standardization (ISO) is briefly reviewed. Following the highly prioritized item of standardization, SPM terminology, the data transfer format shall be standardized in order to enable the access to and processing of SPM data collected by different types of instruments. The present status of the development of open software for import of original data, conversion to standard format, comparison and processing are discussed.

## 1. Introduction

Followed by the pioneering work of *Topografiner* invented by R. Young and coworkers in 1971 [1], scanning tunneling microscopy (STM) was invented by G. Binnig, H. Rohrer and coworkers at IBM Zurich Research Laboratory in 1981 [2]. Due to its outstanding spatial resolution, enabling visualization of individual atoms at surfaces for the first time, the Nobel Prize in physics 1986 was awarded to G. Binnig and H. Rohrer "for their design of the scanning tunneling microscope". In 1986, Atomic Force Microscopy (AFM) was invented by G. Binnig, C.F. Quate and Ch. Gerber, enabled the imaging on insulating surfaces in addition to conductive ones [3]. Since then, various types of scanning probe microscopes (SPMs) have been developed. Measurement and characterization of various surface properties have been realized by using SPMs. Since the SPM measurement head is generally easy to dwarf, it is possible to be used in various environments such as ultrahigh vacuum, liquid, variable temperature, variable magnetic field, stress field, and so on [4]. By utilizing interaction between probe and surface, SPMs can be applied as versatile tools for nanotechnology such as atom operation, nano-deposition, nano-lithography, phase control and so on [5]. During the decade, global market of SPM has been growing steadily with the annual growth rate of about 10 % [6]. Specifically, Asia and the Pacific become the main market and the Europe and North America follow. In the industrial world, the semiconductor and nano-electronics industry is the main market and next, the growth in the life-science biotechnology field is remarkable.

In the case of measurement technique, the technique ripens, and the forming of a worldwide market and the generality rise and the research of the standardization goes into full swing. As for the surface-sensitive measurement techniques, such as Auger electron spectroscopy (AES) and/or X-ray photoelectron spectroscopy (XPS), the research and development began from the 1950s, but the commercial instruments appeared from the 1970s and the market for AES and XPS was formed. After about 20 years lapsed after the appearance, the research of the quantification and the reliability which pointed standardization went into full swing from the 1980s.

As SPM instruments were commercialized in late 1980’s and used as all-round surface analysis tools in research laboratories and manufacturing factories in 1990’s, the needs to the quantification and the standardization rose. Due to the rapid advances in technical innovations and the wide variety of SPMs, relatively little effort has been devoted to the quantification and standardization of SPM as a reliable surface analysis method. For example, the definitions of technical terms used for

SPM had some ambiguity. Different terms were used for almost identical methods, leading to unwanted misunderstandings for users. Therefore, the nomenclature and terminology of SPM shall be given as one of the items with high standardization needs. Since the manufacturers of SPM instruments developed their own data formats using their own terminology, it was difficult to compare the data taken by different instruments. Therefore, the standardization of data transfer format for SPM is highly wanted, which will facilitate access to and processing of SPM data collected by different manufacturer's instruments.

In this paper, we describe recent activities and researches related to SPM standardization, mainly activities performed in the framework of the International Organization for Standardization (ISO). Firstly the activity and future perspective of global standardization of SPM in the ISO framework is summarized. Then the standardization of data transfer format for SPM and the open software for data conversion and processing are introduced.

## 2. SPM standardization in ISO/TC201

Establishment of subcommittee (SC) for SPM global standardization in ISO Technical Committee TC201 (Surface Chemical Analysis) was proposed by Korean Agency of Technology and Standards (KATS) in 2003. As a result, SC9 for SPM was established in 2004. In TC201, SPM is recognized as one of the microscopic measurement techniques for surface chemical analysis. The member body representing Japan in ISO/TC201 is Japanese Industrial Standards Committee (JISC). The domestic deliberation organization to have had entrust member body business on TC201 and TC202 (microbeam analysis) from JISC is Japan National Committee for Standardization of Surface Chemical Analysis (JSCA).

In 2006 D. Fujita *et al.* proposed a roadmap for SPM standardization, in which the terminology for SPM was selected as the top priority item to be standardized [7]. In TC201, the subcommittee SC1 takes charge of the standardization of the terminology commonly used in the surface chemical analysis. The standardization of terminology for SPM was proposed by National Physical Laboratory (NPL) of UK in 2005. M.P. Seah, the chair of SC1, was appointed as the project leader. Finally the ISO document was published in 2010 as ISO 18115-2:2010 (Terms used in scanning probe microscopy) [8]. This International Standard covers 227 terms used in SPM as well as 86 acronyms. The terms cover words or phrases used in describing the samples, instruments and theoretical concepts involved in surface chemical analysis [9].

Since the most common use of SPM is topographic imaging, mainly using dynamic mode AFM, standardizing the methods used for surface topographical analysis should have high priority. Proper procedures for quantitative topographical analysis using SPM shall be standardized: the calibration of the measurement systems and the elimination of the morphological artifacts caused by thermal drift, tip shape, inappropriate scan condition, and so on. However, measurement of the chemical and physical properties and the functionalities of novel materials at the nanoscale is also important function of SPM. Therefore, the study groups for the potential SPM standardization items were firstly established in order to survey the usefulness and industrial demands for the international standards.

The first new work item proposal in SC9 was made by KATS on Near-field Scanning Optical Microscopy (NSOM), of which the leader was J.Y. Kim at Incheon University. International Standard ISO27911:2011 (Definition and calibration of the lateral resolution of a near-field optical microscope) was published in 2011 as the first International Standard from SC9 [10]. It describes a method for determining the spatial (lateral) resolution of an apertured NSOM by imaging an object with a size much smaller than the expected resolution. For the documentation of ISO27911:2011, the contribution by the NSOM experts in JSCA SPM-WG was quite significant. For example, proper reference-material (RM) for the calibration was proposed, in which a nanoscale point light source with the flatness to avoid the influence by the topography is required.

In 2012, the second International Standard ISO 11039:2012 (Measurement of drift rate) was published [11]. The project leader was Prof. W.-H. Huang. This International Standard is suitable for evaluating the drift rate based on SPM images [12,13]. It is intended to help manufacturers quote drift figures in specifications in a meaningful and consistent manner and to aid users to characterize the drift behavior so that effective experiments can be designed. By the quantitative evaluation of the drift rate, the distortion in images can be restored. On the other hand, the establishment of a quantitative technique to compensate thermal drift simultaneously (*in situ* drift compensation) is demanded from the practical viewpoint.

The timeline of the standardization activities in ISO/TC201 and the future plan is summarized in Fig.1. A number of new work item proposals (NWIP) were made during 2006 to 2008 from UK, Korea, China, Japan and Germany. Consequently 6 working groups (WG) for approved work items (AWI) were established from WG1 for NSOM to WG6 for electrical SPM. Already four International Standards were published and 5 work items are ongoing.

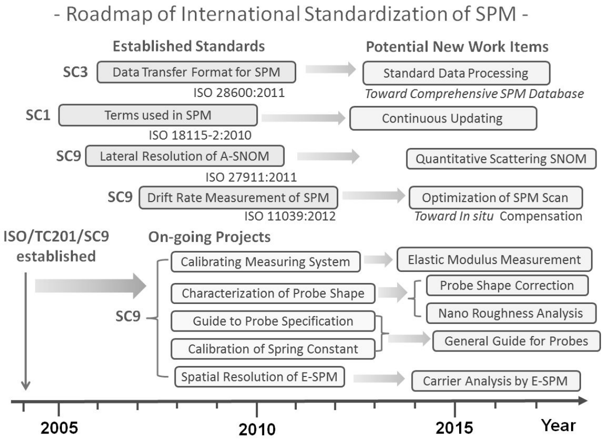


Fig. 1 Timeline of international standardization of scanning probe microscopy on the scheme of ISO TC201 as of FY2013.

## 3. Standardization of Data Transfer Format

### 3.1 Historical Overview

Starting from the standardization of terminology, the SPM standardization proceeds to two directions. One is the standardization of the data management and treatment for SPM, including image processing and image recovery techniques. The other one is the standardization matters about the quantification, the guideline of the use, the calibration procedure, certified reference material (CRM) and so on.

Towards the standardization of data management of SPM, the first step is to standardize the transfer data format for SPM. Previously SPM manufacturers used their own data format for their commercial instruments, so that the SPM data taken by different manufacturer's instruments did not have any compatibility. It was difficult for the SPM users to do quantitative comparison of the data without the detailed knowledge of the data formats.

TC201/SC3 takes charge of the standardization of data management and treatment commonly used in the surface chemical analysis. New Work Item Proposal (NWIP) of the standardization of SPM data transfer format was made by JISC and approved in 2008. D. Fujita, the chair of JSCA/SPM-WG, was appointed as the project leader. Finally the ISO document was published in 2011 as ISO 28600:2011 (Data transfer format for scanning-probe microscopy) [14]. This International Standard specifies a format to transfer SPM data from computer to computer via parallel interfaces or via serial interfaces over direct wire, local area network, global network or other communication links. The transferred data is encoded in those characters that appear on a normal computer display or printer. The format is designed for the data of SPM such as STM, AFM, and related surface analytical methods using pointed probes scanned over sample surfaces. The format covers the data taken by a single-channel imaging, multiple-channel imaging and single-point spectroscopy. The format can be expanded to two-dimensional spectroscopy mapping in the future version.

The basic ideas of the SPM data transfer format are to be readable, writable and transferable by using normal computer systems and communication facilities, to be flexible enough for the future expansion of the SPM derivatives and to be general enough to accommodate various kinds of physical quantities to be measured. To ensure the ease of data operation and telecommunication, it is advantageous to use only those characters that appear on a normal display or printing devices since there is no difficulty in transferring these by communications protocols and manual checking of the data is possible. This is the principle upon which the design of the format is based. This principle is similar to those of the pre-existing international standards ISO 14975 and 14976 for surface chemical analysis and ISO 22029 for micro-beam analysis [15-17].

### 3.2 Basic structure

For the flexibility for the future expansion and the data type generality, the basic structure of the format is a simple sequential text file using ASCII codes that represent alphabetic and numeric characters. Since there are different ASCII sets, it is important to define “character” as in ISO 14976. ASCII text file can be viewed in a text editor. Since the most dominant use of SPM is a two-dimensional single channel mapping, the format should firstly correspond to the major need for image data transfer. Other than the simple image data, the other important uses of SPM are multiple channel imaging and spectroscopy. Thus, the format should cover the multi-channel mapping data and single-point spectroscopy data. The SPM data transfer format can be saved with a filename extension of “.spm”. The file format consists of a header and data. The number and positions of header items are pre-determined so that one can know exactly the positions where the individual header items are located. Following the header items, the data is described in lines depending on the data type. For example, a regularly-spaced single-channel SPM image data can be stored in the format as below;

*data format = header + a single-column data array*

The header consists of 128 lines including blank ones. Each line is terminated by an end-of-line or EOL character which is a special character or a sequence of characters indicating the end of a line of text. In the case of ASCII character set or a compatible character set, EOL is signified by either Carriage Return (CR) or Line Feed (LF) individually, or Carriage Return followed by Line Feed (CR+LF). It should be noted that the actual code representing EOL character is dependent on the operating systems used for individual hardware. The header section shall include the items to specify the measurement specifications of SPM imaging or single-point spectroscopy.

### 3.3 Data array conventions for mapping

Following the common header information, each element of a two dimensional array for a SPM image shall be lined on the x-y plane according to the local x and y coordinates. The temporal order of each pixel of the acquired data array can be deduced by the scanning specifications described in the corresponding header. In the case of single-channel mapping with raster scan mode, a two-dimensional map of a specified physical quantity is represented by a matrix of real numbers. If the sampled map has M rows and N columns, then the corresponding matrix *z(i, j)* is of size *M*×*N*. The coordinate convention to denote such an image array is shown in Fig. 2.

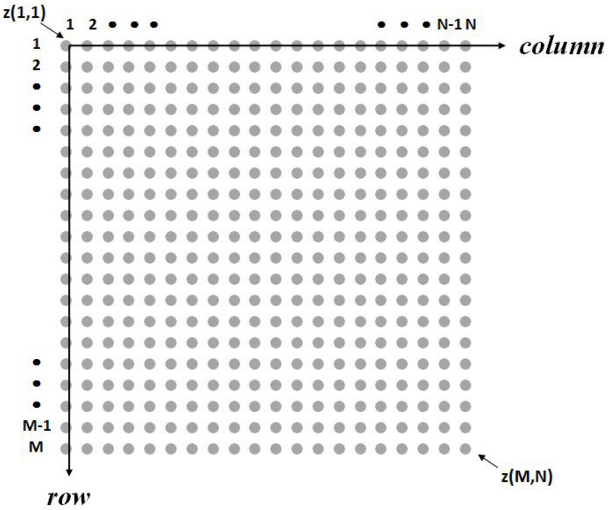
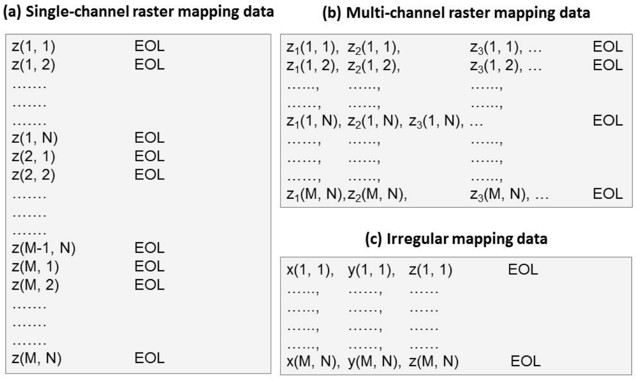


Fig. 2 Coordinate convention for an image matrix $z(i, j)$.

The origin of the coordinate system is at (1, 1). The formats for single-channel and multi-channel mapping data with raster scanning are a single column data array and a multi-column data array as shown in Fig. 3 (a) and (b), respectively. The maximum number of channels is limited by the maximum number of characters acceptable in each text line. The delimiter separating each data element shall be a comma. In the case of irregular mapping, the values of x and y coordinates shall be added as shown in Fig. 3 (c).



**(a) Single-channel raster mapping data**

z(1, 1) EOL
z(1, 2) EOL
…….
…….
…….
z(1, N) EOL
z(2, 1) EOL
z(2, 2) EOL
…….
…….
…….
z(M-1, N) EOL
z(M, 1) EOL
z(M, 2) EOL
…….
…….
…….
z(M, N) EOL

**(b) Multi-channel raster mapping data**

$z_1(1, 1)$, $z_2(1, 1)$, $z_3(1, 1)$, … EOL
$z_1(1, 2)$, $z_2(1, 2)$, $z_3(1, 2)$, … EOL
……, ……, ……,
……, ……, ……,
$z_1(1, N)$, $z_2(1, N)$, $z_3(1, N)$, … EOL
……, ……, ……,
……, ……, ……,
……, ……, ……,
$z_1(M, N)$,$z_2(M, N)$, $z_3(M, N)$, … EOL

**(c) Irregular mapping data**

x(1, 1), y(1, 1), z(1, 1) EOL
……, ……, ……
……, ……, ……
……, ……, ……
……, ……, ……
x(M, N), y(M, N), z(M, N) EOL

Fig. 3 The formats for (a) single-channel raster mapping data, (b) multi-channel raster mapping data, and (c) irregular mapping data.

### 3.4 Spatial geometry

Specification of the measurement geometry of SPM is an essential pre-requisite for quantitative analysis. General relationship between a probe and a sample stage is shown in Fig.4 (a). XYZ coordinates or global coordinates are placed on the plane of a sample stage. Spatial position of a probe can be specified by the XYZ coordinates as shown in Fig. 2 (b). To specify the geometrical arrangement of a probe on the XY plane is particularly important because the tip shape of a general cantilever probe is anisotropic. Therefore, it is required to specify the angle between the probe and X axis in the XY plane in order to correct a possible artifact due to the shape of a probe tip.

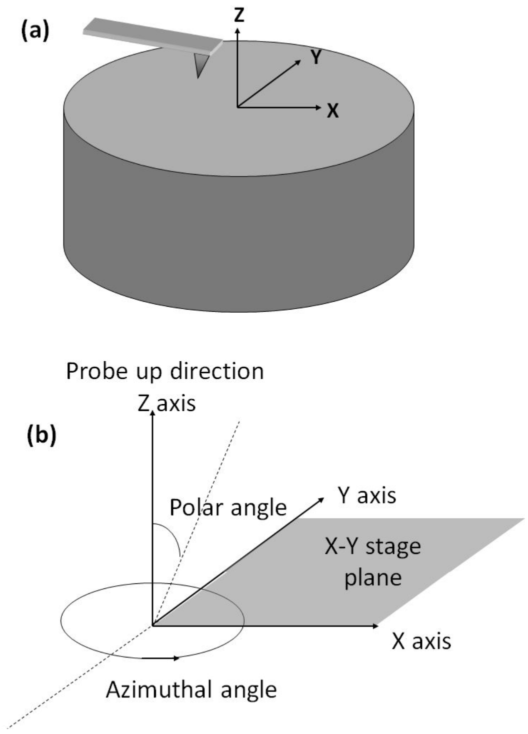


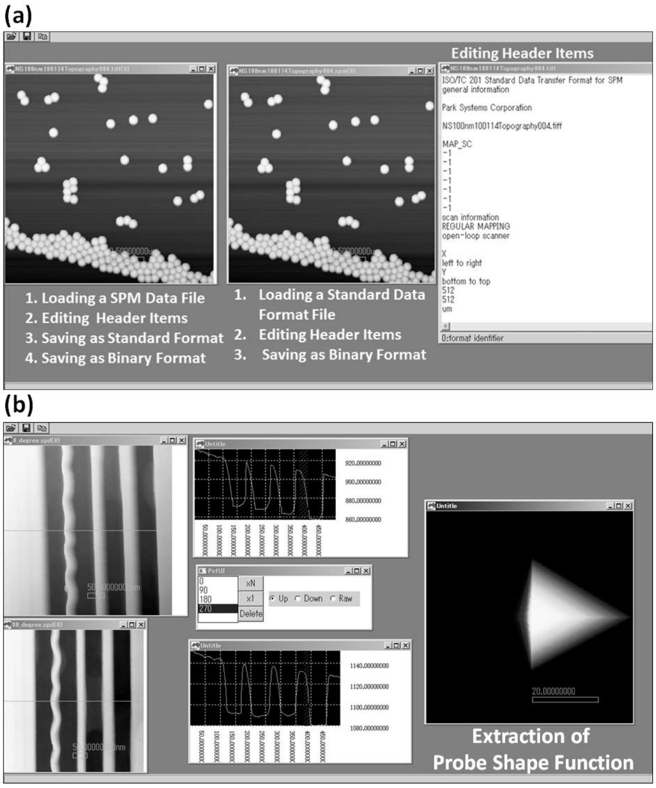
Fig. 4 (a) Geometrical arrangement of a probe and a stage. (b) Geometrical orientations for specifying spatial positions and directions.

### 3.5 Open software for data conversion

The potential benefits of the standardization of data transfer format are as follows; (1) Using the common terminology for the description of instrumental specifications and experimental conditions, SPM data can be treated more quantitatively, (2) SPM data taken by different machines can be shared and treated consistently, and (3) the development of SPM data treatment programs and the establishment of SPM database will be more promoted.

It is highly expected that the conversion program from the original native data format of the SPM manufacturer to the standard data transfer format will facilitate the exchangeability of the SPM data and promote the development of unified data processing programs that contribute for the quantitative analysis to improve. We have developed such data conversion software which is based on ISO 28600:2011 as shown in Fig. 5 (a). It is open software and is made accessible in the home page of National Institute for Materials Science (NIMS) [18]. Not only can the user convert the native SPM data into the standard data format compatible with ISO, but also can edit the header items, and save the data as a binary format file with the same header information.

At the next stage of the data management and treatment, the standardization of SPM data processing methods such as tilt correction, noise reduction, probe shape evaluation, image reconstruction, drift correction, and so on shall be promoted. For example, extraction of probe shape function from the AFM images of a tip characterizer is shown in Fig. 5(b) [19].



1. Loading a SPM Data File
2. Editing Header Items
3. Saving as Standard Format
4. Saving as Binary Format

1. Loading a Standard Data Format File
2. Editing Header Items
3. Saving as Binary Format

```
ISO/TC 201 Standard Data Transfer Format for SPM
general information

Park Systems Corporation

NS100nm100114Topography004.tiff

MAP_SC
-1
-1
-1
-1
-1
-1
-1
scan information
REGULAR MAPPING
open-loop scanner

X
left to right
Y
bottom to top
512
512
um
```

0:format identifier

Fig. 5 (a) Open data conversion software compatible with ISO 28600:2011 and (b) extraction of probe shape function from the tip characterizer.

## 4. Summary

Up to now, four International Standards on SPM were already published. Especially, due to its high priority and industrial demands, ISO 18115-2:2010 for terms used in SPM should be made compatible with the domestic standards such as Japanese Industrial Standards (JIS) in Japan.

In the case of the SPM standardization of the near future, the standardization of physical property measurement techniques for soft materials such as polymer and biomaterials, and electric and magnetic measurement methods for semiconductor and magnetic materials and devices should become more important.

Extensive expansion of the global SPM market is enhancing the needs for quantification and standardization, and becomes the driving force of making global standards. On the contrary, it is expected that global standards may promote the popularization of SPM and the expansion of the use and moreover advancing quantification and accuracy of the measurements.

Before the proposal of NWIs to ISO/TC201, it is important to grasp the industrial needs by market survey, and to implement an international interlaboratory test, so-called round robin test (RRT) for the usability evaluation by using the VAMAS (Versailles Project on Advanced Materials and Standard) scheme.

In the case of the SPM data management and treatment, the final goal is the building of common data processing environment and an integrated SPM database, which provide the environment where one can access and process the SPM data much more easily and effectively.

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## 閲読コメント

**［閲読者 1-1］**

header に書き込めるのは，1 byte（アルファベット，数字）だけでしょうか． 2 bytes（漢字，ひらがな，等）も使用可能でしょうか？

**［著者］**

漢字や平仮名等の 2 バイトの文字については対応しておりません．アルファベットや数字等の ASCII コード文字に限定しております．漢字等 2 バイト文字（UNICODE）は使用することはできますが，欧米等の他の言語圏のユーザーは理解不能となります．そのため，ASCII コード文字としております．

［**閲読者 1-2**］

確認です．試料表面の平均面ではなくて，試料台が XY 面ですね．だとすると試料平均表面が試料台と平行でないと XY がずれ，Z 方向も試料表面鉛直方向とずれます.

［著者］

試料が試料ステージ面と平行にセットされるようにユーザーは試みると思いますが，完全に平行に設置することはできません．SPM 計測では，いかなる場合でも，試料の傾き（Tilt）の影響を含めた試料表面形状を計測することになります．この傾き（Tilt）の補正は，SPM 形状像から判断してユーザーが画像データ処理として行うことになります.

［**閲読者 1-3**］

この報告を読み始めて心配になったのは，ユーザーが現状で使っているソフトに export 機能があるのか（または, 機能が付加されるのを期待するのか），また import はどうするのか, という点でした. また，SPM データを比較するために data transfer が必要だという論理ですから，比較する（引き算や割り算）ためのソフトはどこにあるのか，という点を気遣いながら読ませてもらいました.

この open software には，各社のデータを読み込む機能があると理解しましたが，データを比較する機能はあるのでしょうか？

abstract, introduction で「open software で各社のデータを読み込める」と記述していただけると安心して読み通せるような気がします．open software for data conversion という表現だと，データフォーマットの単なる変換機能と思えましたので.

また，複数データの比較をどのようにするか，またはどのような計画があるかを記述していただくと良いと思います.

［著者］

オープンソフトウェアでは各社のデータを import し，標準データフォーマットに変換し，傾き補正や探針形状評価とその補正などのデータ処理を行えるようになっています．また，ドリフト速度の計測と補正，ノイズ低減などの機能を付加する予定です. また，データ変換形式においてもヘッダー部分は共通ですが，データをバイナリー形式に変換する機能も付けてあります．これらにより，大きなデータについても対応できるようにしております．バイナリー形式のデータフォーマットの標準化は今後の改訂の際に取り組みたいと考えております．ご指摘の複数データの比較演算等の機能についても付加したいと考えております. ご指摘のアブストラクトでは，import of original data, conversion to standard format, comparison and processing と訂正しました.