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Surface chemical analysis — Data transfer format for scanning-probe microscopy

Analyse chimique des surfaces — Format de transfert de données pour la microscopie à sonde à balayage

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Foreword

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The main task of technical committees is to prepare International Standards. Draft International Standards adopted by the technical committees are circulated to the member bodies for voting. Publication as an International Standard requires approval by at least 75 % of the member bodies casting a vote.

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Introduction

In surface topographical and chemical analyses, many commercial instruments for scanning-probe microscopy (SPM) are operated under various environments. These SPM instruments provide the scientists and engineers with a wide range of analytical techniques and many operating parameters to vary. Since the whole of the data acquisition and processing of SPM can be digitally controlled by a computer with data storage devices, all the parameters and data can be recorded in digital files. However, since there has been no standard data format for SPM, the data taken by different manufacturers' instruments are difficult to transfer, exchange, share and archive. Besides, the complexity of the data processing required for the interpretation of the data makes it essential to keep a complete record of data acquisition and data pre-processing. Thus a standard format for the transfer of data is required to enhance communication, to interpret and treat the data taken by different instruments consistently and to reduce the uncertainty of data analysis.

Surface chemical analysis — Data transfer format for scanning-probe microscopy

1 Scope

This International Standard specifies a format for the transfer of scanning-probe microscopy (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 scanning tunnelling microscopy (STM), atomic force microscopy (AFM) and related surface analytical methods using pointed probes scanned over sample surfaces. The format covers the data taken by single-channel imaging, multiple-channel imaging and single-point spectroscopy. The format can be expanded to two-dimensional spectroscopy mapping in a future version.

2 Normative references

The following referenced documents are indispensable for the application of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 14976, *Surface chemical analysis — Data transfer format*

3 Description of the format

3.1 General

The basic ideas of the data transfer format for SPM are for the format to be readable, writable and transferable by using normal computer systems and communication facilities, to be flexible enough for the future expansion of SPM derivatives and to be general enough to accommodate various kinds of physical quantity 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[1] and ISO 14976 (see Clause 2) for surface chemical analysis and ISO 22029[2] for microbeam analysis.

The main body of this International Standard provides the description of the format and relevant conventions. Annex A describes the spatial geometry and types of scanner. Annex B explains typical data acquisition geometries, Annex C gives annotated examples of the format and Annex D gives actual examples of the format.

3.2 The components of the meta-language

The meta-language comprises a notation for specifying a set of rules for generating a linear sequence of characters. Only characters generated by the rules are to be inserted in the sequence. How to define the meta-language should follow ISO 14976.

The following is a summary of the symbols specified in the meta-language:

- `*` follows an integer specifying the number of occurrences.
- `-` precedes a syntactic-exception in a syntactic-term.
- `,` separates successive syntactic-terms in a single-definition.
- `|` separates alternative single-definitions in a definitions-list.
- `=` separates the definitions-list from the meta-identifier being defined in a syntax-rule.
- `;` terminates a syntax-rule.
- ‘ and ‘ or “ and “ enclose characters to form a terminal string, representing the characters as they are generated.
- (* and *) enclose a comment to form a bracketed-textual-comment, giving additional information for the human reader.
- (and) enclose a definitions-list to form a grouped-sequence, grouping items together in the usual algebraic sense.
- { and } enclose a definitions-list to form a repeated-sequence, a syntactic-primary which may occur zero or more times.
- [and] enclose a definitions-list to form an optional-sequence, a syntactic-primary which may be omitted or included once.
- ? and ? enclose text to form a special-sequence, a syntactic-primary described in a language other than the meta-language.

3.3 Basic structure

For the flexibility for future expansion and the generality of data type, the basic structure of the format is a simple sequential text file using ASCII codes that represent alphabetic and numeric characters, where ASCII means American Standard Code for Information Interchange. Since there are different ASCII sets, it is important to define “character” as in ISO 14976. An ASCII text file can be viewed in a text editor.

Because the most predominant 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 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 as *.spm, i.e. with the filename extension .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, regularly spaced single-channel SPM image data can be stored in the following format:

Data format = header items + a single-column data array

Temporal sequences of data resulting from continuous SPM experiments are not covered.

3.4 Header structure

The overall structure of the header shall follow the basic principle of the pre-existing standard data format in ISO 14976. However, a set of modifications with respect to ISO 14976 is needed for the header information of SPM data transfer format. Although it would be helpful to use the same terminology and vocabulary standardized for the conventional surface chemical analysis data transfer format, since a considerable effort was made to ensure a precise form of words[3][4], a significant number of new terms need to be added as the header items for the precise specification of SPM data.

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 the ASCII character set or a compatible character set, an 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 an EOL character is dependent on the operating systems used for individual hardware. The header section shall include the items shown in 3.5 and 3.6 to specify the measurement specifications of SPM imaging or single-point spectroscopy. In order to make it easier for the users to understand the format and to code the data treatment programmes, a format identifier and labels shall be included in the format.

3.5 Basic definitions of the common terms

character = (* A character is the character SPACE or any of the 94 graphic characters specified in the American National Standard for Information Systems — Coded character sets — 7-bit American national standard code for information interchange (7-bit ASCII), ANSI X3.4-1986. *);
decimal number = [sign], [[digit], '.'], [digit] – , EOL;
digit = '0' | '1' | '2' | '3' | '4' | '5' | '6' | '7' | '8' | '9';
EOL = ? 7-bit ASCII character indicating the end of the text line ?;
integer = [sign], [digit] –, EOL;
one or more = integer; (* The value of one or more shall be greater than zero. *);
two or more = integer; (* The value of two or more shall be greater than one. *);
real number = decimal number, ['E', [sign], [digit] –], EOL;
sign = '+' | '–';
text line = 80*[character], EOL;
units = ('A' | 'C' | 'c/s' | 'd' | 'degree' | 'eV' | 'Hz' | 'K' | 'm' | 'micro m' | 'm/s' | 'N' | 'n' | 'nA' | 'nm' | 'N/m' | 'Pa' | 's' | 'V'), EOL;
(* These values are abbreviations for the units listed below:

'A'	amps
'C'	coulombs
'c/s'	counts per second
'd'	dimensionless — just a number, e.g. counts per channel
'degree'	angle in degree
'eV'	electron volts
'Hz'	hertz
'K'	kelvins
'm'	metres
'micro m'	micrometres
'm/s'	metres per second
'N'	newtons
'n'	not defined here — may be given in a label
'nA'	nanoamps
'nm'	nanometres
'N/m'	newtons per metre
'Pa'	pascals
's'	seconds
'V'	volts

*);

3.6 Definitions of header items

(*1*) format identifier = 'ISO/TC 201 SPM data transfer format', EOL;
(*2*) label line = 'general information', EOL;
(*3*) institution identifier = text line;
(* character string identifying the institution responsible for the data, for example: 'NIMS'. *);
(*4*) instrument model identifier = text line;
(* character string identifying the instrument used for the data acquisition.*);
For a commercial SPM system, "manufacturer's name" and "machine-codename" shall be specified to identify the instrument used. In the case of a homemade system, "homemade" and/or "machine-code"

may be used for the identification.
(*5*) operator identifier = text line;
(* character string identifying the operator, for example: ‘Fujita’ *);
(*6*) experiment identifier = text line;
(* character string identifying the experiment *);
Generally, the original file name is a suitable candidate for the experimental identifier in order to identify the raw data file to be transferred.
(*7*) comment line = text line;
(* character strings describing the summary of the SPM measurement. *);
(*8*) experiment mode = (‘MAP_SC’|‘MAP_MC’|‘SPEC_SC’|‘SPEC_MC’|), EOL;
(* character string identifying the SPM measurement.
MAP_SC = A complete set of single-channel data values for every point in a regular two-dimensional spatial array.
MAP_MC = A complete set of multi-channel data values for every point in a regular or irregular two-dimensional spatial array.
SPEC_SC= A complete set of single-channel spectrum taken at a single point in an SPM image.
SPEC_MC= A complete set of multi-channel spectra taken at a single point in an SPM image. *);
(*9*) year in full = integer;
(* Gregorian calendar year, for example: ‘2008’ *);
(*10*) month = integer;
(*11*) day of month = integer;
(*12*) hours = integer; (* 24-hour clock *);
(*13*) minutes = integer;
(*14*) seconds = integer;
(*15*) number of hours in advance of Greenwich Mean Time = integer;
The above seven items are required to represent the date and time of the data measured. This is the time at which the last data point was recorded. If the value of any of the above six items is not known, the value –1 should be entered as a dummy value.

(*16*) label line = ‘scan information’, EOL;
(*17*) scan mode = (‘REGULAR MAPPING’ | ‘IRREGULAR MAPPING’), EOL;
(* character string indicating the type of scanning in an X-Y plane.
‘REGULAR MAPPING’ = two-dimensional mapping by raster scanning in the X-Y plane, where the probe tip is scanned by regular movement along a fast scan axis. The coordinate data on X and Y shall be omitted.
‘IRREGULAR MAPPING’ = two-dimensional mapping by vector scanning in the X-Y plane, where the probe tip is positioned by irregular movements. The coordinate values of X and Y for individual elements shall be added to the data array. *);
(*18*) scanning system = (‘open-loop scanner’ | ‘XY closed-loop scanner’ | ‘XYZ closed-loop scanner’), EOL;
(* character string indicating the type of scanning system. *);
For the positioning of the probe, position scanners based on piezo-electric components are usually used. Without closed-loop control, the position scanning system is called an open-loop scanner. A scanning system with a position sensor and a feedback control is called a closed-loop scanner.
(*19*) scanner type = (‘sample XYZ scan’ | ‘probe XYZ scan’ | ‘sample XY scan and probe Z scan’ | ‘sample Z scan and probe XY scan’), EOL;
(* character string indicating the type of scanner positioning in the X-Y plane *);
(*20*) fast scan axis = (‘X’ | ‘Y’), EOL;
(* character string indicating the scan axis to acquire each line of a map in the case of raster scanning *);
(*21*) fast scan direction = text line;
(* character string indicating the scan direction to acquire each line of a map in the case of raster scanning, for example: ‘left to right’, ‘right to left’, ‘bottom to top’ or ‘top to bottom’, depending on the fast scan axis *);
Maps are for one fast scan direction only. Maps incorporating both directions shall be compiled as two maps with relevant information in the comment line at (*7*).
(*22*) slow scan axis = (‘X’ | ‘Y’), EOL;
(* character string indicating the axis opposite to the fast scan axis in the case of raster scanning *);

(*23*) slow scan direction = text line;
(* character string indicating the slow scan direction to acquire a map, for example: ‘bottom to top’, ‘top to bottom’, ‘left to right’ or ‘right to left’, depending on the slow scan axis*);
(*24*) number of discrete X coordinates available in full map = integer;
(* a value indicating the number of pixel size of a map in the X direction, for example: ‘256’ or ‘512’ *);
(*25*) number of discrete Y coordinates available in full map = integer;
(* a value indicating the number of pixel size of a map in the Y direction *);
(*26*) physical unit of X axis = units;
(* character string indicating the physical unit of X axis, for example: ‘nm’ or ‘V’ *)
(*27*) physical unit of Y axis = units;
(* character string indicating the physical unit of Y axis, for example: ‘nm’ or ‘V’ *);
The length unit, such as ‘nm’, should be used for the X or Y axis if the scanner is properly calibrated. If it is not calibrated, the voltage applied to the corresponding piezo-electric scanner axis may be used.
(*28*) field of view X = real number;
(* a real number indicating the scan width of an image in the X direction *);
(*29*) field of view Y = real number;
(* a real number indicating the scan width of an image in the Y direction *);
The physical units for the field of view X and Y are the same as those of the X and Y axis, respectively.
(*30*) physical unit of X offset = units;
(* character string indicating the physical unit of X axis offset, for example: ‘nanometre’, ‘micrometre’ or ‘V’ *);
(*31*) physical unit of Y offset = units;
(* character string indicating the physical unit of Y axis offset, for example: ‘nanometre’, ‘micrometre’ or ‘V’ *);
(*32*) X offset = real number;
(* a real number indicating the X axis offset value relative to a stage midpoint *);
(*33*) Y offset = real number;
(* a real number indicating the Y axis offset value relative to a stage midpoint *);
(*34*) rotation angle = real number;
(* a real number indicating the degrees of rotation angle that the X axis of scan is rotated anticlockwise from the X coordinate on the sample stage *);
(*35*) physical unit of scan speed = units;
(* character string indicating the physical unit of the scan speed of a probe along the fast scan axis, for example: ‘nm/s’ *);
(*36*) scan speed = real number;
(* a real number indicating the scan speed along a fast scan direction *);
(*37*) physical unit of scan rate = units;
(* character string indicating the physical unit of the rate of scanning, for example: ‘Hz’ *);
(*38*) scan rate = real number;
(* a real number indicating the scan frequency along a fast scan direction *);
(*39*) SPM technique = text line;
(* character string specifying the SPM technique used for measurement, for example:
BEEM = ballistic electron beam microscopy,
CPAFM = conductive probe atomic force microscopy,
contact mode AFM = contact mode atomic force microscopy,
DFM = dynamic force microscopy,
EFM = electrostatic force microscopy,
FMM = force modulation microscopy,
FFM = friction force microscopy,
FM-AFM = frequency modulation atomic force microscopy,
IC-AFM = intermittent contact mode atomic force microscopy,
NC-AFM = non-contact mode atomic force microscopy,
KFM = Kelvin force microscopy,
MFM = magnetic force microscopy,
LFM = lateral force microscopy,
SCM = scanning capacitance microscopy,
SSRM = scanning spreading resistance microscopy,

STM = scanning tunnelling microscopy,
SThM = scanning thermal microscopy,
NSOM = near-field scanning optical microscopy,
SNOM = scanning near-field optical microscopy, and so on *);
(*40*) bias voltage contact = ('sample biased' | 'tip biased'), EOL;
(* character string specifying the electrode where the bias voltage is applied
sample biased = voltage is applied to the sample relative to the grounded probe tip
tip biased = voltage is applied to the probe tip relative to the grounded sample *);
(*41*) bias voltage = real number;
(* a real number indicating the bias voltage in V applied to the sample or probe tip *);
(*42*) number of set items = integer;
(* a value indicating the number of set items of the SPM measurement *);
(*43*) set parameter(s) = text line;
(* character string identifying each of the set parameters, SPs, separated by a comma, for example: 'free-oscillation amplitude, drive frequency' *);
The free-oscillation amplitude of a vibrating probe can be controlled by so-called drive amplitude. It defines the amplitude of the voltage applied to a piezo-electric system which drives the vibration of a cantilever. The drive frequency is the frequency at which an oscillating probe such as a cantilever probe is vibrated.
(*44*) unit(s) of set parameter(s) = units;
(* character string indicating each of the physical units of the set parameters, SPs, separated by a comma in order, for example: 'nm, Hz' *);
(*45*) value of set parameter = real number;
(* real number(s) indicating the value of each of the set parameters, SPs, separated by a comma, for example: '100, 100 000' *);

(*46*) calibration comment for set parameter = text line;
(* character string of relevant comments for each of the set parameters, SPs, separated by a comma, for example: 'SP1 is CV1 times instrumental value, SP2 is CV2 times instrumental value' *);

(*47*) calibration for set parameter = real number;
(* real number(s) indicating the calibration value, CV, of each of the set parameters, SPs, separated by a comma, for example: '1,054, 0,965' *);

(*48*) label line = 'environment description', EOL;
(*49*) environment mode = text line;
(*character string indicating the environment of the analysis space, for example, 'UHV', 'air', 'liquid', 'controlled atmosphere', etc *);
(*50*) sample temperature = real number;
(* a real number indicating the absolute temperature of the sample, expressed by the unit K *);
(*51*) surroundings pressure = real number;
(* a real number indicating the pressure of the sample surroundings, expressed by the unit Pa *);
(*52*) environment humidity = real number;
(* a real number indicating the relative humidity, especially in the case of the ambient or controlled atmosphere environment *);
Relative humidity is defined as the ratio of the partial pressure of water vapour in a gaseous mixture of air and water vapour to the saturated vapour pressure of water at a given temperature. Relative humidity is expressed as a percentage.
(*53*) comment line = text line;
(* character strings describing the environment specifications other than the above items *);
(*54*) label line = 'probe description', EOL;
(*55*) probe identifier = text line;
(*character string identifying the probe tip used for the data acquisition*);
(*56*) probe material = text line;
(*character string indicating the material of the probe tip, for example: Si, Si_3N_4, W, Pt-Ir, and so on *);
(*57*) normal spring constant = real number;
(* a real number indicating the normal spring constant of a force sensor, expressed by the unit N/m *);
(*58*) resonance frequency = real number;
(* a real number indicating the resonance frequency of an oscillating sensor probe, expressed by the unit Hz *);