# INTERNATIONAL STANDARD

ISO 28600

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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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ISO 28600 was prepared by Technical Committee ISO/TC 201, *Surface chemical analysis*, Subcommittee SC 3, *Data management and treatment*.

### 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 scanningprobe 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<sup>[1]</sup> and ISO 14976 (see Clause 2) for surface chemical analysis and ISO 22029<sup>[2]</sup> 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<sup>[3][4]</sup>, 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;
                   integer; (* The value of one or more shall be greater than zero. *);
one or more =
                   integer; (* The value of two or more shall be greater than one. *);
two or more =
                   decimal number, ['E', [sign], [digit] - ], EOL;
real number =
sian =
              80*[character]. EOL:
text line =
              ( 'A' | 'C' | 'c/s', | 'd' | 'degree' | 'eV' | 'Hz' | 'K' | 'm' | 'micro m' | 'm/s' | 'N' | 'n' | 'nA' | 'nm' | 'N/m' |
units =
              'Pa' | 's' | 'V' ), EOL;
        (* These values are abbreviations for the units listed below:
              'A'
                            amps
              'C'
                            coulombs
              'c/s'
                             counts per second
              'ď'
                             dimensionless — just a number, e.g. counts per channel
                             angle in degree
              '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. *);
                               ('MAP_SC'|'MAP_MC'|'SPEC_SC'|'SPEC_MC'|), EOL;
(*8*) experiment mode =
     (* 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.
                           'scan information', EOL;
(*16*) label line =
(*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
        '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
     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*).
                               ( 'X' | 'Y'), EOL;
(*22*) slow scan axis =
     (* 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.
                                real number;
(*28*) field of view X =
     (* 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,
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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<sub>3</sub>N<sub>4</sub>, 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 *);
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(*59*) cantilever sensitivity = real number;
      (*a real number relating the deflection signal of a cantilever probe to the distance of Z travel expressed
     by the unit nm. For the "spectroscopy mode" force distance curves, the value for the cantilever sensitivity
     (V/nm) is required to convert cantilever deflection from volts to nm. *);
(*60*) angle between probe and X axis = real number;
     (*a real number indicating the anticlockwise angle between the probe and the X axis of the sample stage,
     expressed by the unit degrees *);
(*61*) angle between probe vertical movement and Z axis in X azimuth = real number;
     (*a real number, expressed by the unit degrees*)"
(*62*) angle between probe vertical movement and Z axis in Y azimuth = real number;
     (*a real number, expressed by the unit degrees*)
(*63*) comment line =
                           text line;
     (* character strings describing the probe specifications other than the above items *);
                           'sample description', EOL;
(*64*) label line =
                                text line;
(*65*) sample identifier =
     (*character string identifying the sample, for example: 'Si(001) surface: P-doped 0,01 ohm-cm', and so
     on *);
(*66*) species label =
                           text line:
     (*character string identifying the chemical species of the sample, for example: 'Si' *);
(*67*) comment line =
                           text line:
     (*character string describing the sample specifications other than the above items *);
(*68*) label line =
                           'single-channel mapping description', EOL;
(*69*) Z axis channel =
                                text line:
     (*character string indicating the input signal for the intensity of the Z axis when the experiment mode =
     MAP SC, for example: 'height', 'tunnelling current', 'the number of photons', and so on *);
(*70*) physical unit of Z axis channel = units:
     (* character string indicating the physical unit of the Z axis, for example: 'nm', 'nA', 'c/s' *);
(*71*) comment line =
                           text line:
     (*character string describing the information on the Z axis specifications other than the above items *);
(*72*) label line =
                           'spectroscopy description', EOL;
(*73*) spectroscopy mode =
                                text line:
     (*character string describing the SPM spectroscopy mode, for example:
         I-V spectroscopy = the current (I) between the conductive surface and probe tip is measured while
         the bias voltage (V) is ramped.
         I-Z spectroscopy = the current (I) between the conductive surface and probe tip is measured while
         the tip height (Z) is ramped.
         force-distance curve = the force between the probe tip and sample surface is measured while the tip
         height is ramped. *);
(*74*) spectroscopy scan mode = ('REGULAR' | 'IRREGULAR'), EOL;
     (* 'REGULAR' = spectroscopy with regularly separated abscissa values, where the probe tip is located at
     a fixed position. The individual abscissa valued shall be omitted.
     'IRREGULAR' = spectroscopy with irregularly separated abscissa values, where the probe tip is located
     at a fixed position. The individual abscissa values shall be added to the data array *);
(*75*) abscissa label =
                           text line;
     (*character string describing the title of abscissa, for example: 'sample bias voltage' *);
(*76*) abscissa units =
                           units:
     (* character string describing the unit of abscissa of the spectrum, for example: 'V' *);
(*77*) abscissa start =
                           real number:
     (*a real number indicating the start value of the abscissa of the spectrum *);
(*78*) abscissa end =
                           real number;
     (*a real number indicating the end value of the abscissa of the spectrum *);
(*79*) abscissa increment =
                               real number:
     (*a real number indicating the increment value of the abscissa of the spectrum *);
(*80*) calibration constant for abscissa =
                                             real number
     (*a real number indicating the calibration constant for abscissa *);
(*81*) number of points in abscissa =
                                         integer;
     (*a value indicating the number of measured points in abscissa *);
```

```
(*82*) number of ordinate items =
                                         one or more;
      (* a value indicating the number of measured items in ordinate *);
     In the case of SPEC_MC or multi-channel spectra, the number shall be two or more.
(*83*) ordinate label(s) =
                                text line;
     (* character string identifying each of the ordinate labels, separated by a comma, for example: 'tunnelling
     current, phase shift' *);
(*84*) ordinate unit(s) =
                                units;
     (*character string describing each of the ordinate unit(s), separated by a comma, for example: 'nA,
     degree' *);
(*85*) calibration constant(s) for ordinate = real number
     (*a real number indicating each of the calibration constant(s) for ordinate(s) *);
(*86*) comment line =
                           text line;
     (*character string describing the spectroscopy specifications *);
(*87*) label line =
                           'data treatment description', EOL;
(*88*) data treatment = ( 'raw data' | 'pre-treated data' | 'post-treated data'), EOL;
     (* character string indicating the type of data treatment *);
(*89*) plain correction =
                               text line;
     (* character string indicating the type of flattening method used to correct the sample slope or undesired
     plain artifacts *);
(*90*) numerical filtering =
                                text line:
     (* character string indicating the type of data filtering processed, for example: 'Fourier filtering',
      'parametric low pass filter with a weight factor of 1,3', 'median filtering with a kernel size of 1×5', and so
(*91*) image reconstruction = text line;
     (* character string indicating the type of image reconstruction processed, for example: 'blind
     reconstruction' *);
(*92*) comment line =
                           text line:
     (* character string describing the data treatment specifications other than the above items *);
(*93*) label line =
                           'multi-channel mapping description', EOL;
(*94*) number of data channels = two or more;
     (* an integer indicating the number (>1) of data channels when experiment mode = MAP MC *);
(*95*) 1st data channel =
                                text line;
     (* character string indicating the signal source of the 1st data channel of MAP MC *);
(*96*) 1st data channel unit = units;
     (* character string indicating the physical unit of the 1st data channel of MAP MC *);
(*97*) 1st data channel comment = text line:
     (* character string describing the information on the 1st data channel of MAP MC *);
(*98*) 2nd data channel =
                                text line:
     (* character string indicating the signal source of the 2nd data channel of MAP MC *);
(*99*) 2nd data channel unit = units;
     (* character string indicating the physical unit of the 2nd data channel of MAP MC *);
(*100*) 2nd data channel comment = text line;
     (* character string describing the information on the 2nd data channel of MAP_MC *);
(*101*) 3rd data channel =
                               text line;
     (* character string indicating the signal source of the 3rd data channel of MAP_MC *);
(*102*) 3rd data channel unit = units;
     (* character string indicating the physical unit of the 3rd data channel of MAP MC *);
(*103*) 3rd data channel comment =
                                         text line:
     (* character string describing the information on the 3rd data channel of MAP MC *);
(*104*) 4th data channel =
                                text line:
      (* character string indicating the signal source of the 4th data channel of MAP MC *);
(*105*) 4th data channel unit = units;
     (* character string indicating the physical unit of the 4th data channel of MAP_MC *);
(*106*) 4th data channel comment =
                                         text line;
     (* character string describing the information on the 4th data channel of MAP MC *);
(*107*) 5th data channel =
                                text line:
     (* character string indicating the signal source of the 5th data channel of MAP MC *);
```

```
(*108*) 5th data channel unit = units;
     (* character string indicating the physical unit of the 5th data channel of MAP MC *);
(*109*) 5th data channel comment =
                                         text line;
     (* character string describing the information on the 5th data channel of MAP_MC *);
(*110*) 6th data channel =
                                text line;
      (* character string indicating the signal source of the 6th data channel of MAP MC *);
(*111*) 6th data channel unit = units;
      (* character string indicating the physical unit of the 6th data channel of MAP MC *);
(*112*) 6th data channel comment =text line:
     (* character string describing the information on the 6th data channel of MAP MC *);
(*113*) 7th data channel =
                                text line;
     (* character string indicating the signal source of the 7th data channel of MAP MC *);
(*114*) 7th data channel unit = units;
     (* character string indicating the physical unit of the 7th data channel of MAP_MC *);
(*115*) 7th data channel comment =text line;
     (* character string describing the information on the 7th data channel of MAP MC *);
(*116*) 8th data channel =
                                text line:
     (* character string indicating the signal source of the 8th data channel of MAP MC *);
(*117*) 8th data channel unit = units;
      (* character string indicating the physical unit of the 8th Z data channel of MAP MC *);
(*118*) 8th data channel comment =
                                         text line:
     (* character string describing the information on the 8th Z data channel of MAP MC *);
(*119*) comment line =
                                text line:
     (* character string describing the overall information on the multi-channel mapping *);
(*120*) blank line
                           EOL;
(*121*) blank line
                           EOL;
(*122*) blank line
                           EOL:
(*123*) blank line
                           EOL;
(*124*) blank line
                           EOL:
(*125*) blank line
                           EOL:
(*126*) blank line
                           EOL;
(*127*) blank line
                           EOL;
        The blank lines from 120 to 127 are reserved for possible future expansion of the format.
(*128*) end of header identifier = 'end of header', EOL;
```

The header consists of 128 lines followed by the data array. The end of the data file shall be indicated by the experiment terminator:

experiment terminator = 'end of experiment', EOL;

### 3.7 Data array conventions for mapping

Following the common header information, each element of a two-dimensional array for an 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 from the scanning specifications described in the corresponding header.

In the case of single-channel mapping with a 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  $M \times N$ . The coordinate convention to denote such an image array is shown in Figure 1. The origin of the coordinate system is at (1, 1). The format for single-channel mapping data with raster scanning is a single-column data array as shown below:

```
Z(1, 1) EOL
Z(1, 2) EOL
......
Z(1, N) EOL
```

Z(2, 1) Z(2, 2)	EOL EOL
Z(M-1, N) Z(M, 1) Z(M, 2)	EOL EOL
7(M N)	FOI

The format for multi-channel mapping data is composed of a multi-column data array as shown below:

$Z_1(1, 1),$ $Z_1(1, 2),$	$Z_2(1, 1),$ $Z_2(1, 2),$	Z <sub>3</sub> (1, 1), Z <sub>3</sub> (1, 2),	EOL EOL
,	,	,	
Z <sub>1</sub> (1, <i>N</i> ),	Z <sub>2</sub> (1, <i>N</i> ),	Z <sub>3</sub> (1, <i>N</i> ),	EOL
,	,	,	
$Z_1(M, N),$	$Z_2(M, N)$ ,	$Z_3(M, N), \ldots$	EOL

The maximum number of channels is eight, which is actually 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 below:

X(1, 1),	Y(1, 1),	Z(1, 1)	EOL
,	,		
, X(M, N),	······, Y( <i>M</i> , <i>N</i> ),	Z(M, N)	EOL

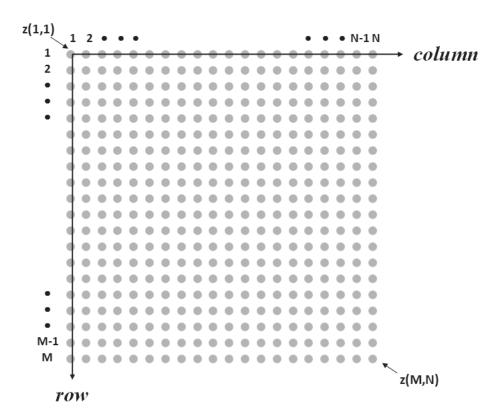


Figure 1 — Coordinate convention for an image matrix Z(i, j)

### 3.8 Measurement geometry

The three-dimensional geometry of the probe and sample is defined in the figures in Annex A, referred to the fixed orthogonal XYZ coordinate system. The Z direction is taken as the upward vertical, the X direction is the horizontal plane to the operator's right and the Y direction is the same horizontal plane but away from the operator standing in front of the instrument. The choice of the front might be arbitrary, but shall be clearly defined at the time the system geometry is evaluated.

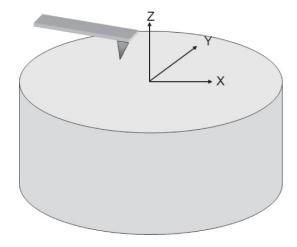
There are three major modes of scanning in SPM. One is with the probe scanning and the sample fixed. An SPM probe can scan over a sample surface using a three-dimensional positioning device or a scanner. The second one is with the sample scanning and the probe fixed. The third type is with both the sample and the probe tip scanning. In the last case, the sample is scanned in the X-Y plane while the probe moves along the Z direction.

# Annex A (informative)

# Spatial geometry and types of scanner

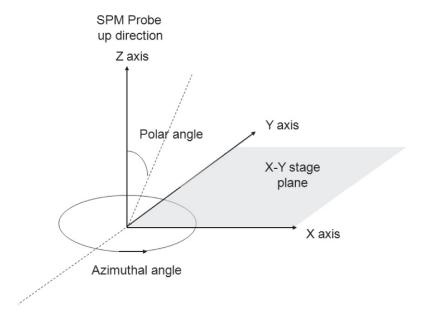
### A.1 Spatial geometry

Specification of the measurement geometry in SPM is an essential pre-requisite for quantitative analysis. The general relationship between the SPM probe and the sample stage is shown in Figure A.1a). XYZ coordinates or global coordinates are placed in the plane of the sample stage. The spatial position of the probe tip can be specified by the XYZ coordinates as shown in Figure A.1b). Specifying the geometrical arrangement of the SPM probe in the X-Y plane is particularly important because the tip shape of a general cantilever probe is anisotropic. Therefore, as shown in Figure A.2, the angle between the probe and the X axis in the X-Y plane has to be specified in order to correct a possible artifact due to the shape of the probe tip.



a) Geometrical arrangement of SPM probe and sample stage

Figure A.1 — General relationship between SPM probe and sample stage (continued on next page)



### b) Geometrical orientations for specifying spatial positions and directions

Figure A.1 — General relationship between SPM probe and sample stage

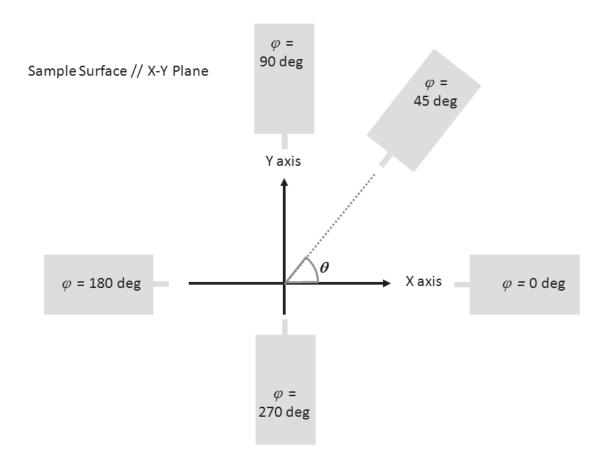
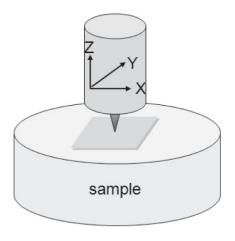
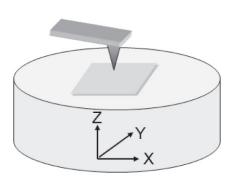


Figure A.2 — Geometrical arrangement of the SPM probe in the X-Y plane, indicating the angle between the probe tip and the X axis

### A.2 Types of scanner

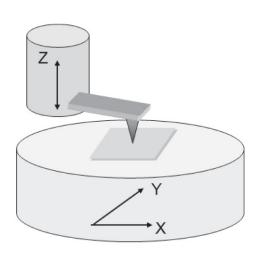
There are several modes of scanning and types of scanner in SPM, which should be properly specified. Raster scanning with data acquisition at equally spaced positions is generally used for SPM imaging. The simplest scanning system uses an open-loop scanner. To avoid the possible artifacts caused by hysteresis or non-linearity of PZT scanners, a closed-loop scanner with X, Y and/or Z position sensors is used. The most accurate and SI-traceable scanning system is based on raster scanning, with a closed-loop feedback using XYZ position sensors that are calibrated to be traceable to the SI unit of length. The four possible types of scanner are shown schematically in Figure A.3, the types shown in Figures A.3 a), A.3 b) and A.3 c) being popularly used for commercial instruments.

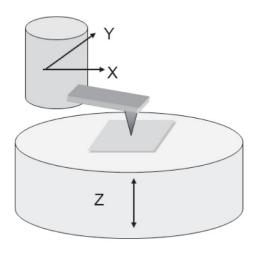




a) Probe scanned in X, Y and Z directions (sample fixed)

b) Sample scanned in X, Y and Z directions (probe fixed)





probe scanned in Z direction

c) Sample scanned in X and Y directions and d) Sample scanned in Z direction and probe scanned in X and Y directions

Figure A.3 — Geometrical arrangement of the SPM probe in the X-Y plane, indicating the angle between the probe tip and the X axis

# Annex B (informative)

# **Data acquisition geometry**

It is important to specify the SPM data acquisition area scanned by an SPM probe using the sample stage XY coordinates, or global coordinates. This area is shown schematically in Figure B.1. The spatial location of the centre of the scanning area or the scanner midpoint has to be the origin of the global coordinates. The centre position of the data acquisition area can be specified by a set of X offset and Y offset values in SI length units. These offsets are the X and Y coordinates of the global X and Y coordinates, respectively. The angle of rotation  $\theta$  of the scan area, expressed in degrees, can be defined as an anticlockwise angle of the fast scan direction measured from the global X axis.

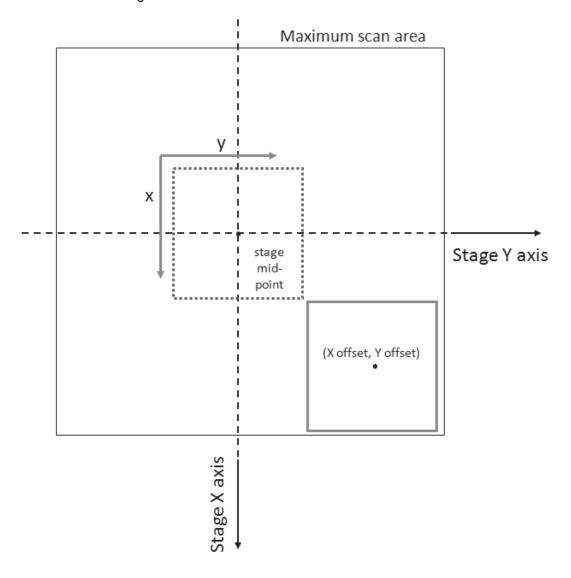


Figure B.1 — Schematic illustration of the data acquisition area scanned by an SPM probe using the sample stage X-Y coordinates or global coordinates

### **Annex C**

(informative)

## Annotated examples of the data format

### C.1 Regularly spaced single-channel SPM data

```
ISO/TC 201 SPM data transfer format
format identifier =
label line =
                                                               general information
institution identifier =
                                                               NIMS
instrument model identifier =
                                                               VT-SPM
operator identifier =
                                                               Fujita
experiment identifier =
                                                               original file name.dat
comment line =
                                                               SiO2/Si(111) surface imaging in UHV at HT
experiment mode =
                                                               MAP SC
                                                               2007
year in full =
month =
                                                               10
day of month =
                                                               11
hours =
                                                               18
minutes =
                                                               15
seconds =
                                                               0
number of hours in advance of Greenwich Mean Time =
                                                               8
label line =
                                                               scan information
                                                               REGULAR MAPPING
scan mode =
                                                               open-loop scanner
scanning system =
                                                               probe XYZ scan
scanner type =
fast scan axis =
                                                               Χ
fast scan direction =
                                                               left to right
slow scan axis =
                                                               Υ
slow scan direction =
                                                               bottom to top
number of discrete X coordinates available in full map =
                                                               256
number of discrete Y coordinates available in full map =
                                                               256
physical unit of X axis =
                                                               nm
physical unit of Y axis =
                                                               nm
field of view X =
                                                               50
field of view Y =
                                                               50
physical unit of X offset =
                                                               nm
physical unit of Y offset =
                                                               nm
X offset =
                                                               1 500
Y offset =
                                                               2 000
rotation angle =
                                                               n
physical unit of scan speed =
                                                               nm/s
                                                               100
scan speed =
physical unit of scan rate =
                                                               Hz
scan rate =
                                                               0.91
SPM method =
                                                               NC-AFM
bias voltage contact =
                                                               sample biased
bias voltage =
                                                               0,2
number of set items =
                                                               1
set parameter(s) =
                                                               phase shift
unit(s) of set parameter(s) =
                                                               degree
value of set parameter =
                                                               -1
calibration comment for set parameter =
```

calibration for set parameter = label line = environment description environment mode = **UHV** 873 sample temperature (K) = surroundings pressure(Pa) = 1,0E-8 environment humidity = comment line = label line = probe description probe identifier = needle sensor probe material = Si normal spring constant (N/m) = 40 resonance frequency (Hz) = 300 000 cantilever sensitivity (V/nm) = 0,04 angle between probe and X axis = 0,0 angle between probe vert. move. and Z axis in X azimuth = 0,0 angle between probe vert. move. and Z axis in Y azimuth = 0,0 comment line = label line = sample description SiO2/Si(111): P-doped 0,01 ohm-cm sample identifier = species label = Si, O comment line = heating at 873 K single-channel mapping description label line = Z axis channel = height physical unit of Z axis channel = nm comment line = label line = spectroscopy description spectroscopy mode = spectroscopy scan mode = abscissa label = abscissa unit = abscissa start = abscissa end = abscissa increment = calibration constant for abscissa = number of points in abscissa = number of ordinate items = ordinates labels = ordinate unit(s) = calibration constant(s) for ordinate = comment line = label line = data treatment description data treatment = raw data plain correction = numerical filtering = image reconstruction = comment line = label line = multi-channel mapping description number of data channels = 1st data channel = 1st data channel unit = 1st data channel comment = 2nd data channel = 2nd data channel unit = 2nd data channel comment = 3rd data channel = 3rd data channel unit = 3rd data channel comment =

```
4th data channel =
4th data channel unit =
4th data channel comment =
5th data channel =
5th data channel unit =
5th data channel comment =
6th data channel =
6th data channel unit =
6th data channel comment =
7th data channel =
7th data channel unit =
7th data channel comment =
8th data channel =
8th data channel unit =
8th data channel comment =
comment line =
blank line
end of header identifier =
                                                                 end of header
followed by 65 536 (256 × 256) lines of single-column data array for the Z axis, as below:
. . . . . . . . .
. . . . . . . .
experiment terminator =
                                                                 end of experiment
```

### C.2 Regularly spaced multi-channel SPM mapping

```
format identifier =
                                                              ISO/TC 201 SPM data transfer format
label line =
                                                             general information
institution identifier =
                                                             NIMS
instrument model identifier =
                                                             homemade SPM
operator identifier =
                                                             Kitahara
experiment identifier =
                                                             original_file_name.dat
comment line =
                                                              Si(111) surface imaging in UHV at RT
                                                             MAP\_MC
experiment mode =
                                                             2007
vear in full =
month =
                                                              12
                                                              15
day of month =
                                                              13
hours =
minutes =
                                                              15
seconds =
                                                              30
number of hours in advance of Greenwich Mean Time =
                                                             8
label line =
                                                             scan information
scan mode =
                                                              REGULAR MAPPING
                                                             open-loop scanner
scanning system =
                                                             probe XYZ scan
scanner type =
fast scan axis =
                                                             left to right
fast scan direction =
slow scan axis =
                                                              Υ
```

slow scan direction =	bottom to top
number of discrete X coordinates available in full map =	256
number of discrete Y coordinates available in full map =	256
physical unit of X axis =	nm
physical unit of Y axis =	nm
field of view X =	50
field of view Y =	50
physical unit of X offset =	nm
physical unit of Y offset =	nm
X offset =	1 500
Y offset =	2 000
rotation angle =	0
physical unit of scan speed =	nm/s
scan speed =	100
physical unit of scan rate =	Hz
scan rate =	0,91
SPM method =	NC-AFM
bias voltage contact =	sample biased
bias voltage =	0,2
number of set items =	1
set parameter(s) =	frequency shift
unit(s) of set parameter(s) =	Hz
value of set parameter =	<b>–15</b>
calibration comment for set parameter =	
calibration for set parameter =	
label line =	environment description
environment mode =	UHV
sample temperature (K) =	295
surroundings pressure (Pa) =	1,0E-8
environment humidity =	
comment line =	
label line =	probe description
probe identifier =	piezo-resistive cantilever
probe material =	Si
normal spring constant (N/m) =	40
resonance frequency (Hz) =	300 000
cantilever sensitivity (V/nm) =	0,037 9
angle between probe and X axis =	0,0
angle between probe vert. move. and Z axis in X azimuth =	0,0
angle between probe vert. move. and Z axis in Y azimuth =	0,0
comment line =	
label line =	sample description
sample identifier =	Si(111) surface: P-doped 0,01 ohm-cm
species label =	Si
comment line =	cleaned by flash up to 1 300 K in UHV
label line =	single-channel mapping description
Z axis channel =	
physical unit of Z axis channel =	
comment line =	
label line=	spectroscopy description
spectroscopy mode =	openiosopy decomplian.
spectroscopy scan mode =	
abscissa label =	
abscissa unit =	
abscissa start =	
abscissa end =	
abscissa increment =	
abbolosa moromoni	

calibration constant for abscissa =	
number of points in abscissa =	
number of ordinate items =	
ordinates labels =	
ordinate unit(s) =	
calibration constant(s) for ordinate =	
comment line =	
label line =	data treatment description
data treatment =	raw data
plain correction =	
numerical filtering =	
image reconstruction =	
comment line =	
label line =	multi-channel mapping description
number of data channels =	3
1st data channel =	height
1st data channel unit =	nm
1st data channel comment =	
2nd data channel =	dissipation
2nd data channel unit =	V .
2nd data channel comment =	
3rd data channel =	current
3rd data channel unit =	nA
3rd data channel comment =	
4th data channel =	
4th data channel unit =	
4th data channel comment =	
5th data channel =	
5th data channel unit =	
5th data channel comment =	
6th data channel =	
6th data channel unit =	
6th data channel comment =	
7th data channel =	
7th data channel unit =	
7th data channel comment =	
8th data channel =	
8th data channel unit =	
8th data channel comment =	
comment line =	
blank line	
end of header identifier =	end of header
followed by 65 536 (256 $\times$ 256) lines of comma-separated 1st,	2nd and 3rd values of corresponding channels
for the Z axis, as below:	
,	
,,	
,,	
experiment terminator =	end of experiment
одрениен испинатог —	она от ехрепшент

# C.3 Irregularly spaced single-channel SPM data

format identifier =	ISO/TC 201 SPM data transfer format
label line =	general information
institution identifier =	NIMS
instrument model identifier =	VT-SPM
operator identifier =	Ohgi
experiment identifier =	original_file_name.dat
comment line =	
	SiO2/Si(111) surface in UHV at HT
experiment mode =	MAP_MC
year in full =	2007
month =	10
day of month =	11
hours =	18
minutes =	15
seconds =	0
number of hours in advance of Greenwich Mean Time =	8
label line =	scan information
scan mode =	IRREGULAR MAPPING
scanning system =	open-loop scanner
scanner type =	probe XYZ scan
fast scan axis =	X
fast scan direction =	left to right
slow scan axis =	Υ
slow scan direction =	bottom to top
number of discrete X coordinates available in full map =	256
number of discrete Y coordinates available in full map =	256
physical unit of X axis =	nm
physical unit of Y axis =	nm
field of view X =	50
field of view Y =	50
physical unit of X offset =	nm
physical unit of Y offset =	nm
X offset =	1 500
Y offset =	2 000
rotation angle =	0
physical unit of scan speed =	nm/s
scan speed =	100
physical unit of scan rate =	Hz
scan rate =	0,91
SPM method =	NC-AFM
bias voltage contact =	sample biased
bias voltage =	0,2
number of set items =	1
set parameter(s) =	phase shift
unit(s) of set parameter(s) =	•
, , , , , , , , , , , , , , , , , , , ,	degree
value of set parameter =	<b>–1</b>
calibration comment for set parameter =	
calibration for set parameter =	
label line =	environment description
environment mode =	UHV
sample temperature (K) =	873
surroundings pressure (Pa) =	1,0E-8
environment humidity =	
comment line =	
label line =	probe description
probe identifier =	cantilever sensor
probe identifier -	Cantile ver sensor

probe material = normal spring constant (N/m) = resonance frequency (Hz) = cantilever sensitivity (V/nm) = angle between probe and X axis = angle between probe vert. move. and Z axis in X azimuth = angle between probe vert. move. and Z axis in Y azimuth = comment line = label line = sample identifier = species label = comment line = label line = Z axis channel =	Si 40 300 000 0,05 0,0 0,0 0,0 sample description SiO2/Si(001): P-doped 0,01 ohm-cm Si, O heating at 873 K single-channel mapping description height
physical unit of Z axis channel =	nm
comment line =	
label line =	spectroscopy description
spectroscopy mode = spectroscopy scan mode =	
abscissa label =	
abscissa unit =	
abscissa start =	
abscissa end =	
abscissa increment =	
calibration constant for abscissa =	
number of points in abscissa =	
number of ordinate items =	
ordinates labels =	
ordinate unit(s) =	
calibration constant(s) for ordinate = comment line =	
label line =	data treatment description
data treatment =	raw data
plain correction =	Tan data
numerical filtering =	
image reconstruction =	
comment line =	
label line =	multi-channel mapping description
number of data channels =	3
1st data channel =	X coordinate value
1st data channel unit =	nm
1st data channel comment =	
2nd data channel =	Y coordinate value
2nd data channel comment =	nm
2nd data channel comment = 3rd data channel =	height
3rd data channel unit =	nm
3rd data channel comment =	11111
4th data channel =	
4th data channel unit =	
4th data channel comment =	
5th data channel =	
5th data channel unit =	
5th data channel comment =	
6th data channel =	
6th data channel unit =	
6th data channel comment =	

```
7th data channel =
7th data channel unit =
7th data channel comment =
8th data channel =
8th data channel unit =
8th data channel comment =
comment line =
blank line
end of header identifier =
                                                               end of header
followed by 65 536 (256 × 256) lines of comma-separated 1st, 2nd and 3rd values of corresponding channels
for the X, Y and Z axes, as below:
....., ....., .....
....., ......, ......
...., ....., .....
....., ....., .....
experiment terminator =
                                                               end of experiment
```

### C.4 Single-channel spectroscopy data

```
format identifier =
                                                               ISO/TC 201 SPM data transfer format
label line =
                                                               general information
institution identifier =
                                                               NIMS
instrument model identifier =
                                                               VT-STM
operator identifier =
                                                               Fujita
experiment identifier =
                                                               original data.spe
comment line =
                                                               Ag nanodots on n-type Si(111)
experiment mode =
                                                               SPEC SC
                                                               2002
year in full =
month =
                                                               1
                                                               10
day of month =
hours =
                                                               11
                                                               12
minutes =
seconds =
number of hours in advance of Greenwich Mean Time =
label line =
                                                               scan information
scan mode =
scanning system =
                                                               open-loop scanner
scanner type =
                                                               probe XYZ scan
fast scan axis =
fast scan direction =
slow scan axis =
slow scan direction =
number of discrete X coordinates available in full map =
number of discrete Y coordinates available in full map =
physical unit of X axis =
physical unit of Y axis =
field of view X =
field of view Y =
physical unit of X offset =
```

physical unit of Y offset =	
X offset =	
Y offset =	
rotation angle =	0
physical unit of scan speed =	
scan speed =	
physical unit of scan rate =	
scan rate =	0.774
SPM method =	STM
bias voltage contact =	tip biased
bias voltage =	0,2
number of set items =	1
set parameter(s) =	tunnelling current nA
unit(s) of set parameter(s) =	0,2
value of set parameter = calibration comment for set parameter =	0,2
calibration for set parameter =	
label line =	environment description
environment mode =	UHV
sample temperature (K) =	275
surroundings pressure (Pa) =	1,0E-8
environment humidity =	1,02 0
comment line =	
label line =	probe description
probe identifier =	Ag-coated tungsten tip
probe material =	Ag, W
normal spring constant (N/m) =	<b>.</b>
resonance frequency (Hz) =	
cantilever sensitivity (V/nm) =	
angle between probe and X axis =	0,0
angle between probe vert. move. and Z axis in X azimuth =	0,0
angle between probe vert. move. and Z axis in Y azimuth =	0,0
comment line =	
label line =	sample description
sample identifier =	Si(111) n-type
species label =	Si
comment line=	Si(111)-(7 $\times$ 7) reconstructed surface
label line =	single-channel mapping description
Z axis channel =	
physical unit of Z axis channel =	
comment line =	anastropopy description
label line =	spectroscopy description
spectroscopy mode = spectroscopy scan mode =	I-V spectroscopy IRREGULAR
abscissa label =	sample bias voltage
abscissa unit =	V
abscissa start =	_1,511
abscissa end =	1,512
abscissa increment =	0,023 8
calibration constant for abscissa =	-,
number of points in abscissa =	128
number of ordinate items =	1
ordinates labels =	tunnelling current
ordinate unit(s) =	nA
calibration constant(s) for ordinate =	
comment line =	
label line =	data treatment description

```
data treatment =
                                                            raw data
plain correction =
numerical filtering =
image reconstruction =
comment line =
label line =
                                                            multi-channel mapping description
number of data channels =
1st data channel =
1st data channel unit =
1st data channel comment =
2nd data channel =
2nd data channel unit =
2nd data channel comment =
3rd data channel =
3rd data channel unit =
3rd data channel comment =
4th data channel =
4th data channel unit =
4th data channel comment =
5th data channel =
5th data channel unit =
5th data channel comment =
6th data channel =
6th data channel unit =
6th data channel comment =
7th data channel =
7th data channel unit =
7th data channel comment =
8th data channel =
8th data channel unit =
8th data channel comment =
comment line =
blank line
end of header identifier =
                                                            end of header
followed by 128 lines of comma-separated values for the abscissa and ordinate, as below:
-1,511, -0,03964
-1,487, -0,03892
.....
.....
......
1,512. 0,085 56
```

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end of experiment

experiment terminator =

# Annex D

(informative)

# **Examples of the data format**

### D.1 General

Examples from Annex C are given below. To save space in printing here, carriage returns have been replaced by a comma plus a space.

### D.2 Example C.1 of the data format

### Regularly spaced single-channel SPM data

ISO/TC 201 SPM data transfer format, general information, NIMS, VT-SPM, Fujita, original_file_name.dat, SiO2/Si(111) surface imaging in UHV at HT, MAP_SC, 2007, 10, 11, 18, 15, 0, 8, scan information, REGULAR MAPPING, open-loop scanner, probe XYZ scan, X, left to right, Y, bottom to top, 256, 256, nm, nm, 50, 50, nm, nm, 1 500, 2 000, 0, nm/s, 100, Hz, 0,91, NC-AFM, sample biased, 0,2, 1, phase shift, the second state of t
degree, -1, , , environment description, UHV, 873, 1,0E-8, , , probe description, cantilever sensor, Si, 40,
300 000, 0,04, 0,0, 0,0, 0,0, , sample description, SiO2/Si(111): P-doped 0,01 ohm-cm, Si, O, heating at
873 K, single-channel mapping description, height, nm, , spectroscopy description, , , , , , , , , , , data
treatment description, raw data, , , , multi-channel mapping
description, , , , , , , , , , , , , , , , , , ,
followed by 65 536 (256 $ imes$ 256) lines of single-column data array for the Z axis, as below:
end of experiment

### D.3 Example C.2 of the data format

### Regularly spaced multi-channel SPM data

# **Bibliography**

- [1] ISO 14975, Surface chemical analysis Information formats
- [2] ISO 22029, Standard file format for spectral data exchange
- [3] ISO 18115-1, Surface chemical analysis Vocabulary Part 1: General terms and terms used in spectroscopy
- [4] ISO 18115-2, Surface chemical analysis Vocabulary Part 2: Terms used in scanning-probe microscopy



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