INTERNATIONAL STANDARD

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Surface chemical analysis — Information formats

Analyse chimique des surfaces — Protocoles de l'information

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Contents

Page

Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

International Standards are drafted in accordance with the rules given in the ISO/IEC Directives, Part 3.

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.

Attention is drawn to the possibility that some of the elements of this International Standard may be the subject of patent rights. ISO shall not be held responsible for identifying any or all such patent rights.

International Standard ISO 14975 was prepared by Technical Committee ISO/TC 201, *Surface chemical analysis*, Subcommittee SC 3, *Data management and treatment*.

Annexes A and B of this International Standard are for information only.

Introduction

ISO 14976 provides a digital data transfer format for communicating surface chemical analysis data. Since the importance of databases is increasing in many scientific fields, storage and manipulation of spectral data in databases have become necessary. The structure of ISO 14976 is suitable for communication, but database manipulation is quite different from data communication. Information additional to that contained in ISO 14976 is necessary to handle the data in the databases, so this International Standard proposes three formats which define information packages for (1) specimen information, (2) calibration information and (3) data processing information, which are important to manipulate spectral data in databases. The future compatibility of the format is essential. This format is designed to work with ISO 14976 so that software designed to read the latter will still function correctly with these information packages added. This International Standard, therefore, is supplementary to and compatible with ISO 14976.

The motivation behind the choices made in defining the textual form of the data files described in this International Standard are important. To make it easy for programmers to implement the format reliably in new software, aspects of the Microsoft Windows™ ".INI" file structure are followed. Most modern computers have facilities to read and write this format from a wide range of computer languages via the Windows Application Programming Interface™.

Surface chemical analysis — Information formats

1 Scope

This International Standard specifies a format to supplement ISO 14976 to transfer data for the creation, expansion and revision of a surface chemical analysis spectral database. The format is applied to Auger electron spectroscopy (AES) and X-ray photoelectron spectroscopy (XPS) spectral data.

2 Normative reference

The following normative document contains provisions which, through reference in this text, constitute provisions of this International Standard. For dated references, subsequent amendments to, or revisions of, any of these publications do not apply. However, parties to agreements based on this International Standard are encouraged to investigate the possibility of applying the most recent edition of the normative document indicated below. For undated references, the latest edition of the normative document referred to applies. Members of ISO and IEC maintain registers of currently valid International Standards.

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

3 Terms and definitions

For the purposes of this International Standard, the following terms and definitions apply.

3.1
spectral database
set of retrievable spectral data

3.2
information
information about specimens and/or the procedures of analyser calibration and/or data processing procedures and/or the information necessary to create spectral databases

3.3
package
set of text lines which describe information on spectral data

4 Symbols and abbreviated terms

CAS Chemical Abstracts Service

DTF data transfer format (as specified in ISO 14976)

IUPAC International Union of Pure and Applied Chemistry

N/A not applicable

5 Description of information formats

5.1 General

Information is inserted into the comment lines of the DTF or attached to the DTF as packages. As a result, the existing DTF could be used, without alteration, as a carrier for the information packages; these packages occupy the experiment-comment line or the block-comment lines in the DTF, or build blocks outside the DTF.

With this structure, the reading program, which utilizes information packages, can look for the format identifiers in either the experiment-comment lines, where they apply to all blocks, or in the block-comment lines, where they apply to just one block, or outside the DTF. Existing reading programs would interpret these packages as comments intended for human readers and ignore them.

In this International Standard, the information packages for “specimen information format”, “calibration information format”, and “data processing format” are described. It is a modular structure so that compatibility with software previously written is always maintained.

5.2 Additional rules and definitions

text line: up to 80 characters, followed by carriage return

character: one alternative from the following set comprising the character SPACE and the 7-bit ASCII character set:

‘ ’ | ‘!’ | ‘"’ | ‘#’ | ‘$’ | ‘%’ | ‘&’ | “'” | ‘(’ | ‘)’ | ‘*’ | ‘+’ | ‘,’ | ‘-’ | ‘.’ | ‘/’

| ‘0’ | ‘1’ | ‘2’ | ‘3’ | ‘4’ | ‘5’ | ‘6’ | ‘7’ | ‘8’ | ‘9’ | ‘:’ | ‘;’ | ‘<’ | ‘=’ | ‘>’ | ‘?’

| ‘@’ | ‘A’ | ‘B’ | ‘C’ | ‘D’ | ‘E’ | ‘F’ | ‘G’ | ‘H’ | ‘I’ | ‘J’ | ‘K’ | ‘L’ | ‘M’ | ‘N’ | ‘O’

| ‘P’ | ‘Q’ | ‘R’ | ‘S’ | ‘T’ | ‘U’ | ‘V’ | ‘W’ | ‘X’ | ‘Y’ | ‘Z’ | ‘[’ | ‘\’ | ‘]’ | ‘^’ | ‘_’

| ‘`’ | ‘a’ | ‘b’ | ‘c’ | ‘d’ | ‘e’ | ‘f’ | ‘g’ | ‘h’ | ‘i’ | ‘j’ | ‘k’ | ‘l’ | ‘m’ | ‘n’ | ‘o’

| ‘p’ | ‘q’ | ‘r’ | ‘s’ | ‘t’ | ‘u’ | ‘v’ | ‘w’ | ‘x’ | ‘y’ | ‘z’ | ‘{’ | ‘|’ | ‘}’ | ‘~’

where the vertical bar separates alternatives, given between quotation marks.

carriage return: 7-bit ASCII character CARRIAGE RETURN followed by 7-bit ASCII character LINE FEED

multiple text lines: a set of text lines which identify one item

The decimal sign is given as a point in the format items for computer entry and in examples of verbatim computer entries although, in conformance with the ISO/IEC Directives, Part 3, the decimal sign is given as a comma in the rest of the text.

5.3 The formats

5.3.1 Structures

5.3.1.1 Contents of the specimen information package

The specimen information package consists of the following items shown in bold, on contiguous lines of the text file. Bold items are defined in 5.3.2. All items shall be present and in the order given.

specimen information format identifier

host material

IUPAC chemical name

chemical abstracts registry number

host material composition

bulk purity

known impurities

structure

form of product

supplier

lot number

homogeneity

crystallinity

material family

special material classes

specimen mounting

ex situ preparation

in situ preparation

charge control conditions

specimen temperature

comment on specimen information

end of specimen information format identifier

5.3.1.2 Contents of calibration information package

The calibration information package consists of the following items shown in bold, on contiguous lines of the text file. Bold items are defined in 5.3.2. All items shall be present and in the order given.

calibration information format identifier

energy scale calibration

intensity scale calibration

resolution calibration

end of calibration information format identifier

5.3.1.3 Contents of data processing information package

The data processing information package consists of the following items shown in bold, on contiguous lines of the text file. Bold items are defined in 5.3.2. All items shall be present and in the order given.

data processing information format identifier

data-handling procedure

end of data processing information format identifier

5.3.2 Definition of the items in the formats

5.3.2.1 Specimen information format

Items in bold not defined here are defined in 5.2. Texts in italic characters enclosed by quotation marks are used to code the format, although they do not appear in italics in the formatted data. IUPAC nomenclature and CAS registry number are referred to to code the format.

specimen information format identifier is the **text line**:

"*[ISO_Specimen_Information_Format_1998_October_15]*"

host material is a **text line**. This text line starts with "*host_material*=", followed by a generic description of the specimen. For layered structures, the host material is the "bulk" substance near the surface.

IUPAC chemical name is a **text line**. This text line starts with "*IUPAC_chemical_name*=", followed by the IUPAC chemical name of the host material or, if there is no specification, followed by "*none*", "*unknown*" or "*N/A*".

chemical abstracts registry number is a **text line**. This text line starts with "*chemical_abstracts_registry_number*=", followed by the CAS registry number of the host material or, if there is no specification, followed by "*none*", "*unknown*" or "*N/A*".

host material composition is a **text line**. This text line starts with "*host_material_composition*=", followed by the list of the principal elements present or the chemical formula. When the principal elements' names are used, the composition is given by a real number followed by "*mass%*" or "*atomic%*". If the composition cannot be specified, use "-" instead of a real number.

bulk purity is a **text line**. This text line starts with "*bulk_purity*=", followed by the purity of the material and guarantor (if possible) or, if there is no specification, followed by "*unknown*" or "*N/A*". The purity is given by a real number, and the units acceptable are mass% and atomic%. The units shall be given. An expression like "4N" is not acceptable.

known impurities is a **text line**. This text line starts with "*known_impurities*=", followed by the impurity name(s), concentration(s) and guarantor (if possible) or, if there is no specification, followed by "*none*", "*unknown*" or "*N/A*". The units acceptable are as follows: mass%, atomic%, ppm, ppb, atoms/cm3, and atoms/cm2. The units shall be given.

structure is a **text line**. This text line starts with "*structure*=", followed by information such as a description of the crystal lattice and orientation, e.g. hexagonal close-packed, and/or comments such as fracture surface at grain boundary, etc., or, if there is no specification, followed by "*unknown*" or "*N/A*".

form of product is a **text line**. This text line starts with "*form_of_product*=", followed by the form of the product that the specimen is used for or, if there is no specification, followed by "*unknown*" or "*N/A*".

supplier is a **text line**. This text line starts with "*supplier*=", followed by the name of the manufacturer and/or supplier of the host material or by a reference to how the host was made or, if there is no specification, followed by "*unknown*" or "*N/A*".

lot number is a **text line**. This text line starts with "*lot_number*=", followed by the code that identifies the production run, etc., or, if there is no specification, followed by "*unknown*" or "*N/A*".

homogeneity is a **text line**. This text line starts with "*homogeneity*=", followed by "*homogeneous*" or "*inhomogeneous*" or "*unknown*" or "*N/A*" or another description of the homogeneity of the specimen if none of these is appropriate. This may be followed by a comment, provided the comment is preceded by "*;*".

crystallinity is a **text line**. This text line starts with "*crystallinity*=", followed by "*single*" (single crystal, together with Miller indices of the surface connected by "_") or "*poly*" (polycrystalline) or "*amorphous*" or "*unknown*" or "*N/A*" or another description of the crystallinity of the specimen if none of these is appropriate. This may be followed by a comment, provided the comment is preceded by "*;*".

material family is a **text line**. This text line starts with "*material_family*=", followed by "*metal*" or "*inorganic*" (inorganic compound) or "*organic*" (organic compound) or "*polymer*" or "*semi*" (semiconductor) or "*bio*" (biological material) or "*composite*" or "*super_conductive*" (super-conductive material) or another description of the crystallinity of the specimen if none of these is appropriate. This may be followed by a comment, provided the comment is preceded by "*;*".

special material classes is a **text line**. This text line starts with "*special_material_classes*=", followed by "*rod*" (rod or ingot) or "*sheet*" [sheet or foil (without substrate)] or "*film_single*" [single-layer thin film or coating (on substrate)] or "*film_multi*" [multi-layered thin film or multi-layered coating (on substrate)] or "*sinter*" (sintered material) or "*wafer*" or "*powder*" or "*fibre*" or another description of the special material class of the specimen if none of these is appropriate. This may be followed by a comment, provided the comment is preceded by "*;*".

specimen mounting is a **text line**. This line starts with "*specimen_mounting*=", followed by "*mechanical*" (mechanically mounted using a screw, spring, etc.) or "*mechanically_under_grid*" (mechanically pressed to a grid by a spring) or "*conductive_adhesive*" (fixed by conductive adhesive material) or "*nonconductive_adhesive*" (fixed by non-conducting adhesive material) or "*powder_compact_In*" (powder compact in indium foil, indium pressure pad) or "*powder_put_into*" [powder put into a conductive material (for example, a hole in a copper block)] or another description of the specimen mounting if none of these is appropriate. This may be followed by a comment, provided the comment is preceded by "*;*".

ex situ preparation is a **text line**. This text line starts with "*ex_situ_preparation*=", followed by "*none*" or "*polish*" or "*cleavage*" or "*ion*" (cut by ion beam) or "*powder_compact_steel_pad*" (powder compacted using steel pressure pad) or "*acetone*" (degreased by acetone) or another description of ex situ preparation of the specimen if none of these is appropriate. If ex situ preparation is carried out by a series of the above procedures, **multiple text lines** are used, and the label for each text line is numbered, i.e. "*ex_situ_preparation_1*=", "*ex_situ_preparation_2*=", etc. The number indicates the order of the ex situ preparation procedures. If different kinds of ex situ preparation are carried out simultaneously, the ex situ preparation procedures are combined with "+" following the single label "*ex_situ_preparation*=". The text line may be followed by a comment, provided the comment is preceded by "*;*".

in situ preparation is a **text line**. This text line starts with "*in_situ_preparation*", followed by "*none*" or "*ion*" (ion sputtering, together with ion gun voltage, ion gun current and ion species connected by "_") or "*cleavage*" or "*heating*" or "*scratch*" or another description of the in situ preparation of the specimen if none of these is appropriate. If in situ preparation is carried out by a series of the above procedures, **multiple text lines** are used, and the label for each text line is numbered, i.e. "*in_situ_preparation_1=*", "*in_situ_preparation_2=*", etc. The number indicates the order of the in situ preparation procedures. If different kinds of in situ preparation are carried out simultaneously, the in situ preparation procedures are combined with "+" following the single label "*in_situ_preparation=*". The text line may be followed by a comment, provided the comment is preceded by "*;*".

charge control condition is a **text line**. This text line starts with "*charge_control_condition=*", followed by "*none*" or "*flood*" (flood gun, together with flood gun voltage and flood gun current connected by "_") or "*screen*" (cover with mesh, metal foil, etc.) or another description of the charge control condition of the specimen if none of these is appropriate. If charge control procedures are carried out by a series of the above operations, **multiple text lines** are used, and the label for each text line is numbered, i.e. "*charge_control_condition_1=*", "*charge_control_condition_2=*", etc. The number indicates the order of the charge control procedures. If different kinds of charge control procedure are carried out simultaneously, each charge control condition is combined with "+" following the single label "*charge_control_condition=*". The text line may be followed by a comment, provided the comment is preceded by "*;*".

specimen temperature is a **text line**. This text line starts with "*specimen_temperature=*", followed by the ambient temperature or heating temperature or, if there is no specification, followed by "*unknown*". The temperature is given in kelvins and expressed by a real number followed by "*K*". The text line may be followed by a comment, provided the comment is preceded by "*;*".

comment on specimen information is a **text line**. This text line starts with "*comment=*", followed by the comment. If **multiple text lines** are necessary, each text line starts with a numbered label, i.e. "*comment_1=*", "*comment_2=*", etc. If there is no comment, it is not necessary to attach any word after "*comment=*".

end of specimen information format identifier is the **text line**:

"*[end_of_specimen_information_format]*"

5.3.2.2 Calibration information format

calibration information format identifier is the **text line**:

for AES "*[ISO_AES_Calibration_Information_Format_1998_October_15]*"

for XPS "*[ISO_XPS_Calibration_Information_Format_1998_October_15]*"

energy scale calibration is a **text line**. This text line starts with "*energy_scale_calibration_feature_label=*", followed by the technique, the element name and the transition used for the calibration. The technique and element name are connected with "_". This text line is followed by the text line which starts with "*energy_scale_calibration_feature_measured_energy=*", followed by the energy scale label and measured peak value. The energy scale label and measured peak value are connected with "_". If calibration is done by using multiple peaks, each technique and element name are indicated with the numbered label "*energy_scale_calibration_feature_label_1=*" and energy scale label and measured peak value are indicated with the numbered label "*energy_scale_calibration_feature_measured_energy_1=*". This combination is followed by "*energy_scale_calibration_feature_label_2=*" and "*energy_scale_calibration_feature_measured_energy_2=*", and so on.

When the charge control condition is carried out, indicate the referencing element name with the transition and referencing peak value following the text line label "*energy_scale_calibration_charge_compensation=*". The referencing element name and peak value are connected with "_". When a flood gun is used, enter "*flood*" instead of the referencing element name.

When a spectrum is calibrated using a defined procedure, the text line starts with "*energy_scale_calibration=*", followed by the relevant standard document reference (source, number and year) and the tolerance in eV. The

document source and number are joined with the year which is, in turn, joined with the tolerance by "_". The text line may be followed by a comment, provided the comment is preceded by ";".

When a spectrum is not calibrated, the text line is "*energy_scale_calibration=uncalibrated*".

intensity scale calibration is a **text line**. This text line starts with the label "*intensity_scale_calibration=*", followed by the intensity scale calibration procedure. It is acceptable to indicate only the name(s) of journal(s) or document(s). When **multiple text lines** are necessary to describe the procedure, use the numbered labels "*intensity_scale_calibration_1=*", "*intensity_scale_calibration_2=*", etc.

When a spectrum is calibrated using a defined procedure, the text line starts with "*intensity_scale_calibration=*", followed by the relevant standard document reference (source, number and year) and textual comment, if appropriate. The document source and number are joined with the year by "_", and the textual comment is preceded by ";".

When a spectrum is not calibrated, the text line is "*intensity_scale_calibration=uncalibrated*".

resolution calibration is a **text line**. This text line starts with "*resolution_calibration=*", followed by the resolution scale calibration procedure. When **multiple text lines** are necessary to describe the procedure, use the numbered labels "*resolution_calibration_1=*", "*resolution_calibration_2=*", etc.

When a spectrum is calibrated using a defined procedure, the text line starts with "*resolution_calibration=*", followed by the relevant standard document reference (source, number and year) and the energy resolution. The document source and number are joined with the year which is, in turn, joined with the energy resolution by "_". The text line may be followed by a comment, provided the comment is preceded by ";".

When a spectrum is not calibrated, the text line is "*resolution_calibration=uncalibrated*".

end of calibration information format identifier is the **text line**:

"*[end_of_calibration_information_format]*"

5.3.2.3 Data processing information format

Items in bold not defined here are defined in 5.2. Text in italic characters enclosed by quotation marks is used to code the format.

data processing information format identifier is the **text line**:

for AES "*[ISO_AES_Data_Processing_Information_Format_1998_October_15]*"

for XPS "*[ISO_XPS_Data_Processing_Information_Format_1998_October_15]*"

data processing procedure is a **text line**. This text line starts with "*data_processing_procedure=*", followed by the specification of the data processing procedure. When different data processing procedures are carried out sequentially, each data processing procedure is indicated in one text line with the numbered labels "*data_processing_procedure_1=*", "*data_processing_procedure_2=*", etc. The number indicates the order of the data processing procedures.

When a spectrum is not processed, the text line is "*data_processing_procedure=unprocessed*".

end of data processing information format identifier is the **text line**:

"*[end_of_data_processing_information_format]*"

Annex A
(informative)

Examples of specific entries in formats

A.1 Host material

Examples of a generic description of the specimen are stainless steel, gold copper alloy, 6061 Al, polyamide, nylon, alumina and gallium arsenide. For a layered strucuture, for instance, XPS of an ultra-thin metal film on a thick SiO_2 layer on a Si substrate would be “silica” because the XPS would not probe the Si.

A.2 Host material composition

When the chemical formula of a host material is known, the expression could be Li3PO4, SiO2 or W(CO)6. When the composition is expressed as an atomic concentration or a mass concentration, the description could be Au50Cu50atomic% or Fe74Cr18Ni8mass%, respectively. If the composition cannot be specified, the expression could be of the form Li-P-O-.

A.3 Bulk purity

An expression could be 99.99mass% checked by NISSAN ARC LTD.

A.4 Known impurities

An expression could be N_0.01mass%, O_0.02mass% checked by NISSAN ARC LTD., or S_4E17atoms/cm3.

A.5 Forms of product

Examples of forms of the product that the specimen is used for are MOSFET, reagent, magnetic disk, single-crystal wafer, stub from corroded fender, and lubricant film on the hard disk.

A.6 Energy scale calibration

When the XPS energy scale calibration is carried out using Cu, Ag and Au, then the expression could be as follows:

energy_scale_calibration_feature_label_1=XPS_Cu2p3/2

energy_scale_calibration_feature_measured_energy_1=BE_932.66eV

energy_scale_calibration_feature_label_2=XPS_Ag3d5/2

energy_scale_calibration_feature_measured_energy_2=BE_368.27eV

energy_scale_calibration_feature_label_3=XPS_Au4f7/2

energy_scale_calibration_feature_measured_energy_3=BE_84.00eV

If energy calibration is carried out by the charge compensation procedure by referencing C1s peak value, the expression could be as follows:

energy_scale_calibration_charge_compensation=C1s_285eV

In the case of AES, examples are as follows:

energy_scale_calibration_feature_label_1=AES_CuMVV

energy_scale_calibration_feature_measured_energy_1=KE_61.16eV

energy_scale_calibration_feature_label_2=AES_AuNVV

energy_scale_calibration_feature_measured_energy_2=KE_72.21eV

energy_scale_calibration_feature_label_3=AES_CuLVV

energy_scale_calibration_feature_measured_energy_3=KE_918.62eV

The peak values for the energy scale calibration for XPS and AES are listed in references [9] and [10] in the bibliography.

When a spectrum is calibrated using a defined procedure, the expression could be as follows:

energy_scale_calibration_procedure=ISO9999_1998_0.25eV

A.7 Intensity scale calibration

Intensity scale calibration procedures are reported in references [11], [12] and [13], and in NPL calibration procedure NPL A1 for AES and NPL calibration procedure NPL X1 for XPS.

When a spectrum is calibrated using a defined procedure, the expression could be as follows:

intensity_scale_calibration_procedure=ISO9999_1998;attach Cu spectrum

A.8 Resolution calibration

It is recommended that simple expressions are used. "FWHM of Ag3d5/2_0.97eV" means that the energy resolution of the electron energy analyser is estimated by the full width at half maximum of the silver peak $Ag3d_{5/2}$, which equals 0.97eV."

When a spectrum is calibrated using a defined procedure, the expression could be as follows:

resolution_calibration_procedure=ISO9999_1998_0.5eV

A.9 Data processing calibration

It is acceptable to use abbreviations like “S-G” instead of “Savitzky-Golay”. or “Tougaard” instead of “Tougaard background subtraction”. One processing procedure is written in one text line.

Annex B
(informative)

Examples of formatted data

B.1 Example 1: Formats for describing a processed and calibrated X-ray photoelectron spectrum from a supermarket bag

[ISO_Specimen_Information_Format_1998_October_15]

host_material=polyethylene

IUPAC_chemical_name=polyethylene

chemical_abstracts_registry_number=9002-88-4

host_material_composition=C2H4

bulk_purity=99.5mass% checked by NISSAN ARC LTD.

known_impurities=O_0.3mass%, N_0.1mass% checked by NISSAN ARC LTD.

structure=none

form_of_product=supermarket bag

supplier=Mitsubishi Chemical Co.

lot_number=961017PE

homogeneity=homogeneous

crystallinity=amorphous

material_family=polymer

special_material_classes=sheet

specimen_mounting=mechanically_under_grid

ex_situ_preparation=degreased by n-hexane

in_situ_preparation=none

charge_control_conditions=flood+screen

specimen_temperature=298K

comment=sample is linear low density polyethylene sheet

[end_of_specimen_information_format]

[ISO_XPS_Calibration_Information_Format_1998_October_15]

energy_scale_calibration_feature_label_1=XPS_Cu2p3/2

energy_scale_calibration_feature_measured_energy_1=BE_932.7eV

energy_scale_calibration_feature_label_2=XPS_Au4f7/2

energy_scale_calibration_feature_measured_energy_2=BE_84.0eV

energy_scale_calibration_charge_compensation=flood_6eV

intensity_scale_calibration=NPL_X1

resolution_calibration=FWHM of Ag3d5/2_0.97eV

[end_of_calibration_information_format]

[ISO_XPS_Data_Processing_Information_Format_1998_October_15]

data_processing_procedure_1=smoothing by 5 points Savitzky-Golay

data_processing_procedure_2=Shirley background subtraction

[end_of_data_processing_information_format]

B.2 Example 2: Formats for describing a processed and calibrated X-ray photoelectron spectrum from a multi-layered semiconductor film

[ISO_Specimen_Information_Format_1998_October_15]

host_material=indium gallium arsenide

IUPAC_chemical_name=N/A

chemical_abstracts_registry_number=none

host_material_composition=In0.52Ga0.48As

bulk_purity=99.999mass% checked by NISSAN ARC LTD.

known_impurities=S_1.8E17 atoms/cm3 checked by NISSAN ARC LTD.

structure=cubic; a=0.5868nm

form_of_product=laser diode

supplier=Japan Energy

lot_number=#2845

homogeneity=homogeneous

crystallinity=single_(100)

material_family=semi

special_material_classes=film_multi; total_thickness = 50nm

specimen_mounting=mechanical; with 4 screws

ex_situ_preparation=ethanol

in_situ_preparation=ion_2kV_10uA_Ar

charge_control_conditions=none

specimen_temperature=298K

comment=atomically flat interface

[end_of_specimen_information_format]

[ISO_XPS_Calibration_Information_Format_1998_October_15]

energy_scale_calibration_feature_label_1=XPS_Au4f7/2

energy_scale_calibration_feature_measured_energy_1=BE_84.00eV

energy_scale_calibration_feature_label_2=XPS_Cu2p3/2

energy_scale_calibration_feature_measured_energy_2=BE_932.67eV

intensity_scale_calibration=uncalibrated;Cu and Au spectra acquired together

resolution_calibration=FWHM of Ag3d5/2_0.78eV

[end_of_calibration_information_format]

[ISO_XPS_Data_Processing_Information_Format_1998_October_15]

data_processing_procedure=subtraction of X-ray ghosts

[end_of_data_processing_information_format]

B.3 Example 3: Formats for describing a processed and calibrated Auger electron spectrum from powder of an inorganic material

[ISO_Specimen_Information_Format_1998_October_15]

host_material=strontium chloride

IUPAC_chemical_name=strontium dichloride

chemical_abstracts_registry_number=0476-85-4

host_material_composition=SrCl2

bulk_purity=99.9mass% checked by NISSAN ARC LTD.

known_impurities=N_0.01mass%, O_0.02mass% checked by NISSAN ARC LTD.

structure=cubic fluoride; a=0.698nm

form_of_product=unknown

supplier=Johnson Matthey

lot_number=EP01007

homogeneity=homogeneous

crystallinity=poly

material_family=inorganic

special_material_classes=powder

specimen_mounting=powder_compact_In

ex_situ_preparation=none

in_situ_preparation=ion_2kV_10uA_Ar

charge_control_conditions=none

specimen_temperature=298K

comment=

[end_of_specimen_information_format]

[ISO_AES_Calibration_Information_Format_1998_October_15]

energy_scale_calibration_feature_label_1=AES_CuMVV

energy_scale_calibration_feature_measured_energy_1=KE_61.16eV

energy_scale_calibration_feature_label_2=AES_AuNVV

energy_scale_calibration_feature_measured_energy_2=KE_72.21eV

energy_scale_calibration_feature_label_3=AES_CuLVV

energy_scale_calibration_feature_measured_energy_3=KE_918.62eV

intensity_scale_calibration=J. Surf. Sci. Soc. Jpn., 15, 376(1994)

resolution_calibration=uncalibrated

[end_of_calibration_information_format]

[ISO_AES_Data_Processing_Information_Format_1998_October_15]

data_processing_procedure_1=smoothing by 7 points Savitzky-Golay

data_processing_procedure_2=Shirley background subtraction

[end_of_data_processing_information_format]