INTERNATIONAL STANDARD

ISO
22048

First edition
2004-08-15

Surface chemical analysis — Information format for static secondary-ion mass spectrometry

Analyse chimique des surfaces — Protocole de l'information pour la spectrométrie de masse des ions secondaires (SIMS) en mode statique

© ISO 2004

PDF disclaimer

This PDF file may contain embedded typefaces. In accordance with Adobe's licensing policy, this file may be printed or viewed but shall not be edited unless the typefaces which are embedded are licensed to and installed on the computer performing the editing. In downloading this file, parties accept therein the responsibility of not infringing Adobe's licensing policy. The ISO Central Secretariat accepts no liability in this area.

Adobe is a trademark of Adobe Systems Incorporated.

Details of the software products used to create this PDF file can be found in the General Info relative to the file; the PDF-creation parameters were optimized for printing. Every care has been taken to ensure that the file is suitable for use by ISO member bodies. In the unlikely event that a problem relating to it is found, please inform the Central Secretariat at the address given below.

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 2.

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.

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

ISO 22048 was prepared by Technical Committee ISO/TC 201, *Surface chemical analysis*, Subcommittee SC 3, *Data management and treatment*.

Introduction

ISO 14976 provides a digital data transfer format for surface chemical analysis. That format provides basic information about the data acquisition, but data required for calibration does not specifically include certain detailed aspects necessary to interpret static secondary-ion mass spectrometry (static SIMS) data. That format also contains the spectral data and information about the abscissa increment and its value in the spectrum. Additional data, such as the mass scale calibration data are assembled into information packages with a defined format to be transmitted either within a file conforming to ISO 14976 or separately. In this way, information formats for AES and XPS have been defined in ISO 14975[1]. For static SIMS, it is important to be able to store and transfer the data, as acquired, for instance using the time-of-flight time scale. Each spectrum then needs associated calibration parameters to convert the time scale to a mass scale, where the mass increment in the spectrum varies with mass. The information format defined here contains these data and can be inserted into the block comment lines of ISO 14976. This format is designed to work with ISO 14976 in such a way that software designed to read the latter functions correctly with this information package added. This International Standard is therefore supplementary to and compatible with ISO 14976. The format is also compatible with ISO 14975 and follows a similar structure.

Surface chemical analysis — Information format for static secondary-ion mass spectrometry

1   Scope

This International Standard provides a digital format to store, and transfer between computers, in a compact way, important calibration and instrumental-parameter data necessary to make effective use of spectral-data files from static SIMS instruments. This format is designed to supplement the data transfer format specified in ISO 14976.

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   Terms, definitions and conventions

For the purposes of this document, the terms and definitions given in ISO 14976 and the following terms and definitions apply, as well as the convention, stated at the end of this clause, concerning the use of the decimal sign.

3.1
package
set of text lines which describes information about spectral data

In conformance with common usage, the decimal sign is given as a point for all items or examples of verbatim computer entries although, in conformance with the ISO/IEC Directives, Part 2, the decimal sign is given as a comma in the rest of the text.

4   Symbols (and abbreviated terms)

A ToF calibration coefficient

α calibration coefficient for the term x^2 in Equation (4)

B ToF calibration coefficient

β calibration coefficient for the term x in Equation (4)

γ calibration constant in Equation (4)

E ion energy in the flight path of a mass spectrometer, in electron volts

1

L	total path length of the spectrometer, in metres
u	unified atomic mass unit
M	mass scale in units of u divided by the modulus of the charge number of the ion
m	mass of ion in units of M
t	measured arrival time referenced to the beam chopper
T	flight time of ion, in seconds
Δt	flight time offset, in seconds
x	abcissa increment (e.g. channel number, time or mass)
SIMS	secondary-ion mass spectrometry
ToF	time-of-flight

5 Description of information format

5.1 General

This information format is designed to be inserted into the comment lines of the block in ISO 14976. Thus, extant software programmes, developed to read ISO 14976, will continue to work effectively. In the case of static SIMS using time-of-flight mass spectrometers, the abscissa scale would have uniform time increments and the supplementary information will be in a human-readable form in the comment lines. Additionally, software designed to interpret the present information format will be able to convert the data to a calibrated mass scale and be able to calculate additional parameters to assist analysts. This could have been done prior to transmission and storage of the data but, in that case, to retain optimum mass resolution, the whole spectrum would need to be interpolated to the smallest mass increment. That would lead to very large data files and be unwieldy.

In order to define the calibration parameters for the mass scale, a generic quadratic function, which encompasses most types of mass analyser, is used. In a time-of-flight mass spectrometer with an effective flight path of length L, the mass, m, of an ion with energy, E, along the flight path is simply related to the measured arrival time referenced to the beam chopper, t, by

$$m = \frac{2E(t - \Delta t)^2}{L^2} \tag{1}$$

where Δt is a delay offset to allow for the time taken for the primary ion to travel from the beam chopper to the sample. For a ToF system, two calibration coefficients are now defined, where

$$A = \frac{2E}{L^2} \tag{2}$$

and

$$B = \Delta t \tag{3}$$

The mass, m, may now be described by a quadratic equation in terms of the abscissa increment, x, which may represent either time or channel number:

$$m = \alpha x^2 + \beta x + \gamma \tag{4}$$

where $\alpha = A$, $\beta = -2AB$ and $\gamma = AB^2$. Whilst this equation uses an extra non-independent coefficient, it does give the flexibility to describe the mass scale for most spectrometers. For example, a quadrupole spectrometer with a linear mass scale will have $\alpha = 0$ whereas a magnetic-sector mass spectrometer may require all three independent coefficients. Thus, a three-term calibration, where one term may be zero, covers a wide range of instruments without the software having to read if/then choices.
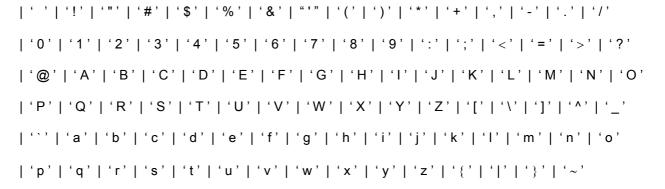
The mass scale calibration shall be calculated using the correct physical model appropriate to the spectrometer, such as Equation (1) for a ToF spectrometer.

In the above, it has been assumed that the ion has unit charge. In practice, this is generally true. However, a few ions are multiply charged. This increases E by the multiplicative factor so that the ion mass appears reduced by that factor. In using Equation (4), therefore, m represents the mass divided by the number of electrons representing the charge imbalance of the ion. We will denote this scale by units of "M".

Three archetypal examples of this format are given in Annex A. The first example is for a ToF SIMS instrument where the mass scale is non-linear in time and the abscissa is recorded in channel numbers in the ISO 14976 file. The spectrometer mass calibration gives $A = 3.683406219931798 \times 10^{-9}$ and $B = 3.674421716518492 \times 10^3$ which were used to calculate the calibration coefficients α, β and γ. The second example is for a magnetic-sector instrument with a non-linear mass scale which requires all three independent calibration coefficients. The third example is for a quadrupole instrument with an incorrect linear mass scale recorded in the ISO 14976 file due to instrument drift. Two calibration coefficients, β and γ, are used to correct the mass scale.

5.2 Additional rules and definitions

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

character: the character SPACE or any of the 94 graphic characters specified in the 7-bit ASCII character set

The 94 graphic characters are:

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

| '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 'and' or "and".

integer: integer number followed by **carriage return**

real number: decimal number or decimal number in exponential notation followed by **carriage return**

text line: line of up to 80 characters

If the value of any **real number** or **integer** in the format is not known, then 1E37 shall be entered.

5.3   The format

5.3.1   Content of the information format

The static SIMS information format consists of the following items shown in bold, on contiguous lines of the text file. All items shall be present and in the order given.

static SIMS instrumental-parameter information format identifier

primary-ion mass

primary-ion pulsed current

primary-ion direct current

primary-ion pulse width

primary-ion bunched-pulse width

number of ions per pulse

primary-ion dose

primary-ion cycle time

number of ion pulses

extraction voltage

sample holder voltage

post-acceleration voltage

calibration coefficient alpha

calibration coefficient beta

calibration coefficient gamma

flood gun energy

flood gun cycle time

flood gun pulsed current

end of static SIMS instrumental-parameter information format identifier

The analysis source label of ISO 14976 shall be used to identify the primary particle species. Extensible markup language, XML[2], is the recommended format. For example, SF_5, is written as SF₅.

5.3.2 Definition of items in the format

The items below are in the order given in 5.3.1. All texts enclosed by quotation marks define items of the format and are shown in italics here for clarity but are not actually coded in the data files in italics.

static SIMS instrumental parameter information format identifier is the **text line** "*[ISO_Static_SIMS_Instrumental_Parameter_Information_Format_1999_September_1]*", followed by **carriage return**.

primary-ion mass is a **text line**. This text line starts with "*primary_ion_mass*=", followed by a **real number** giving the value of the mass of the primary ion in unified atomic mass units.

primary-ion pulsed current is a **text line**. This text line starts with "*primary_ion_pulsed_current*=", followed by a **real number** giving the value of the pulsed primary-ion current, in pA.

primary-ion direct current is a **text line**. This text line starts with "*primary_ion_direct_current*=", followed by a **real number** giving the value of the primary-ion direct current, in nA.

primary-ion pulse width is a **text line**. This text line starts with "*primary_ion_pulse_width*=", followed by a **real number** giving the value of the primary-ion pulse width, in ns, before any bunching.

primary-ion bunched pulse width is a **text line**. This text line starts with "*primary_ion_bunched_pulse_width*=", followed by a **real number** giving the value of the primary-ion pulse width, in ns, after bunching.

number of ions per pulse is a **text line**. This text line starts with "*number_of_ions_per_pulse*=", followed by an **integer** giving the value of the number of primary ions in each pulse.

primary-ion dose is a **text line**. This text line starts with "*primary_ion_dose*=", followed by a **real number** giving the value of the total ion dose accumulated during the acquisition of the associated data, in units of ions/m^2.

primary-ion cycle time is a **text line**. This text line starts with "*primary_ion_cycle_time*=", followed by a **real number** giving the value of the time, in µs, between the start of each ion pulse.

number of ion pulses is a **text line**. This text line starts with "*number_of_ion_pulses*=", followed by a **real number** giving the value of the number of primary-ion pulses used to acquire the data.

extraction voltage is a **text line**. This text line starts with "*extraction_voltage*=", followed by a **real number** giving the value of the potential with respect to ground, in volts, to which the extraction electrode is pulsed.

sample holder voltage is a **text line**. This text line starts with "*sample_holder_voltage*=", followed by a **real number** giving the value of the potential with respect to ground, in volts, to which the sample holder is pulsed.

post acceleration voltage is a **text line**. This text line starts with "*post_acceleration_voltage*=", followed by a **real number** giving the value of the potential, in volts, through which the ions are accelerated onto the detector.

calibration coefficient alpha is a **text line**. This text line starts with "*calibration_coefficient_alpha*=", followed by a **real number** giving the value of the mass scale calibration coefficient, α.

NOTE   If the unit of abscissa increment, x, is time or is dimensionless or is mass, then the units of the calibration coefficient, α, are M·s^{-2} or M or M^{-1}, respectively.

calibration coefficient beta is a **text line**. This text line starts with "*calibration_coefficient_beta*=", followed by a **real number** giving the value of the mass scale calibration coefficient, β.

NOTE   If the unit of abscissa increment, x, is time or is dimensionless or is mass, then the units of the calibration coefficient, β, are $M \cdot s^{-1}$ or M or dimensionless, respectively.

calibration coefficient gamma is a **text line**. This text line starts with "*calibration_coefficient_gamma*=", followed by a **real number** giving the value of the mass scale calibration coefficient, γ, in M.

flood gun energy is a **text line**. This text line starts with "*flood_gun_energy*=", followed by a **real number** giving the value of the electron energy, in eV, when striking the sample.

flood gun cycle time is a **text line**. This text line starts with "*flood_gun_cycle_time*=", followed by a **real number** giving the value of the time, in µs, between the start of each electron pulse.

flood gun pulsed current is a **text line**. This text line starts with "*flood_gun_pulsed_current*=", followed by a **real number** giving the value of the pulsed flood gun current, in nA.

end of static SIMS instrumental-parameter information format identifier is the **text line** "*[end_of_ISO_Static_SIMS_Instrumental_Parameter_Information_Format]*" followed by **carriage return**.

Annex A
(informative)

Examples of formatted data

A.1 Example of data acquired using a time-of-flight mass spectrometer

This example illustrates a pulsed ion source with a three-parameter calibration with two independent coefficients for the mass scale. Note that these items are not italicized.

[ISO_Static_SIMS_Instrumental_Parameter_Information_Format_1999_September_1]

primary_ion_mass=127

primary_ion_pulsed_current=0.9

primary_ion_direct_current=1E37

primary_ion_pulse_width=25

primary_ion_bunched_pulse_width=0.9

number_of_ions_per_pulse=1E37

primary_ion_dose=1E16

primary_ion_cycle_time=100

number_of_ion_pulses=600000

extraction_voltage=-2000

sample_holder_voltage=0

post_acceleration_voltage=-13500

calibration_coefficient_alpha=3.6834062199317976E-9

calibration_coefficient_beta=-2.7068775610553372E-5

calibration_coefficient_gamma=0.04973104847149

flood_gun_energy=15

flood_gun_cycle_time=100

flood_gun_pulsed_current=5

[end_of_ISO_Static_SIMS_Instrumental_Parameter_Information_Format]

A.2 Example of data acquired using a magnetic sector mass spectrometer

This example illustrates a continuous ion source with a three-parameter calibration with three independent coefficients for the mass scale.

[ISO_Static_SIMS_Instrumental_Parameter_Information_Format_1999_September_1]

primary_ion_mass=40

primary_ion_pulsed_current=1E37

primary_ion_direct_current=0.5

primary_ion_pulse_width=1E37

primary_ion_bunched_pulse_width=1E37

number_of_ions_per_pulse=1E37

primary_ion_dose=5.1E16

primary_ion_cycle_time=1E37

number_of_ion_pulses=1E37

extraction_voltage=0

sample_holder_voltage=-4000

post_acceleration_voltage=-1000

calibration_coefficient_alpha=0.0000831

calibration_coefficient_beta=0.0007635

calibration_coefficient_gamma=0.0123011

flood_gun_energy=1E37

flood_gun_cycle_time=0

flood_gun_pulsed_current=0

[end_of_ISO_Static_SIMS_Instrumental_Parameter_Information_Format]

A.3 Example of data acquired using a quadrupole mass spectrometer

This example illustrates a continuous ion source with a three-parameter calibration with two independent coefficients for the mass scale.

[ISO_Static_SIMS_Instrumental_Parameter_Information_Format_1999_September_1]

primary_ion_mass=132

primary_ion_pulsed_current=1E37

primary_ion_direct_current=1.5

primary_ion_pulse_width=1E37

primary_ion_bunched_pulse_width=1E37

number_of_ions_per_pulse=1E37

primary_ion_dose=8.1E16

primary_ion_cycle_time=1E37

number_of_ion_pulses=1E37

extraction_voltage=-20

sample_holder_voltage=0

post_acceleration_voltage=-3000

calibration_coefficient_alpha=0

calibration_coefficient_beta=0.9992

calibration_coefficient_gamma=0.034
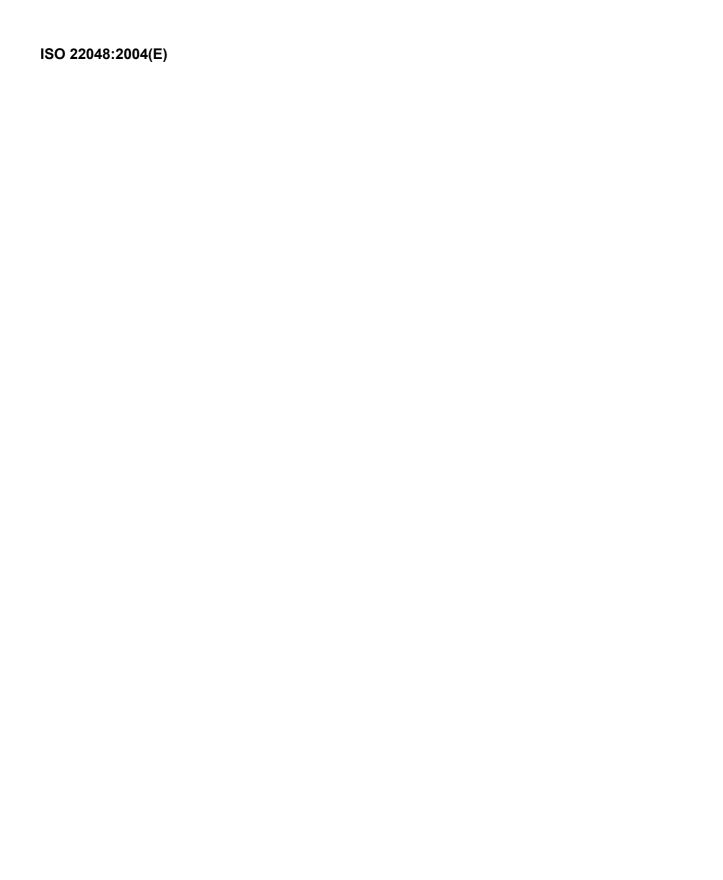
flood_gun_energy=1E37

flood_gun_cycle_time=0

flood_gun_pulsed_current=0

[end_of_ISO_Static_SIMS_Instrumental_Parameter_Information_Format]

Bibliography

[1]   ISO 14975, *Surface chemical analysis — Information formats*

[2]   ISO/IEC 13522-8, *Information technology — Coding of multimedia and hypermedia information — Part 8: XML notation for ISO/IEC 13522-5*

ISO 22048:2004(E)

ICS 71.040.40

Price based on 10 pages