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

Reference number
ISO 22048:2004(E)

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Published in Switzerland

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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

 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

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.