INTERNATIONAL STANDARD

ISO 13084

First edition
2011-05-15

Surface chemical analysis — Secondary-ion mass spectrometry — Calibration of the mass scale for a time-of-flight secondary-ion mass spectrometer

Analyse chimique des surfaces — Spectrométrie de masse des ions secondaires — Étalonnage de l'échelle de masse pour un spectromètre de masse des ions secondaires à temps de vol

Reference number
ISO 13084:2011(E)

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Published in Switzerland

Foreword

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ISO 13084 was prepared by Technical Committee ISO/TC 201, *Surface chemical analysis*, Subcommittee SC 6, *Secondary ion mass spectrometry*.

Introduction

Secondary-ion mass spectrometry (SIMS) is a powerful technique for the analysis of organic and molecular surfaces. Over the last decade, instrumentation has improved significantly so that modern instruments now have very high repeatability and constancy (Reference [2] in the Bibliography). An increasing requirement is for the identification of the chemical composition of complex molecules from accurate measurements of the mass of the secondary ions. The relative mass accuracy to do this and to distinguish between molecules that contain different chemical constituents, but are of the same nominal mass (rounded to the nearest integer mass), is thus an important parameter. A relative mass accuracy of better than 10 ppm is required to distinguish between C_2H_4 (28,031 30 u) and Si (27,976 92 u) in a parent ion with total mass up to 1 000 u, and between CH_2 (14,015 65 u) and N (14,003 07 u) in parent ions with total mass up to 300 u. However, in a recent interlaboratory study (Reference [3] in the Bibliography), the average fractional mass accuracy was found to be 150 ppm. This is significantly worse than is required for unambiguous identification of ions. A detailed study (Reference [4] in the Bibliography) shows that the key factors degrading the accuracy include the large kinetic energy distribution of secondary ions, non-optimized instrument parameters and extrapolation of the mass scale calibration.

This International Standard describes a simple method, using locally sourced material, to optimize the instrumental parameters, as well as a procedure to ensure that accurate calibration of the mass scale is achieved within a selectable uncertainty.

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1 Scope

This International Standard specifies a method to optimize the mass calibration accuracy in time-of-flight SIMS instruments used for general analytical purposes. It is only applicable to time-of-flight instruments but is not restricted to any particular instrument design. Guidance is provided for some of the instrumental parameters that can be optimized using this procedure and the types of generic peaks suitable to calibrate the mass scale for optimum mass accuracy.

2 Symbols and abbreviated terms

2.1 Symbols

m	mass of interest
m_1	calibration mass 1
m_2	calibration mass 2
ΔM	mass accuracy (u)
M_P	measured peak mass (u)
M_T	true mass (u)
$U(m)$	mass uncertainty for a mass m, arising from calibration
U_1	uncertainty in the accurate mass measurement of m_1
U_2	uncertainty in the accurate mass measurement of m_2
U_0	average uncertainty in an accurate mass measurement
V_R	reflector or acceptance voltage (V)
W	relative mass accuracy
x	number of carbon atoms
y	number of hydrogen atoms
$\sigma(\Delta M)$	standard deviation of the mass accuracy for a number of peaks
σ_M	average of the standard deviations of ΔM for each of the four $C_xH_y^+$ cascades with 4, 6, 7 and 8 carbon atoms

2.2 Abbreviated terms

MEMS	micro-electromechanical system
PC	polycarbonate
ppm	parts per million
r/min	revolutions per minute
SIMS	secondary-ion mass spectrometry
THF	tetrahydrofuran
ToF	time of flight