
**Surface chemical analysis —
Secondary ion mass spectrometry —
Method for the measurement of mass
resolution in SIMS**





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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.

The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular, the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

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For an explanation of the voluntary nature of standards, the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the World Trade Organization (WTO) principles in the Technical Barriers to Trade (TBT), see www.iso.org/iso/foreword.html.

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

Any feedback or questions on this document should be directed to the user's national standards body. A complete listing of these bodies can be found at www.iso.org/members.html.

Introduction

Mass resolution is one of the most important instrumental parameters in mass spectrometry (MS). For any MS experiments, an unambiguous result can only be acquired if sufficient mass resolution is reached to separate the target analytes from any possible interference. If the mass resolution of the instrument is insufficient, it can result in a false positive or negative signal. Therefore, the mass resolution is the primary consideration for determining whether an instrument is adequate for the intended purpose. For routine applications, the mass resolution should be adjusted based on the analytical requirements of the sample. Mass resolution is important not only for the instrument acceptance tests and fundamental studies, but also for almost all routine applications.

This document gives guidance for the measurement of mass resolution in SIMS. Various definitions of mass resolution have been summarized and common problems with popular definitions have been discussed elsewhere^[18]. To compare mass resolution between different instrument or/and different types of instruments (e.g. TOF-SIMS, Magnetic SIMS, Quadrupole SIMS, Fourier Transform SIMS and Orbitrap-SIMS, etc.), it is necessary to show the measured peak shape and define mass resolution correctly.

After introducing a reasonable new definition for mass resolution and a method considering the peak shape to compare the mass resolution between TOF-SIMS, Magnetic SIMS, Quadrupole SIMS and Fourier Transform SIMS, this document specifies a method to measure the mass resolution in SIMS.

Surface chemical analysis — Secondary ion mass spectrometry — Method for the measurement of mass resolution in SIMS

1 Scope

This document specifies a method for measuring the mass resolution in SIMS, and how to compare the mass resolution between different instruments (e.g. TOF-SIMS, Magnetic SIMS, Quadrupole SIMS, Fourier Transform SIMS, etc.) by considering the peak shapes.

2 Normative references

The following documents are referred to in the text in such a way that some or all of their content constitutes requirements 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 18115-1, *Surface chemical analysis — Vocabulary — Part 1: General terms and terms used in spectroscopy*

3 Terms and definitions

For the purposes of this document, the terms and definitions given in ISO 18115 and the following apply.

ISO and IEC maintain terminology databases for use in standardization at the following addresses:

- ISO Online browsing platform: available at <https://www.iso.org/obp>
- IEC Electropedia: available at <https://www.electropedia.org/>

3.1

mass resolution

measurement of the ability of a mass spectrometer to separate mass peaks in a mass spectrum

Note 1 to entry: For a mass peak at position M and a mass peak at position $M+\Delta M$ which can be separated in a mass spectrum then ΔM is the mass resolution of the mass spectrometer at M under these conditions. The peak shape as well as the method of measurement of ΔM should be reported.

Note 2 to entry: If M and $M+\Delta M$ can be separated, ΔM , $M/\Delta M$ or $\Delta M/M$ are defined as mass resolution, mass resolving power or relative mass resolution respectively. Designs of mass spectrometer generally maintain the resolution either to be constant throughout the mass spectrum or to be proportional to mass being scanned. For the former, the mass resolution is a useful term whereas, for the latter, the relative mass resolution and resolving power are more useful.

Note 3 to entry: The sensitivity required to detect the presence of a peak at a position $M+\Delta M$ depends upon the shape of the peak at M and the degree to which peak tails place limits on the magnitude of a peak at $M+\Delta M$ which can be detected. Simple measures of resolution may not represent the actual or practical resolution needed for particular applications.

Note 4 to entry: Usually, normalized output signal distribution from an instrument is a function of variable input measurand values which arises from a feature with a single measurand value. However, in mass spectrometry community, because “mass” is a single measurand value, the peak shape is normally used for the resolution function.