



Designation: E 1504 – 92 (Reapproved 1996)

Standard Practice for Reporting Mass Spectral Data in Secondary Ion Mass Spectrometry (SIMS)¹

This standard is issued under the fixed designation E 1504; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ϵ) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 This practice provides the minimum information necessary to describe the instrumental, experimental, and data reduction procedures used in acquiring and reporting secondary ion mass spectrometry (SIMS) mass spectral data.

1.2 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.*

2. Referenced Documents

2.1 *ASTM Standards:*

E 673 Terminology Relating to Surface Analysis²

3. Terminology

3.1 *Definitions*—For definitions of terms used in this practice, refer to Terminology E 673.

4. Summary of Practice

4.1 Experimental conditions and reporting procedures that affect SIMS mass spectral data are presented in order to standardize the reporting of such data to facilitate comparisons with other laboratories and analytical techniques.

5. Significance and Use

5.1 This practice is intended for use in reporting the experimental and data reduction procedures described in other publications.

6. Information to be Reported

6.1 *Instrumentation:*

6.1.1 If a standard commercial SIMS instrument is used, specify the manufacturer and model number. Specify the manufacturer and model number of any accessory or auxiliary equipment that would affect the data contained within the mass spectrum (for example, additional vacuum pumping attachments, primary ion mass filter, electron flood guns, etc.). If any nonstandard modification has been made to the instrumentation, describe the modification in detail.

6.1.2 If a noncommercial SIMS system is used, specify the components composing the system (for example, ion gun, pumping system, vacuum chamber, and mass filter). Specify the manufacturer and model number if the components are of commercial origin. If the components are home-built, specify them in such detail that their potential effect on the obtained mass spectrum may be deduced by an individual experienced in SIMS and vacuum technology.

6.2 *Specimen:*

6.2.1 Describe the specimen in as much detail as possible. Such factors would include, but are not limited to, sample history, bulk and trace composition (especially electronic dopants), physical dimensions, sample homogeneity, crystallinity, and any preanalysis cleaning procedure used.

6.2.2 State the method of sample mounting. When analyzing vacuum-compatible liquids, describe the substrate onto which the sample was deposited. In the case of particulate samples pressed into metal foils, state the nature and purity of the foil. Describe any conductive coating or grids placed on the sample for charge compensation.

6.3 *Experimental Conditions:*

6.3.1 *Primary Ion Source*—If a mass-filtered primary ion beam is used, specify the isotope and charge state of the primary ion species. If not mass-filtered, state the nature and purity of the source material used for ion production. State the impact energy, the angle of incidence (relative to the sample normal), the ion current (also the manner of current determination), whether the primary ion beam was rastered, the unrastered beam diameter, and the total irradiated area. Specify the primary ion dose, in ions-cm⁻², that was used to acquire that mass spectrum.

6.3.2 *Secondary Ion Mass Spectrometer*—Specify the analyzed area, any electronic gating parameters used including, but not limited to, the size of the gated area, the size of any apertures in the secondary ion optical column, the secondary ion collection angle, the energy bandpass of the secondary ion mass spectrometer (note particularly whether any energy discrimination was used to reduce the signal intensity of polyatomic ions), whether electrostatic or magnetic peak switching was used for double focussing instruments, the type of sample charge compensation, the type of measurement system used to measure secondary ion intensity (for example, Faraday cup, electron multiplier, microchannel plate), and the secondary ion impact energy on the detector.

¹ This practice is under the jurisdiction of ASTM Committee E-42 on Surface Analysis and is the direct responsibility of Subcommittee E42.06 on SIMS.

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² *Annual Book of ASTM Standards*, Vol 03.06.

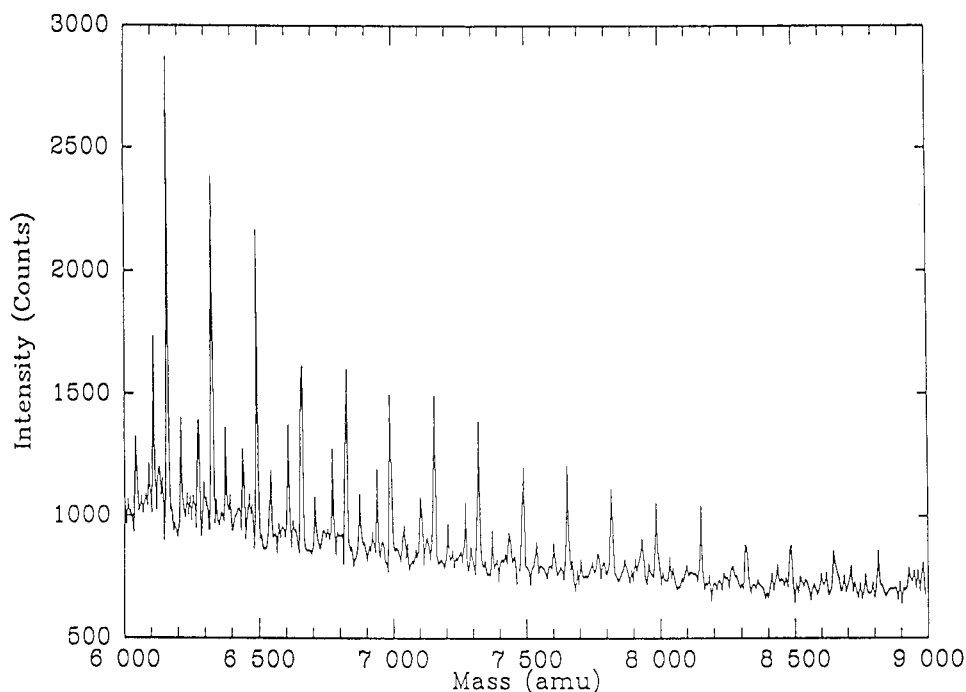


FIG. 1 Static SIMS Mass Spectrum of Perfluorinated Polyakylether

6.3.3 *Mass Spectral Background*—Specify the pressure in the primary ion column, specimen chamber, and mass spectrometer prior to sample introduction and during analysis. Specify the type of vacuum pumping in each section of the instrument. Describe any significant or unusual contaminants, if known. Provide the composition of any reactive gas used for sample flooding,³ along with the method used to determine the partial pressure of the reactive gas.

6.4 Results:

6.4.1 *Display of Mass Spectral Data*—The vertical axis of a SIMS mass spectral display gives the secondary ion intensity in units of either counts/s, total integrated counts (specify whether the integration is over total spectra acquired or time), or percent of the most intense peak displayed in the spectrum. The

integrated horizontal axis displays the mass/charge ratio. An example of a SIMS mass spectrum is shown in Fig. 1.⁴

6.4.2 *Calibration*—Specify the method used to establish the mass scale, especially the number of calibration points used and the form of any algorithm used.

6.4.3 *Mass Resolution*—Specify the mass resolution of the mass spectrometer. This should be calculated as $M/\Delta M$, where ΔM is the full width at half maximum intensity for an ion peak at mass M . Because many mass spectrometers vary in mass resolution over their mass range, specify both the ΔM and M values used to calculate the specified mass resolution.

7. Keywords

7.1 mass spectral data; SIMS

³ Barnheim, M. and Slodzian, G., "Effect of Oxygen on the Sputtering of Aluminum Targets Bombarded with Argon Ions", *International Journal of Mass Spectrometry and Ion Physics*, Vol 12, 1973, p. 93.

⁴ Hues, S. M., Colton, R. J., Wyatt, J. R., and Schultz, J. A., "A Pulsed Alkali-Ion Gun for Time-of-Flight Secondary Ion Mass Spectrometry", *Review of Scientific Instruments*, Vol 60, 1989, p. 1239.

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