Designation: E1504 – 11

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

This standard is issued under the fixed designation E1504; 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 The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.

1.3 *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:*[2]

E673 Terminology Relating to Surface Analysis (Withdrawn 2012)[3]

3. Terminology

3.1 *Definitions*—For definitions of terms used in this practice, refer to Terminology E673.

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, model number, and type of analyzer used. 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, primary ion sources, 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*—Describe the specimen in as much detail as possible. Such factors would include, but are not limited to, sample preparation and handling, sample history, bulk and trace composition, physical dimensions, sample homogeneity, crystallinity, and any preanalysis cleaning procedure used. Describe in detail the method of sample mounting. Describe any conductive coating or grids placed on the sample for charge compensation. If a substrate is used, include substrate composition, purity, and any methods of cleaning.

6.3 *Experimental Conditions:*

6.3.1 *Primary Ion Source and Ion Optical Column*—If a commercial ion source is being used, then the manufacturer and model number should be specified. If the ion source is a custom design, then it should be described in detail and appropriate literature references given, if applicable. The species extracted from the ion source must be specified. If the primary ion column provides mass filtering, then the selected mass-filtered species must be specified. If there is no mass-filtering, then the purity of the material used for ion production must be specified. State the ion energy and the impact energy of the primary beam. State the angle of incidence of the primary ion beam with respect to the surface normal of the

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

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[2] For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

[3] The last approved version of this historical standard is referenced on www.astm.org.

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sample as well as the ion current (and the method by which this is measured). State whether the ion beam is rastered and if so, state the dwell time, the spot size, and the total irradiated area. Specify the primary ion dose (ions-m^2) that was used to obtain the spectrum. If the primary ion beam is pulsed (that is, Time-of-Flight SIMS), details of the pulsing should be described (pulse width, repetition rate, extent of beam bunching, and so forth). In addition, any special alignment or tuning of the primary column should be specified or referenced.

6.3.2 Other experimental conditions: If non-standard operating are employed, such as application of low/high temperatures or sample rotation during analysis, please state this and any additional information that may be required, such as rotation speed (in rad/s).

6.3.3 *Secondary Ion Mass Spectrometer*—Specify the area of the sample from which the ions were collected. Specify whether any electronic gating methods were used, the parameters of the gating, and how the gating method affects the spectrum (such as, raster gating for crater edge rejection or spectral gating for selecting a mass spectral region in a Time-of-Flight spectrometer). Specify the conditions of the mass spectrometer, such as, but not limited to, collection angle, energy-filtering parameters, reflectron voltages, pulsing conditions, the use of collimation or beam-defining apertures and slits, post-acceleration voltages, and so forth. If appropriate, state how the condition influenced the mass spectral data (that is, energy filtering to reduce polyatomic ion species). If charge compensation is used, describe the type of system used and the parameters of the system. If an electron flood gun is used, then the current or dose (electrons/m^2) should be specified. Specify and describe the type of secondary ion detection system used (such as, Faraday cup, pulse-counting electron multiplier, resistive anode encoder, and so forth).

6.3.4 *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,[4] 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 horizontal axis should display the mass/charge ratio. Any corrections (such as for dead time, or background subtraction) applied to the spectrum must be stated.

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

[4] Bernheim, 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.

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