SIMS Template Instructions

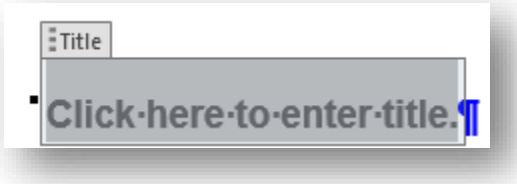
Guide to using this Template

For ease-of-use, this template has been designed as a Microsoft Word form that when filled out, will closely resemble a published ***Surface Science Spectra*** article. Authors are encouraged to consult published articles for additional guidance. The form consists of two types of fields: standard and drop down.

Standard Fields

To enter content into a standard field, click on the grey field instructive label.

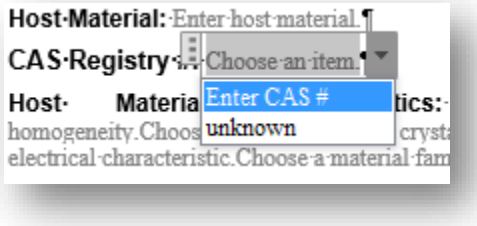
The field will open, and content can be added either by typing directly, or by copy/paste from another document.



Drop-down Fields:

To choose content from a drop-down field, click on the grey field instructive label.

The field will open, and content can be chosen from the menu by clicking on the appropriate item.



Figures:

A key feature of ***Surface Science Spectra*** is the uniformity of its figures. As such, SSS adheres to strict figure formatting guidelines (described below).

Initial submission process: Authors may copy/paste (as a picture) spectra into the appropriate spectrum placeholder as indicated. Leave the "Accession #" label shown in the figure template as is during this phase. Unique accession numbers will be assigned to each specimen in the submission once the manuscript has been accepted. The accession number(s) will be sent to the authors to add to the final versions of the figures.

Final submission process: Authors need to send each figure (as a separate file) in one of the following formats: PostScript (.ps), Encapsulated PostScript (.eps), TIFF, JPG, or production-ready PDF. You can name each Figure file with a descriptive title such as Figure1, Figure 2, etc.

Instructions for Figures:

Font sizes:

1. Accession# label inside plot is **Arial 16 bold**.
2. Axis labels are Arial 14.
3. Tick labels are Arial 11.
4. Peak labels are Arial 11.

Plotting:

Figures can be plotted in the software of your choice as long as they follow the font and formatting guidelines. The X axis of the figure should be labelled 'm/z'. The Y axis of the figure should be plotted in 'Counts'. Only label major peaks in the spectrum that can be accurately identified. Include one figure per specimen submitted. If you need to show 2 spectral regions to accomplish this, please present them as a stacked plot in 1 figure.

Labelling:

Additional labelling of the figures can be done using the software of your choice. If you use PowerPoint to create figures for production, define the slide area as 8.5 x 11 portrait mode and then copy/paste each figure on individual slides.

Submission Overview

Title: Enter title, beginning with a descriptive reference to the specimen or other characteristics specific to this data record. Avoid titles which begin with the technique, such as SIMS Study of....'

Authors: Enter authors names as you wish them to appear in *SSS*.

Affiliations: Enter authors affiliations as you wish them to appear in *SSS*.

Abstract: Summarize and include key information about the specimens and spectra, such as specimen material, measurement procedures, and significance of the research. The abstract will be printed verbatim. Because the abstract must stand alone in some databases, **please do not cite references in the abstract**. You may include references beginning with the **Introduction**.

Keywords: Include keywords relevant to your samples.

Technique: SIMS

Specimen: Provide a generic description of the specimen, such as nylon, 6061 Al, or SiO_2. For layered structures, the specimen is the 'bulk' substance near the surface.

Manufacturer and Model: Enter the instrument manufacturer name. If the instrument was custom-built, enter the designer's name and reference a published article, if applicable. Enter the manufacturer's model number.

Major Species in Spectra: Specify the major components present.

Minor Species in Spectra: Specify other notable species present.

Published Spectra: Enter the number of specimen spectra for which you are requesting hard-copy publication. An opportunity to identify specific spectra for publication is given in the template figure caption.

Spectral Category: Choose the suggested category of the data record **drop down with choices: Technical**, **Comparison**, or **Reference** (see overview of instructions for definitions). The editors may suggest an alternate category, based on the recommendations of referees.

Introduction

Enter any descriptive, explanatory, or introductory comments that pertain to your entire submission, *e.g.,* why the work is significant, or what the conclusions show. You may cite references.

Specimen Description

Each specimen will need a unique number. Please copy and complete a Specimen Description section for each specimen.

Specimen: Provide a generic description of the specimen, such as nylon, 6061 Al, or SiO_2. For layered structures, the specimen is the 'bulk' substance near the surface.

Chemical Abstract Service (CAS) Registry #: Enter the CAS registry number of the specimen. Enter 'unknown' if not known.

Specimen Characteristics: Homogeneity: (drop down with choices – Homogeneous, Inhomogeneous, Unknown), choose the one that best applies. **Phase:** (drop down with choices – Gas, Liquid, Powder, Solid), **c**hoose the one that best applies. **Crystallinity:** (drop down with choices – Amorphous, Polycrystalline, Single Crystal, Unknown Crystallinity), **c**hoose the one that best applies. **Electrical Characteristics:** (drop down with choices – Conductor, Dielectric, Semiconductor, Superconductor, Unknown Conductivity), choose the one that best applies. **Material Family:** (drop down with choices – Biological Material, Composite, Inorganic Compound, Metal, Organic Compound, Polymer, Semiconductor), choose the one that best applies. **Special Material Classes:** (drop down with choices – Ceramic, Coating, Fiber, Glass, Other, Powder, Thin Film), choose all appropriate responses. Leave blank if Special Classes do not apply. If 'Other,' describe in 'As Received Condition' (copy/paste this field as necessary).

Chemical Name: Enter the full chemical name of the specimen according to IUPAC conventions, *e.g.*, for Li_3PO_4 you would enter lithium orthophosphate.

Source: Provide the name of the manufacturer and/or supplier of the specimen or give a reference to how the was made, *e.g.,* thermally grown SiO_2 on Si.

Specimen Composition: List the principal elements present or the chemical formula, if practical.

Form: Give a physical description of the specimen, *e.g.,* MOSFET, reagent, single-crystal wafer, stub from corroded fender from brand X pickup truck, etc.

Structure: Include information such as a description of the crystal lattice and orientation, *e.g.* [1 0 -1 0] hexagonal close-packed, and/or comments such as fracture surface at grain boundary, etc. You may also submit a hard-copy bonding diagram.

History and Significance: Comment field for background information about the specimen, *e.g.,* moon rock retrieved by Apollo IX mission, or a discussion of why the spectra were taken. Include comments on purity, known contaminants, results of other analytical techniques. Identify the organization that developed any specified alternate standard designator, *e.g.,* AISI in the case of 1003 carbon steel.

As Received Condition: Describe the physical condition of the specimen as it was supplied, *e.g.,* as grown, paint delaminating from metal stub, etc. Include the thermal and storage history of the specimen as well as physical condition.

Analyzed Region: Describe the specimen analyzed qualitatively, *e.g.,* shorted FET gate, same as specimen, or weld bead.

***Ex Situ* Preparation and Mounting:** Describe specimen preparation prior to introduction into the spectrometer vacuum system, *e.g.,* as received, washed in ethanol, scraped with a well-pickled file, etc. Also, describe the specimen mounting technique.

***In Situ* Preparation:** Describe specimen preparation or treatment procedures within the spectrometer vacuum system prior to analysis, *e.g.,* ion sputter cleaning and annealing.

Charge Control Conditions and Procedures: Describe the equipment used to control charge of the specimen during measurement. Include flood gun voltages and current, target bias, etc. Also describe the procedures used to determine the charge control.

Temperature During Analysis: Enter the specimen temperature during analysis, in Kelvin. Use 300 for 'room temperature' if not otherwise measured.

Pressure During Analysis (in Pa): Enter the maximum pressure chamber pressure during analysis in Pascal (1 Torr = 133 Pascal). Normally expressed using powers of 10, for example 1.33×10^{-6}.

Pre-Analysis Beam Exposure: Describe procedures and include comments on the amount of time the analyzed region was exposed to the ion gun or electron irradiation prior to the measurements for these spectra (especially important for beam-sensitive specimens).

Instrument Configuration

Manufacturer and Model: Enter the instrument manufacturer name. If the instrument was custom-built, enter the designer's name and reference a published article, if applicable. Enter the manufacturer's model number.

Analyzer Type: Drop down with choices – magnetic sector, quadrupole, time-of-flight. Choose the analyzer type that best applies. If 'Other,' include a description of the ‘Non-Standard Analyzer or Lens’ by entering this information after the analyzer type drop-down menu.

Sample Rotation: Drop down with choices- yes or no.

Rotation Rate: If sample was rotated, give the rate in revolutions per min. If sample was not rotated, enter zero.

Oxygen Flood Source: Describe oxygen flood system.

Oxygen Flood Source Pressure: Analyzer chamber pressure with oxygen flood in use, in Pa (1 Torr = 133 Pa).

Other flood Source: Describe other flood system.

Other flood Source Pressure: If applicable, analyzer chamber pressure with other flood source in use, in Pa (1 Torr = 133 Pa).

Unique Instrument Features Used: *E.g.*, sample can be tilted.

Energy Acceptance Window: Enter the analyzer acceptance window width, in eV. For a reflectron this would be set by the reflection voltage. For a TRIFT, it would be determined by the energy-slit width.

Post-acceleration Voltage: Provide the post-acceleration voltage, in kV.

Sample Bias: Enter the sample potential with respect to ground, in eV.

Specimen Normal-to-analyzer: Enter specimen emission angle, in degrees.

Ion Sources

Note: if multiple ion sources were used, copy/paste the ion sources section as necessary.

Ion Source 1 of: Enter the number of ion sources used.

Purpose of this Ion Source: Drop down with choices – analysis beam, sputtering beam, or other. If other, enter description following this field.

Ion Source Manufacturer: If non-standard ion source, describe ion source after this field.

Ion Source Model and Type: No instructions

Beam Mass Filter: Drop down with choices - yes or no. If a Beam Mass Filter was employed, enter Manufacturer and Type, relevant operating parameters, etc. after this field.

Beam Species and Charge State: *E.g.,* Au^{+}.

Beam Gating Used: Drop down with choices - yes or no. If beam gating was used, describe Beam gating implementation method.

Additional Beam Comments: Please provide any additional information and/or comments about this beam's source, implementation, and purpose.

Beam Voltage (eV): Enter the source voltage with respect to ground, in eV.

Net Beam Voltage (impact voltage) (eV): Enter difference between accelerating voltage and sample potential, in eV.

Ion Pulse Width: Enter time duration of single pulse (ns), after bunching if bunching applied.

Ion Pulse Rate: Enter repetition rate of pulses, in kHz.

DC Beam Current: Enter beam current when pulsing is off, in nA.

Pulsed Beam Current: Enter beam current when pulsing is on, in nA.

Current Measurement Method: Drop down with choices – biased stage or Faraday cup.

Beam Diameter: Enter diameter of unrastered beam as full width half-maximum, in μm.

Beam Raster Size: Enter X and Y dimensions of raster on the sample in micrometers. If non-standard raster (*e.g.,* spiral) describe after this field.

Raster Pixel Dimensions: Enter the number of pixels in the X direction by the number by the number of pixels in the Y direction.

Beam Incident Angle: Angle, in degrees, between specimen normal and this ion source axis (uncorrected for change due to deflection by sample voltage).

Source to Analyzer Angle (degrees): Enter the angle, in degrees, between analyzer axis and this ion source axis.

Acknowledgments

Acknowledge grants and other people who have contributed to the work (other than authors) here. Any funding information provided in your Acknowledgements should also be listed in your manuscript details in the submission system. Under “Manuscript Information”, please click on "Publication Charges and Funding". Enter any funding sources in the "Funding Sources" section. Please be concise. Acknowledgements text should be styled as AckText. Acknowledgement title should be styled as AckHead

Author Declarations

Conflicts of Interest *(required)*

If there are conflicts to report, a statement to that effect must be included. If there are no conflicts to report, the statement "The authors have no conflicts to disclose" must be included.

Ethics Approval *(if applicable)*

Research articles containing experiments on animals and/or human subjects must include a statement that the authors obtained ethics approval. For more information, see author instructions for *SSS*.

Author Contributions *(if applicable)*

Statements about author contributions can be added here if needed.

Data Availability Statement

Since you are using this manuscript template, the appropriate statement likely is: "The data that supports the findings of this study are available within the article and its supplementary material." To confirm, you can review the instructions and templates, using the following link: https://publishing.aip.org/resources/researchers/open-science/research-data-policy.

References

References to be published in *Surface Science Spectra*.

Spectral Features Table

Note: One spectral features table per specimen and it should highlight the unique peaks within that spectrum. If there are peaks that occur in all spectra within the submission, they should be placed in a spectral features table at the end of the submission. There is an 'optional' table at the end of the template if needed.

Spectrum ID#: The official ID number will be assigned to you on acceptance. For initial submission, please enter the first part of the data (X,Y) file name (minus the extension), in the rows that relate to that file. Note: There are instructions on the required file naming scheme for initial submission found in *Information for Contributors*.

Mass (Δm), Da: List the experimental mass "Mass" and the deviation from the theoretical mass (Δm) for each unique major peak in the spectrum. If the same peaks show up in each spectrum in the submission, please do not include them in the individual tables and place them in a separate table at the end of the template instead.

Species: List the chemical formulas for the listed masses. Only include formulas for species that you are certain of. Peak identifications should only be provided for species where the centroid mass matches within ~+/- 65 ppm and where the peak pattern matches the expected isotopic pattern.

Peak Assignment: If known, state the likely source of the stated peaks. This could include things like 'surface contamination', 'sample material', 'molecular ion', or [M-H]'. If not known, please leave blank as this field should be used only if it provides additional insight into the source of the identified peak.

Spectra

Paste the spectrum as you would like it published. Only label major peaks in the spectrum that can be accurately identified. Include one figure per specimen submitted. If you need to show 2 spectral regions to accomplish this, please present them as a stacked plot in 1 figure. File formats for plots are PostScript, EPS, TIFF, JPG or production-ready PDF.

Specimen: Provide a generic description of the specimen, such as nylon, 6061 Al, or SiO_2. For layered structures, the specimen is the 'bulk' substance near the surface.

Technique: SIMS

Instrument: Enter the instrument manufacturer name. If the instrument was custom-built, enter the designer's name and reference a published article, if applicable. Enter the manufacturer's model number.

Analyzer Type: Drop down with choices – magnetic sector, quadrupole, time-of-flight, other. Choose the analyzer type that best applies. If 'Other,' include a description of the 'Non-Standard Analyzer or Lens' by entering this information after the analyzer type drop-down menu.

Analyzer Mass Resolution: Specify the mass resolution (m/Δm) of the spectrum. When specifying the mass resolution from each spectrum, please choose a peak that is found in all spectra presented in your submission. If a peak cannot be found in all spectra, then please choose a peak that is within a similar mass range. This will enable comparison of the spectral resolution since mass resolution is dependent on the mass chosen.

Mass Resolution Determined at: Specify the mass (m/z) that the mass resolution was determine at. It is recommended that you use a peak below m/z 100 to avoid artificially inflating the mass resolution by choosing a high mass peak.

Species Used for Mass Calibration: List the species used to calibrate the spectra. The calibration should include at least 3 peaks. If possible, calibrate all submitted spectra with the same calibration set. If a different calibration set needs to be used, please clarify why this was done.

Specimen Normal-to-Analyzer: Enter specimen emission angle, in degrees.

Source-to-Analyzer Angle: Enter the angle, in degrees, between analyzer axis and this ion source axis.

Primary Beam Ion Gun: List the type of primary ion gun used.

Primary Ion Species: List the primary ion species used.

Primary Ion Dose: List the primary ion dose used in ions/cm^2.

Primary Ion Pulse Width: State the primary ion pulse width used.

Primary Ion Pulse Rate: Enter repetition rate of pulses, in kHz.

Net Beam Voltage: Enter difference between accelerating voltage and sample potential, in eV.

Pulsed Beam Current: Enter beam current when pulsing is on, in nA.

DC Beam Current: Enter beam current when pulsing is off, in nA.

Beam Diameter: Enter diameter of unrastered beam as full width half-maximum, in μm.

Beam Raster Size: Enter X and Y dimensions of raster on the sample in micrometers. If non-standard raster (*e.g.,* spiral) describe after this field.

Beam Incident Angle: Angle, in degrees, between specimen normal and this ion source axis (uncorrected for change due to deflection by sample voltage).

Secondary Source Polarity: State the polarity of the collected secondary ions.

Mass Range Minimum: State the minimum value of the mass range.

Mass Range Maximum: State the maximum value of the mass range.

Spectrum Dead Time Corrected: Drop down menu with choices Yes, No or 'Not specified'.

Total Spectral Acquisition Time: State the total acquisition time for the spectrum.

Comment: Note any additional comments about the spectrum that would be useful for the reader.