IUPAC Recommendations

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Glossary of methods and terms used in surface chemical analysis (IUPAC Recommendations 2020)

Abstract: This glossary provides a formal vocabulary of terms for concepts in surface analysis and gives clear definitions to those who utilize surface chemical analysis or need to interpret surface chemical analysis results but are not themselves surface chemists or surface spectroscopists.

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1 Introduction

This Glossary on Methods and Terms used in Surface Chemical Analysis includes definitions of analytical methods and terms used in surface analysis techniques that yield atomic and molecular information, but does not include methods that yield purely structural and morphological information, such as diffraction methods and microscopies. The general scope of the chapter includes analytical techniques in which beams of electrons, ions, or photons are incident on a material surface and scattered or emitted electrons, ions, or photons detected from within about 10 nm of the surface are spectroscopically analysed. The glossary includes methods and terms for chemical analysis of surfaces under vacuum, as well as surfaces immersed in liquid.

This glossary serves as a necessary update to the previous version of the Orange Book, published in 1997 [1]. The advances in surface analysis during the intervening years have been many. Our purpose is to ensure the universality of terminology in the field of Surface Analytical Chemistry. Consistency in terminology is key to assuring reproducibility and consistency in results.

The International Organisation for Standardization (ISO) has published ISO 18115 Surface Chemical Analysis – Vocabulary, which consists of two parts: ISO 18115-1, General terms and terms used in spectroscopy (2013) [2], and ISO 18115-2, Terms used in scanning probe microscopy (2013)[3]. Part 1 mainly covers spectroscopic techniques, while Part 2 includes some surface spectroscopies that have been used in the scanning probe mode. The present Recommendation selectively includes topics contained in the two parts of ISO 18115 without including microscopic methods. The terminology taken from ISO 18115-1 and -2 for this IUPAC Compendium is reproduced with permission of the International Organisation for Standardisation. Terms and definitions also comply with the International Vocabulary of Metrology (VIM) [4]. Where reference is first made to a VIM-defined term it is identified by [VIM x.y]. Where a definition from [2] is used with only minor edits in accommodation of layout, the ISO number is given "Source: [2] entry x.y". Otherwise the source is given as "Modified from [2] x.y".

Section 2 of this Glossary contains definitions of the principal methods used in surface chemical analysis along with Notes giving the more common variants of these principal methods. This section introduces the range of surface chemical analysis methods available. Section 3 provides definitions of terms associated with the various methods of section 2. In each of these sections, a term printed in italics in a definition or a note is defined in another entry in this section of the Glossary.

Also noted is a recent (2019) Technical Report on recent advances in trace element analysis in environmental samples by X-ray based techniques, which gives an excellent overview of recent methods, some of them applicable to surfaces [5].

To avoid unneccesary duplication, where a term is already defined in the recent "Glossary of Methods and Terms used in Analytical Spectroscopy (IUPAC Recommendations 2020)" [6], we do not repeat it here, but cross reference to that publication.

2 Surface Chemical Analytical Principles of Measurement and Methods

2.1 Electron Spectroscopies

1 Auger spectroscopy
   Auger electron spectroscopy, (AES)

Measurement method [VIM 2.5] of electron emission spectroscopy that utilizes Auger electrons emitted from the target following excitation with an electron beam or X-ray beam.

Note 1: Chemical species are identified from the energies of the emitted Auger electrons and the typically low energies of the emitted electrons and resulting escape depth mean the technique is particularly sensitive for surface species analysis.

Note 2: Most AES is performed under high vacuum or ultra-high vacuum. Source: [6] entry 342.

Note 3: An electron beam in the energy range 2 keV to 30 keV is often used for excitation of the Auger electrons. Auger electrons can also be excited with X-rays, ions, and other sources, but the term Auger electron spectroscopy, without additional qualifiers, is usually reserved for electron-beam-induced excitation. Where an X-ray source is used, the Auger electron energies are referenced to the Fermi level, but, where an electron beam is used, the reference may either be the Fermi level or the vacuum level. Conventionally, spectra may be presented in the direct or differential forms.

2 Auger photoelectron coincidence spectroscopy, (APECS)

Detection of an *Auger electron* and a core-level photoelectron, emitted from a solid irradiated by monoenergetic X-rays, within a sufficiently short time that the Auger electron shall arise from the decay of the particular core-hole associated with the photoelectron.

Source: [2] entry 6.1.

3 elastic peak electron spectroscopy, (EPES)

Measurement method [VIM 2.5] in which an *electron spectrometer* is used to measure the energy, intensity, and/or energy broadening distribution of quasi-elastically scattered electrons from a solid or liquid surface.

Note 1: An electron beam in the energy range 100 eV to 3 keV is often used for this kind of spectroscopy.

Note 2: In general, electron sources with energy spreads that are less than 1 eV are required to provide adequate information.

Note 3: EPES is often an auxiliary method of *Auger electron spectroscopy* and *reflection electron energy loss spectroscopy* (REELS), providing information on the composition of the surface layer. EPES is suitable for the experimental determination of the *electron inelastic mean free path*, the electron differential *elastic scattering cross section*, and the surface excitation parameter.

Source: [2] entry 3.4.

4 electron spectroscopy for chemical analysis, (ESCA)

See: *X-ray photoelectron spectroscopy*.

5 reflection electron energy loss spectroscopy, (REELS)

Measurement method [VIM 2.5] in which an *electron spectrometer* is used to measure the energy distribution of electrons quasi-elastically scattered by atoms at or in a surface layer and the associated *electron energy loss spectrum*.

Source: Modified from [2] entry 3.16. See also: *elastic peak electron spectroscopy*.

6 ultraviolet photoelectron spectroscopy, (UPS)

Measurement method [VIM 2.5] in which an *electron spectrometer* is used to measure the energy distribution of electrons emitted from a *surface* irradiated by ultraviolet photons.

Note: Ultraviolet sources in common use include various types of discharges that can generate the resonance lines of various gases (*e.g.* the He I and He II emission lines at energies of 21.2 eV and 40.8 eV, respectively). For variable energies, synchrotron radiation is used.

Source: Modified from [2] entry 3.22.

7 X-ray photoelectron spectroscopy, (XPS)

electron spectroscopy for chemical analysis, (ESCA)

Measurement method [VIM 2.5] of *electron emission spectroscopy* that uses an X-ray source to stimulate the emission of photoelectrons from a surface. These photoelectrons have energies characteristic of transitions specific to the chemical elements from which they were emitted.

Note 1: Laboratory XPS systems usually operate under high or ultra-high vacuum.

Note 2: Synchrotron X-ray XPS can be performed under vacuum, ambient, or high pressure, enabling investigations of surfaces under ambient and extreme conditions.

Source: [6] entry 489.

Note 3: Emitted electrons include photoelectrons and *Auger electrons*.

2.2 Ion scattering spectroscopies

8 direct recoil spectroscopy, (DRS)
elastic recoil detection, (ERD)
elastic recoil detection analysis, (ERDA)

Measurement method [VIM 2.5] to elucidate composition and structure of the outermost atomic layers of a solid material, in which principally monoenergetic neutral atoms or singly charged *probe ions* are used to sputter atoms or ions out of the solid surface, their energy being recorded at one or more *angle of scattering*.

Note 1: In the analysis, it is assumed that the recoiled atom or ion is from a single binary elastic scattering event. The energy is the complement of the primary ion scattered ion energy.

Note 2: The scattered primary ions can be removed from the spectrum by a suitable choice of angle of scattering.

Note 3: This method is often combined with rutherford backscattering spectrometry, as they share many concepts and instrumental items.

Source: [2] entry 6.5. See also *Rutherford backscattering spectrometry*.

9 ion beam analysis, (IBA)

Measurement method [VIM 2.5] to elucidate the composition and structure of the near-surface atomic layers of a solid material, in which principally monoenergetic, singly charged *probe ions* scattered from the *surface* are detected and recorded as a function of their energy, *angle of scattering*, or both.

Note: *Low-energy ion scattering spectrometry*, *medium-energy ion scattering spectrometry*, and *Rutherford backscattering spectrometry* are all forms of IBA in which the probe ion energies are typically in the ranges 0.1 keV to 10 keV, 100 keV to 200 keV, and 1 MeV to 2 MeV, respectively. These classifications represent three ranges in which fundamentally different physics are involved.

Source: [2] entry 3.11.

10 low-energy ion scattering spectrometry, (LEIS(S))

Measurement method [VIM 2.5] to elucidate the composition and structure of the very outermost atomic layers of a solid material, in which principally monoenergetic, singly-charged *probe ions* scattered from the *surface* are detected and recorded as a function of their energy, *angle of scattering*, or both.

Note 1: LEIS(S) is a form of *ion beam analysis* in which the *probe ions*, typically He^+ or Ne^+, have energies in the range 0.1 keV to 10 keV.

Note 2: The acronym usually has only one "S".

Source: [2] entry 3.12.

11 medium-energy ion scattering spectrometry, (MEIS(S))

Measurement method [VIM 2.5] to elucidate the composition and structure of the outermost atomic layers of a solid material, in which principally monoenergetic, singly-charged *probe ions* scattered from the *surface* are detected and recorded as a function of their energy, *angle of scattering*, or both.

Note 1: MEIS is a form of *ion beam analysis* in which the probe ions, typically protons, have energies in the range 100 keV to 200 keV.

Note 2: By using channelling and aligning the incident-ion beam along a crystal axis, the scattering from the substrate can be suppressed, enhancing the signal quality and visibility obtained for amorphous overlayers. By further aligning the detector along a second crystal axis, the double-alignment mode, the scattering from the substrate can be further suppressed, improving the signal quality and visibility for amorphous overlayers to a high level.

Note 3: In some cases, an angle-sensitive detector is used that allows extensive structure and depth profile (see *depth profiling*) information to be obtained.

Note 4: The acronym usually has only one "S".

Source: [2] entry 3.13.

12 Rutherford backscattering spectrometry, (RBS)

Measurement method [VIM 2.5] to elucidate composition and structure of layers at the *surface* of a solid material, in which principally monoenergetic, singly charged *probe ions* scattered from the surface with a *Rutherford cross section* are detected and recorded as a function of their energy or *angle of scattering*, or both.

Note 1: RBS is a form of *ion beam analysis* in which the probe ions, typically He^+ but sometimes H^+, have energies in the range 1 MeV to 2 MeV. In its traditional form, a solid-state energy-dispersive detector is used. In the form of high-resolution RBS, the energy can be reduced to 300 keV and a high-resolution (ion optical) spectrometer can be used.

Note 2: By using channelling and aligning the incident-ion beam along a crystal axis, the scattering from the substrate can be suppressed so that enhanced signal quality and visibility are obtained for amorphous overlayers.

Source: [2] entry 3.15.

2.3 Mass spectrometries

13 desorption atmospheric pressure chemical ionization (DAPCI) mass spectrometry

Measurement method [VIM 2.5] in which a *mass spectrometer* is used to measure the ratio of mass to charge and the abundance of ionized entities emitted from a sample in air as a result of a nearby corona discharge in a humid carrier gas.

Note 1: The carrier gas is usually nitrogen.

Note 2: Both positive and negative ions are observed with the mechanisms involving protonation through water molecules and ionization through the Penning process.

Source: [2] entry 6.4. See also: *direct analysis in real time, plasma assisted desorption ionization*.

14 desorption atmospheric pressure photoionization (DAPPI) mass spectrometry

Measurement method [VIM 2.5] in which a *mass spectrometer* is used to measure the ratio of mass to charge and the abundance of ionized entities emitted from a sample in air as a result of desorption by a jet of hot solvent vapour and ionization by ultraviolet light.

Note 1: The desorption mechanism is thermal.
Note 2: Both positive and negative ions are observed.

Source: [2] entry 6.2. See also: *desorption electrospray ionization*, *extractive electrospray ionization*, *electrospray laser desorption ionization mass spectrometry* and *matrix-assisted laser desorption electrospray ionization*.

15 desorption electrospray ionization (DESI) mass spectrometry

Measurement method [VIM 2.5] in which a *mass spectrometer* is used to measure the ratio of mass to charge and the abundance of ionized entities emitted from a sample in air as a result of the bombardment by ionized solvent droplets generated by pneumatically assisted electrospray ionization.

Note 1: Water and methanol are often used as the solvents to create the droplets. Acids and alkalis are added to control the solution pH.
Note 2: DESI is one of the few surface analysis methods designed to analyse materials without exposure to vacuum. It is used for complex molecules, organic molecules, and biomolecules. *In vivo* analysis is claimed to be possible.

Source: [2] entry 3.2.

16 direct analysis in real time, (DART)

Measurement method [VIM 2.5] in which a *mass spectrometer* is used to measure the ratio of mass to charge and the abundance of ionized entities emitted from a sample in air as a result of the interaction with a beam containing metastable, excited atoms heated to about 500 °C.

Note 1: DART is the registered trademark of JEOL, USA, Inc.
Note 2: The beam atoms usually used are helium, nitrogen, or neon.
Note 3: Both positive and negative ions are observed, although the mechanism for positive ions can be through protonation involving water molecules and the process for negative ions through Penning ionization.

Source: [2] entry 6.3. See also *plasma assisted desorption ionization*.

17 dynamic secondary-ion mass spectrometry, (DSIMS)

Secondary-ion mass spectrometry analysis with primary ion current density sufficiently high for use in the analysis of sample surface layers in the depth direction.

Source: [7] entry 142.

Note: Dynamic SIMS is often simply termed SIMS.

18 electrospray laser desorption ionization mass spectrometry, (ELDIMS)

Measurement method [VIM 2.5] in which a *mass spectrometer* is used to measure the ratio of mass to charge quotient and the abundance of ionized entities emitted from a sample in air *via* ablation by a focused pulsed laser while simultaneously directing an electrospray jet through the desorbed plume to enhance sample ionization.

Note 1: The desorption mechanism is thermal.
Note 2: Both positive and negative ions are observed.

Note 3: With the addition of a matrix on the sample, this is termed *matrix-assisted laser desorption electrospray ionization* (MALDESI).

Note 4: With the use of an infrared laser for ablation, this has sometimes been termed *laser ablation electrospray ionization* (LAESI).

Source: [2] entry 6.6. See also: *desorption atmospheric pressure photoionization, desorption electrospray ionization, extractive electrospray ionization.*

19 extractive electrospray ionization (EESI) mass spectrometry

Measurement method [VIM 2.5] in which a *mass spectrometer* is used to measure the ratio of mass to charge and the abundance of ionized entities emitted from a sample in air as a result of an inert gas being passed over the sample to pick up the molecules, which are subsequently ionized by ionized solvent droplets generated by pneumatically assisted electrospray ionization.

Note: Both positive and negative ions are observed.

Source: [2] entry 6.7. See also: *desorption atmospheric pressure photoionization, desorption electrospray ionization, electrospray laser desorption ionization mass spectrometry* and *matrix-assisted laser desorption electrospray ionization.*

20 fast atom bombardment (FAB) mass spectrometry

Measurement method [VIM 2.5] in which a *mass spectrometer* is used to measure the ratio of mass to charge and the abundance of *secondary ions* emitted from a sample as a result of the bombardment by fast neutral atoms.

Source: Modified from [2] entry 3.6. See also: [7]

21 G-SIMS

Variant of *static secondary-ion mass spectrometry* in which the intensities for each mass in two spectra from the same area, recorded with different beam energies or different bombarding ions, are ratioed to each other and the result is used to scale one of the spectra to generate a new spectrum.

Note 1: As with static SIMS, the ion *areic dose* during measurement is restricted to less than 10^{16} ions per m^2 to an extent that depends on both the material of the sample and the size of the molecular fragments being analysed.

Note 2: The G-SIMS spectrum enables the mass of whole molecules on the *surface* to be determined more readily than in static SIMS.

Note 3: The "G" in G-SIMS originally indicated the gentleness of the process generated.

Source: [2] entry 3.7.

22 laser ablation electrospray ionization (LAESI) mass spectrometry

Measurement method [VIM 2.5] in which a *mass spectrometer* is used to measure the ratio of mass to charge and the abundance of ionized entities emitted from a sample in air as a result of laser ablation and electrospray ionization.

Note 1: The laser wavelength is usually in the infrared region.

Note 2: Both positive and negative ions are observed with the mechanisms involving protonation through water molecules and ionization through the Penning process.

Source: [2] entry 6.10. See also: *desorption atmospheric pressure photoionization, desorption electrospray ionization, extractive electrospray ionization, electrospray laser desorption ionization mass spectrometry, matrix-assisted laser desorption electrospray ionization.*

23 mass spectrometry, (MS)

Obsolete: mass spectroscopy

Study of matter through the formation of gas-phase ions that are characterized using *mass spectrometers* by their mass, charge, structure, and/or physico-chemical properties.

Note 1: The term is a misnomer because it is m/z, rather than mass, that is the independent variable in a *mass spectrum*.

Note 2: 'Mass spectroscopy' is an obsolete synonym for *mass spectrometry* that should not be used in order to avoid confusion with spectroscopies in which the measured quantity is the absorption or emission of electromagnetic radiation.

Source: [7] entry 320.

24 matrix-assisted laser desorption electrospray ionization (MALDESI) mass spectrometry

Measurement method [VIM 2.5] in which a *mass spectrometer* is used to measure the ratio of mass to charge and the abundance of ionized entities from a sample that has been mixed with a matrix whose role is enhancing the ion yield produced by laser ablation and electrospray ionization.

Note 1: The matrix, *e.g.* glycerol, allows efficient absorption of the laser energy and assists the desorption of the analyte molecules in the ejected charged droplets.

Note 2: Both positive and negative ions are observed.

Source: [2] entry 6.12. See also: *desorption atmospheric pressure photoionization*, *desorption electrospray ionization*, *extractive electrospray ionization*, *electrospray laser desorption ionization mass spectrometry*, *laser ablation electrospray ionization*.

25 matrix-assisted laser desorption/ionization mass spectrometry (MALDI) mass spectrometry

Measurement method [VIM 2.5] in which a *time-of-flight* mass spectrometer is used to measure the ratio of mass to charge and the abundance of ions emitted, as a result of a short pulse of laser illumination, from a sample whose analyte is contained in a matrix that assists the formation of ions.

Note 1: The matrix used for assisting the ion emission needs a strong absorbance at the laser wavelength and a low enough mass to sublime. Examples of matrices for 337 nm wavelength laser light are 2,5-dihydroxybenzoic acid (DHB), 3,5-dimethoxy-4-hydroxycinnamic acid (sinapinic acid), and α-cyano-4-hydroxycinnamic acid (CHCA).

Note 2: MALDI is used to analyse non-volatile polar biological and organic macromolecules, as well as polymers, to masses of over 3 000 ku.

Source: [2] entry 3.14.

26 plasma assisted desorption ionization (PADI) mass spectrometry

Measurement method [VIM 2.5] in which a *mass spectrometer* is used to measure the ratio of mass to charge and the abundance of ionized entities emitted from a sample in air as a result of the bombardment by a focused plasma.

Note 1: The energy of the plasma ions is very low.

Note 2: The beam atoms usually used are helium, nitrogen, air, or argon.

Note 3: Both positive and negative ions are observed, although the mechanism for positive ions can be through protonation involving water molecules and the process for negative ions through Penning ionization.

Source: [2] entry 6.15. See also: *direct analysis in real time*.

27 reactive desorption electrospray ionization mass spectrometry

Mode of *desorption electrospray ionization mass spectrometry* with reactive chemicals within the spray solution to enhance the analytical specificity.

Source: [2] entry 6.16.

Note: The method has been used to detect chemical warefare agents [8], as well as natural products in marine alga [9].

28 secondary-ion mass spectrometry, (SIMS)

Measurement method [VIM 2.5] in which a focused beam of primary ions produces secondary ions by sputtering from a solid *surface*. The secondary ions are analysed by mass spectrometry.

Note: SIMS is, by convention, generally classified as either dynamic, in which the material surface layers are continually removed as they are being measured, or static, in which the ion *areic dose* during measurement is restricted to less than 10^{16} ions per m^2 in order to retain the surface in an essentially undamaged state.

See also: *dynamic secondary-ion mass spectrometry*, *static secondary-ion mass spectrometry*.

Source: [7] entry 475.

29 static secondary-ion mass spectrometry, (SSIMS)

Method of *secondary-ion mass spectrometry* using low current densities for analysis of sample *surface* components, in contrast with *dynamic secondary-ion mass spectrometry*, which is used for analysis of components in the depth direction.

Note 1: When the sample is an organic molecule in solid form, the term is often changed to organic SIMS or molecular SIMS.

Source: [7] entry 501.

Note 2: The ion *areic dose* during measurement is restricted to less than 10^{16} ions per m^2 to an extent that depends on both the material of the sample and the size of the molecular fragments being analysed. See [2] entry 3.20.

Note 3: Ions are usually detected by a *time of flight mass spectrometer* (TOF-SIMS).

30 surface-assisted laser desorption/ionization (SALDI) mass spectrometry

Matrix-assisted laser desorption/ionization mass spectrometry using a combined liquid and particulate matrix.

Note: The first particulate matrix to be used was graphite. More recently, nano particle matrices have been used. Ethane-1,2-diol (ethylene glycol) is a typical liquid.

Source: [2] entry 6.18.

2.4 Optical and X-ray spectroscopies

31 attenuated total reflection infrared spectroscopy, (ATRIRS)

Attenuated total reflection spectroscopy in which the infrared absorption spectrum of a sample in contact with a prism is measured.

Note 1: Most ATRIR work is carried out with an angle of incidence of 45 degrees inside a ZnSe or diamond prism, both with a refractive index of 2.4. With such optical conditions, total internal reflection is achieved with an effective sample refractive index less than about 1.7 for almost all powdered samples.

Note 2: ATRIRS has particular application in the surface chemical analysis of solid particle films immersed in aqueous solution.

Source: [10, 11].

32 attenuated total reflection (ATR) spectroscopy
internal reflection spectroscopy (IRS)
frustrated total internal reflection spectroscopy

Measurement method [VIM 2.5] of *molecular spectroscopy* based on *total internal reflection* within a prism attenuated by absorbing material in contact with the prism (*attenuated total reflection*).

Note: A spectrum resembles an absorption spectrum of the sample.

Source: Modified from [6] entry 499, [10, 11].

33 diffuse reflection-absorption infrared spectroscopy, (DRAIRS)
diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS)

Measurement method [VIM 2.5] in which the infrared absorption spectrum of light reflected and transmitted from powdered samples is measured.

Note: Used for the analysis of weakly-reflective surfaces in gas phase or vacuum.

34 diffuse X-ray reflectometry

See: *off-specular X-ray reflectometry*.

35 ellipsometry

Measurement method [VIM 2.5] for the thickness of transparent surface films and layers and for the refractive index of a reflecting material.

Note 1: Radiation that is linearly polarized oblique to the surface becomes elliptically polarized after reflection at non-normal incidence. The *ellipticity* is obtained from measurements of the intensity and polarization of the incident and the reflected radiation.

Source: [6] entry 531.

Note 2: Ellipsometry may utilise monochromatic light, while spectroscopic ellipsometry employs a range of frequencies.

36 extended X-ray absorption fine structure spectroscopy, (EXAFS)

X-ray absorption fine structure spectroscopy in the energy region from the core-level edge to an energy several hundred eV greater.

Note 1: Extended X-ray absorption fine structure results mainly from the single scattering of the photoelectron from surrounding atoms and is exhibited as oscillations in the absorption *cross section* with increasing photon energy. Analysis of the oscillations provides information, through bond lengths, on the local chemical environment of the emitting atom.

Source: [2] entry 6.8.

Note 2: EXAFS has been used as an alternate term for the superordinate concept of XAFS.

37 frustrated total internal reflection

See: *attenuated total reflection*.

38 grazing-incidence small-angle X-ray scattering analysis, (GISAXS)

Measurement method [VIM 2.5] in which the elastically scattered intensity of X-rays from a reflecting surface is measured for small-angle deflections at grazing incidence.

Note 1: The grazing incidence angle depends on photon energy and material and is typically less than 2°.

Note 2: GISAXS provides structural information for the surface or for particles on the surface, with lengths scales between several nm and several hundred nm.

Source: [2] entry 6.9.

39 infrared reflection-absorption spectroscopy, (IRRAS)

See: *reflection-absorption infrared spectroscopy*.

40 internal reflection spectroscopy, (IRS)

See: *attenuated total reflection spectroscopy*.

41 near-edge extended X-ray absorption fine structure spectroscopy, (NEXAFS)

See: *X-ray absorption near-edge spectroscopy*.

42 near-field scanning optical microscopy, (NSOM)

See: *scanning near-field optical microscopy*.

43 off-specular X-ray reflectometry
   diffuse X-ray reflectometry

X-ray reflectometry in which significant scattered intensity arises from imperfections in the specimen, the scattered intensity falling outside the specular condition (see *specular X-ray reflectometry*).

Note: Imperfections generating diffuse XRR include surface and interface roughnesses, film defects, and inhomogeneities. Quantitative estimates of these can be made by modelling.

Source: [2] entry 6.13.

44 particle-induced X-ray emission analysis, (PIXE)

Measurement method [VIM 2.5] in which the energies and intensities of X-rays emitted from a solid surface, under the action of a beam of atoms or ions, are detected.

Note: Unlike electron microprobe X-ray analysis, where the generating radiation is an electron beam, in PIXE the X-ray background is much reduced so that the detection limits are significantly improved while *lateral resolution* can be maintained.

Source: [2] entry 6.14.

45 reflection-absorption infrared spectroscopy, (RAIRS)
infrared reflection-absorption spectroscopy (IRRAS)

Spectroscopy based on *reflection-absorption*.

Note 1: RAIRS allows improved discrimination between species at the surface and those in the bulk.

Note 2: RAIRS is most sensitive at metal surfaces with grazing incidence.

Note 3: RAIRS is usually employed with the sample in a vacuum or gas.

Note 4: RAIRS may be employed with polarization modulation to minimize background absorption.

Source: Modified from [6] entry 636.

46 scanning near-field optical microscopy, (SNOM)
near-field scanning optical microscopy (NSOM)
near-field optical microscopy

Measurement method [VIM 2.5] in microscopy in which spectroscopic data may be collected with the detector closer to the sample than the optical wavelength employed.

Note: Includes near-field infrared, Raman, and fluorescence spectroscopies.

Source: [3] entry 3.17.

47 second harmonic generation, (SHG)

Non-linear optical effect in which light is emitted with twice the frequency of the incident light.

Note 1: In *scanning near-field optical microscopy*, tip enhancement can lead to second harmonic generation when a metal tip is used, or can lead to an increase in second harmonic generation from the surface in close proximity to the tip.

Note 2: For incident light, the lack of symmetry at a surface or at a buried interface can lead to SHG.

Source: Modified from [3] entry 5.140.

48 small-angle X-ray scattering

Measurement method [VIM 2.5] in which the elastically scattered intensity of X-rays is measured for small-angle deflections.

Note 1: Angular scattering is usually measured within the range 0.1° to 10°. This provides structural information on macromolecules, as well as periodicity on length scales typically larger than 5 nm and less than 200 nm for ordered or partially ordered systems.

Note 2: Wide-angle X-ray scattering (WAXS) is an analogous technique, similar to X-ray crystallography, in which scattering at larger angles, which is sensitive to periodicity on smaller length scales, is measured.

Note 3: The X-ray source can be a synchrotron, in which case the term synchrotron radiation small-angle X-ray scattering (SRXAS) is occasionally encountered.

Source: [2] entry 3.18.

49 specular X-ray reflectometry

Mode of *X-ray reflectometry* in which the angle between the detected beam and the sample surface is equal to that of the incident beam and the sample surface. See also *off-specular X-ray reflectometry*.

Note 1: Specular XRR is the plainary mode for XRR and is often meant when the term XRR is used.

Note 2: In this case, the *angle scattering 2θ* is twice the incidence angle, ω. The detected, scattered X-ray intensity is measured as a function of either ω or 2θ or the scattering vector, q_z. The intensity data are usually presented as a function of q_z or ω.

Source: [2] entry 6.17.

50 sum frequency generation spectroscopy, (SFGS)
vibrational sum frequency spectroscopy, (VSFS)

Measurement method [VIM 2.5] from non-linear optics in which a structurally-ordered sample at an interface between two phases is irradiated by single frequency visible and variable frequency infrared pulses of light to generate a sum frequency vibrational spectrum of the interfacial species without any bulk phase contribution.

Note: Closely related to *second harmonic generation*.

51 surface extended X-ray absorption fine structure spectroscopy, (SEXAFS)

Extended X-ray absorption fine structure spectroscopy in which, instead of measuring X-ray absorption, electron emission arising from that absorption is measured.

Note 1: Emitted electrons include *Auger electrons* and *secondary electrons*.
Note 2: The detection of emitted electrons provides greater surface sensitivity than is generally found with extended X-ray absorption fine structure measurements.

Source: Modified [2] entry 6.19.

52 surface plasmon resonance

Resonant interaction between the natural frequency of a *surface plasmon* and incident light of the same frequency.

53 surface-enhanced infrared spectroscopy, (SEIRAS)

Measurement method [VIM 2.5] giving enhanced infrared absorption in the measured infrared spectrum of a sample adsorbed on a roughened thin metal substrate. The metal substrate is deposited onto a prism and data is collected by total internal reflection.

Note: SEIRAS enhancements can be 10^2 or greater.

53 surface-enhanced Raman spectroscopy, (SERS)

Measurement method [VIM 2.5] of Raman spectroscopy by which the intensity of vibrational bands in the Raman spectra of molecules within a few nanometers of the surface of microscopically rough metals, metal colloids, and metal nanoparticles is increased by up to 10^6.

Note 1: The metals that give the largest enhancement are silver, gold, and copper, but this phenomenon has been reported to occur with a range of other metals.
Note 2: Other mechanisms of enhancement are known, but the common usage of SERS is with a metal or related systems and implies enhancement through interaction with a surface plasmon.

Source: Modified from [6] entry 654.

54 surface-enhanced resonant Raman spectroscopy, (SERRS)

Measurement method [VIM 2.5] of s*urface-enhanced Raman spectroscopy* (SERS) by which the Raman spectrum is significantly enhanced under the conditions that, whilst undergoing SERS, the molecules are excited by radiation that is in resonance with electronic transitions in the sample.

Note 1: Enhancements of up to and greater than 10^{10} have been measured.
Note 2: The acronym SERRS is used for both surface-enhanced resonant Raman scattering and spectroscopy.
Source: Modified from [6] entry 655.

55 synchrotron radiation small-angle X-ray scattering, (SRXAS)

See: *small-angle X-ray scattering.*

57 tip enhanced Raman spectroscopy, (TERS)

Measurement method [VIM 2.5] of Raman spectroscopy combining *surface-enhanced Raman spectroscopy* and scanning using an atomic force microscope or scanning tunnelling microscope to produce maps of a surface.
Source: Modified from [6] entry 665.

Note: TERS is one of several near-field optical spectroscopic techniques.

58 total reflection X-ray fluorescence spectroscopy, (TXRF)

Measurement method [VIM 2.5] in which an X-ray spectrometer is used to measure the energy distribution of *fluorescence* X-rays emitted from a *surface* irradiated by primary X-rays under the condition of *total reflection.*
Source: [2] entry 3.21.

59 vibrational sum frequency spectroscopy, (VSFS)

See: *sum frequency generation spectroscopy.*

60 wide-angle X-ray scattering, (WAXS)

See: *small-angle X-ray scattering.*

61 X-ray absorption fine structure spectroscopy, (XAFS)

Measurement method [VIM 2.5] to measure the absorption of X-rays at energies near and above (typically several hundred eV greater) an absorption edge, over which fine structure (modulation of the X-ray absorption coefficient) can be detected.

Note 1: XAFS includes both *extended X-ray absorption fine structure spectroscopy* and *X-ray absorption near-edge spectroscopy.* It involves transitions from a core-level to an unoccupied orbital or band and mainly reflects the local atomic structure and bonding (SEXAFS) and the density of the unoccupied electronic states (XANES).
Note 2: XAFS measurements usually start some 10 eV before the core-level binding energy (the absorption edge) of the emitting atoms, because in many cases pre-edge features are used to identify chemical bonds [example: π* resonances (excitation into lowest unoccupied molecular orbitals) in C K-edge spectra of polymer samples].

Note 3: Usefully sharp absorption edges are commonly observed in X-ray absorption spectra, although broader increases can be observed for some inner-shell excitations with short lifetimes.

Source: [2] entry 6.20.

Note 4: XAFS spectra are best recorded when a highly intense beam of X-rays from a synchrotron is used along with a high *resolution* double crystal or curved crystal spectrometer. Detectors include ionization chambers, scintillation counters, and solid state detectors. [12].

62 X-ray absorption near-edge spectroscopy, (XANES)

near-edge extended X-ray absorption fine structure spectroscopy, (NEXAFS)

X-ray absorption fine structure spectroscopy in the energy region near (within approximately 100 eV) an absorption edge.

Note 1: XANES results from interference in multiple scattering of low-energy photoelectrons by surrounding atoms. It provides information on the local coordination environment, oxidation state, molecular orbitals, hybridization, and band structure (unoccupied electronic states).

Note 2: XANES measurements usually start some 10 eV before the core-level binding energy (the absorption edge) of the emitting atoms, because in many cases pre-edge features are used to identify chemical bonds, *e.g.* π* resonances (excitation into lowest unoccupied molecular orbitals) in C K-edge spectra of polymer samples.

Note 3: Usefully sharp absorption edges are commonly observed in X-ray absorption spectra, although broader increases can be observed for some inner-shell excitations with short lifetimes.

Source: [2] entry 6.21.

63 X-ray reflectometry, (XRR)

Measurement method [VIM 2.5] for surface and interface roughness and density, layer thickness of thin layers, and electron density profile achieved by reflecting X-rays from a flat sample and analysing the reflected intensity as a function of angle (See also *specular X-ray reflectometry*)

Note: Monochromatic X-rays of low divergence are required. Many layers can be modelled, with thicknesses between about 1 nm and a few μm, and (subject to conditions) fitted to the data. The surface needs to be flat over the *beam footprint* of typically 10 mm to 40 mm.

Source: [2] entry 6.22.

64 X-ray standing waves, (XSW)

Measurement method [VIM 2.5] based on the interference of X-rays that occurs near the Bragg condition at the surface of a crystalline solid, which leads to intensity maxima in yields of photoelectrons as the Bragg condition is scanned by tilting the sample.

Note 1: Intensity nodes are scanned from one lattice plane to the next as the sample is tilted. Atomic positions in the crystalline lattice can be determined from comparisons of measured scans of photoelectron intensity *versus* tilt angle with calculated scans from dynamical scattering theory.

Source: [2] entry 6.23.

Note 2: For defect-rich substrates, such as metal single crystals, a normal-incidence or back-reflection geometry may be used. Instead of rocking the crystal in space, the energy of the incident beam is tuned through the Bragg condition.

3 Terms used in surface chemical analysis

3.1 General terms

65 absolute elemental sensitivity factor

Coefficient for an element by which the measured intensity for that element is divided to yield the atomic concentration or atomic fraction of the element present in the sample.

Note 1: The choice of atomic concentration or atomic fraction should be made clear.

Note 2: The type of sensitivity factor utilized should be appropriate for the formulae used in the quantification process and for the type of sample analysed, *e.g.* for homogeneous samples or segregated layers.

Note 3: The source of sensitivity factors should be given to ensure that the correct *matrix factors* or other parameters are used.

Note 4: Sensitivity factors depend on parameters of the excitation source, the spectrometer, and the orientation of the sample to these parts of the instrument. Sensitivity factors also depend on the matrix being analysed. Sensitivity factors also depend on the matrix being analysed. In *secondary ion mass spectrometry* this has a dominating influence.

Source: [2] entry 4.415.

66 adsorbate

Material accumulated on the *surface* of an *adsorbent* by the process of *adsorption*.

Source: [1] section 9.5.

67 adsorbent

Condensed phase where *adsorption* occurs at the surface.

Source: Modified from [1] section 9.5.

68 adsorption

Increase in the concentration of an *adsorbate* at an *interface* of a condensed phase (*adsorbent*) and a liquid or gaseous layer due to the operation of surface forces.

Source: Modified from [1] section 9.5. See also: *surface excess*.

69 adsorption isotherm

Relationship between the amount, number, or mass of a substance adsorbed and the composition of the bulk phase (or the partial pressure in the gas phase) under equilibrium conditions at constant temperature.

Source: Modified from [13] p 585.

Example: Langmuir adsorption isotherm for the surface coverage of an adsorbing ideal gas B, θ_B, as a function of partial pressure of B, p_B.

$$\theta_B = K_{eq}^B p_B / (1 + K_{eq}^B p_B).$$

70 altered layer

Surface region of a material under particle bombardment where the chemical state or physical structure is modified by the effects of the bombardment.

Note 1: For silicon bombarded by 4 keV O_2^+ at near-normal incidence, after *sputtering* for a sufficient time to reach a steady state, the *surface* is converted to stoichiometric SiO_2 to a depth of around 15 nm, with lower oxygen concentrations at greater depths. At 2 keV, this is reduced to 7 nm, these thicknesses being approximately twice the *projected range*.

Note 2: The *observed interface width* (depth resolution) in *secondary-ion mass spectrometry* can be greater or smaller than the altered-layer thickness, depending on the analyte and bombarding-ion species.

Source: [2] entry 4.6.

71 analyser transmission function

See: *spectrometer transmission function*.

72 analysis area (of sample)

Two-dimensional region of a sample *surface* measured in the plane of that surface, from which the entire analytical signal or a specified fraction of that signal is detected.

Source: [2] entry 4.8.

73 analysis area (of spectrometer)

Two-dimensional region of a sample *surface* at the analytical point, but set in the plane at right angles to the spectrometer axis, from which the entire analytical signal or a specified fraction of that signal is detected.

Source: [2] entry 4.9.

74 angle lapping

Sample preparation in which a sample is mechanically polished at an angle to the original *surface*.

Note: This angle can often be less than 1°, so that depth information with respect to the original surface is transformed to lateral information.

Source: [2] entry 4.14. See also *radial sectioning*.

75 angle of emission
   emission angle

Angle between the trajectory of a particle or photon, as it leaves a *surface*, and the local or average surface normal.

Note 1: The particular surface normal needs to be specified.

Source: [2] entry 4.16.

Note 2: In *XPS* and other techniques, the *take-off angle*, which is referred to the sample surface, is quoted.

76 angle of incidence, ω
   incidence angle

Angle between the incident beam and the local or average surface normal.

Note 1: The particular surface normal, such as the surface normal to an elementary portion of a rough *surface* or the normal to the average surface plane, needs to be specified.

Source: [2] entry 4.17.

Note 2: In *XPS* and other techniques, the angle may be referenced to the sample surface.

77 areic dose rate, *G*

Areic dose introduced into a solid in time interval *t* divided by *t*.

Note 1: For a stationary parallel beam, the areic dose rate equals the *flux* times $\cos\theta$, where θ is the *angle of incidence* of the beam.

Source: [2] entry 4.179.

78 areic dose, *D*
dose

Number, *N*, of energetic particles of a specified type introduced into a solid through a surface area *A* divided by *A*. $D = N/A$.

Note 1: The energetic particles are atoms or atom clusters, which can be electrically charged or neutral, and the surface area *A* is the geometric surface area.

Note 2: For a stationary parallel beam, the areic dose equals the *fluence* times $\cos\theta$, where θ is the *angle of incidence* of the beam to the surface normal. Therefore, the use of 'fluence' for 'dose' is not recommended.

Note 3: In some texts, the term dose density is used, but the term dose (more correctly areic dose) is more widespread. The term dose has been defined very differently in the fields of radiation and the medical sciences. Some have taken the total amount of particle radiation impacting the *surface* to be the dose, while others consider the amount divided by the area of the surface to be the dose. Here, dose is taken to be the latter. Dose density and dose, where they occur, are to be taken as the areic dose.

Note 4: For a discussion of areic dose in relation to ion-implanted *reference materials* [VIM 5.14], see Reference [14].

Source: [2] entry 4.175.

79 areic surface energy
surface energy

Energy required to increase a surface area at thermodynamic equilibrium divided by that increase in area.

Note 1: SI unit J m^{-2}.

Note 2: This term has no relation to surface energy approximation, used in energetic-ion analysis and *Rutherford backscattering spectrometry*.

80 atomic mixing

Migration of sample atoms due to energy transfer with incident particles in the surface region.

Source: [2] entry 4.32. See also: *cascade mixing, collision cascade*.

81 Auger neutralization

Process in which an electron, tunnelling from the conduction band of a solid, neutralizes an incoming ion and an electron is ejected from a surface atom.

Note: The ejected electron can be emitted into the vacuum.

Source: [2] entry 4.40.

82 average beam current, I_{av}

Electric charge of specified polarity in a beam passing in time interval t, divided by t.

Note: For beams in which the instantaneous current varies periodically with time, the time interval t is an integral number of periods.

Source: [2] entry 4.69.

83 backscattering energy

Energy of a particle from the primary beam after it has undergone a backscattering collision and escaped from the sample.

Source: [2] entry 4.60.

84 ball cratering

Procedure in which the sample is abraded by a sphere in order to expose compositional changes in layers below the original *surface*, with the intent that the depth of those layers can be related to the lateral position in the crater created by the abrasion.

Source: [2] entry 4.64. See also: *radial sectioning*.

85 beam diameter

Full width of a particle beam of circular cross section at half maximum intensity measured in a plane normal to the beam direction.
Source: [15].

Note: The beam diameter is usually specified at a given point in space, such as the position of the sample.

Source: [2] entry 4.73.

86 binary elastic scattering (of particles)
elastic scattering

Collision between a moving particle and a second particle in which total kinetic energy and total momentum are conserved.

Note: In elastic scattering interactions, the moving particle can be deflected through angles of up to 180°.

Source: [2] entry 4.80. See also: *inelastic scattering*.

87 Bragg's rule

Empirical rule formulated by W.H. Bragg and R. Kleeman that states that the *stopping cross section* of a compound sample is equal to the sum of the products of the elemental stopping cross sections for each constituent and its atomic fraction.

$$S_{AB}(\varepsilon) = xS_A(\varepsilon) + yS_B(\varepsilon)$$

where $S_{AB}(\varepsilon)$ is the stopping cross section of the compound A_xB_y, and $S_A(\varepsilon)$ and $S_B(\varepsilon)$ are the stopping cross sections of elements A and B, respectively.

Source: [2] entry 4.85, modified from [15].

88 bulk plasmon

See: *plasmon*.

89 cascade mixing

Diffusion-like process in which atoms of material are moved randomly by energy deposited by incident particles slowing down in the sample surface region.

Source: [2] entry 4.87, without notes. See also: *atomic mixing, collision cascade*.

90 channeling

Preferential motion of energetic particles along the crystal axes of a crystalline solid as the particles move through the sample.

Source: [2] entry 4.94, without notes.

91 charge neutralization

Maintenance at a fixed potential, usually near neutrality, of the *surface* of a non-conducting or poorly conducting sample material under bombardment by primary particles or photons.

Note 1: Charge neutralization can be accomplished by bombarding the surface with electrons or, more rarely, ions or photons.

Source: [2] entry 4.98.

92 charging potential

Electric potential of the *surface* region of an insulating sample, caused by irradiation.

Note 1: Different charging potentials can occur on different areas or at different depths in a sample, arising from sample inhomogeneities or non-uniform intensity of the incident *flux* of radiation.

Note 2: The surface and bulk potentials can differ, for example as a result of band bending, *interface* dipoles, and charge centres.

Source: [2] entry 4.103.

93 chemical map

Surface map using signals proportional to the amount of an element in a particular chemical state in the sample.

Source: [2] entry 4.290.

94 chromatic aberration

Non-ideal focus of an electron or ion optical system for electrons or ions of different energies.

Source: [2] entry 4.110.

95 cluster ion

Ion formed by the combination, *via* noncovalent forces, of two or more atoms or molecules of one or more chemical species with an ion.

Example: $[(H_2O)_nH]^+$, $[(H_2O)_n (CH_3OH)_mH]^+$, $[(NaCl)_nNa]^+$, Au_{10}^-, or $[M + Na + CH_3OH]^+$, where M represents a molecule.

Source: [7] entry 80.

Note 1: The cluster can have a positive or negative charge.
Note 2: Cluster ions are used for primary-ion sources with enhanced properties compared with those of monatomic ions.
Examples: Ar_n^+ is often used. Other examples of such sources are Au_3^+, Au_5^+, Bi_3^+, Bi_5^+, C_{60}^+, $H_3O^+(H_2O)_n$, $[Os_3(CO)_{12}]^+$, and SF_5^+.

96 collision cascade

Sequential energy transfer between atoms in a solid as a result of bombardment by an energetic species.

Source: [15]. See also: *atomic mixing*, *cascade mixing*.

97 compositional depth profile, (CDP)

Chemical composition measured as a function of distance normal to the *surface*.

Source: [2] entry 4.115.

98 counts

Number of pulses recorded by a detector system in a defined time interval.

Note 1: Counts can be representative, one-for-one with particles being detected (in the absence of dead time losses in the counting measurement), in which case they follow Poisson statistics (unless other *noise* sources are present), or they can simply be proportional to the number of particles being detected. The type of measure needs to be clearly stated.
Note 2: In multi-detector systems, the apportion of counts into relevant channels of the spectrum can lead to changes from the expected Poisson statistics in each channel, since the counts in neighbouring channels can be partly correlated.

Source: Modified from [2] entry 4.120.

99 crater depth

Average depth of the region of a crater from which the measured signal is derived.

Note 1: The crater is generally formed by ion bombardment in sputter *depth profiling* and, in this case, can be different from the thickness of sample material removed by *sputtering* due to dilation of the altered layer.
Note 2: The crater depth can be modified by the formation of a reacted layer (*e.g.* an oxide) following any exposure to the atmosphere or other environments necessary when conducting the crater depth measurement.

Source: [2] entry 4.121.

100 cross section, σ

Probability of reaction or process for a specified target entity divided by the incident particle *fluence*.
Source: [2] entry 4.123, without notes.

Note: SI unit m^2.

Source: [16] p 24.

101 cross-sectioning

Sample preparation in which the sample is cleaved, cut, or polished in a plane perpendicular to the *interface* under study, so that associated compositional differences or gradients can be observed in that plane.

Source: [2] entry 4.137.

102 damage limit

Particle *fluence* above which significant changes in the spectrum or in a stated peak, arising from damage processes, are observed.

Source: [2] entry 4.138. See also: *static limit*.

103 delta layer

Layer of discrete composition, one atom thick, formed during the growth of material on a substrate.

Note: These films are often formed during epitaxial growth on single-crystal substrates.

Source: [2] entry 4.158.

104 depth profile
vertical profile

Chemical or elemental composition, signal intensity, or processed intensity information from the available software measured in a direction normal to the *surface*.

See also: *compositional depth profile*.

105 depth profiling

Monitoring of signal intensity as a function of a variable that can be related to distance normal to the *surface*.

Note: Signal intensity is usually measured as a function of the *sputtering* time.

Source: [2] entry 4.163. See also: *compositional depth profile*.

106 depth resolution

See: *observed interface width*.

107 depth resolution parameter

Parameter that can be used as a coefficient in an analytic fit to a measured compositional *depth profile* or as a qualitative way of describing that profile.

Examples: Standard deviation (for a Gaussian response function), full width at half maximum intensity (for any bell-shaped distribution), and *decay length* (for an exponentially increasing or decreasing region of the response function).

Note 1: Standard deviations can be used for any bell-shaped curve. If parameters are measured for a step change in composition, care must be taken that the depth range for the measurements is large enough to ensure that the signal becomes constant with depth on either side of the step.

Note 2: Parameter definitions should be used consistently.

Note 3: Depth resolution parameters usually give no indication of distinguishability, but are useful in instrumental evaluation and profile deconvolution.

Source: [2] entry 4.167. See also *observed interface width*.

108 dose

See: *areic dose*.

109 elastic scattering

See: *binary elastic scattering*.

110 emission angle

See: *angle of emission*.

111 elastic scattering cross section, σ_e

Cross section for *binary elastic scattering*.
Source: [2] entry 4.126.

112 electron flooding

Irradiation of a sample with low-energy electrons in order to change or stabilize the *charging potential*.
Source: [2] entry 4.188.

113 elemental map

Surface map using signals proportional to the amount of an element present in a sample.
Source: [2] entry 4.291.

114 energy resolution

Full width at half maximum (See: [6] entry 61) intensity of the measured energy distribution for monoenergetic particles.
Source: [2] entry 4.384. See also: *resolution*.

115 equilibrium surface composition sputtering

See: *steady-state surface composition sputtering*.

116 erosion rate (of a surface)

Change in the position of the *surface* as a result of particle or photon irradiation divided by time of irradiation.

Note 1: Erosion rate can be deduced from surface profilometer measurements of a crater after analysis. In this case, the effects of the altered layer and post-profile oxidation need to be considered.

Note 2: Where the erosion is caused by *sputtering*, initially the erosion rate can be less than the *sputtering rate* as a result of the retention of sputtering particles.

Note 3: The rate can be measured as a velocity.

Source: [2] entry 4.202.

117 Faraday cup

Detector with a cup-shaped electrode for collection of the electric charge carried by a beam of charged particles passing into the cup, designed such that the emission of charged particles from the detector is minimized.

Note: A Faraday cup is of "black hole" quality if it is open only to charged particles moving from outside in, but not to charged particles of any type moving from inside out. As a detector for ions in a beam, a Faraday cup is "ideal" if it combines a black-hole capability with a filter for electrons and *secondary ions* (*i.e.* the Faraday cup is open only to forward-moving ions of the beam, but is closed to all electrons and secondary ions from both inside and outside the cup).

Source: [7] entry168.

118 Fermi level

See: *standard vacuum level.*

119 field-induced migration

Effect occurring in insulators or semi-conductors where internal electric fields cause the migration of sample atoms.

Source: Modified from [2] entry 4.214.

120 fluence of a parallel beam of particles, *F*

For particles of a specified type incident normally at a *surface*, $F = dN/dA$, where N is number of particles and A is area.

Note 1: For a scanned parallel beam, the fluence can be referenced to the laboratory coordinate system or to the scanned beam's own moving coordinate system. The latter will generally give the higher value. The usage of fluence in these situations requires a clear statement of the coordinate system being used.
Note 2: In some texts, the term fluence is used for *areic dose*. This is incorrect and has led to confusion. See Note 2 in areic dose.
Note 3: For a parallel beam, fluence rate and *flux* density are equivalent measures.

Source: [2] entry 4.217.

Note 4: SI unit m^{-2}. In spectroscopy, fluence is the energy of electromagnetic radiation delivered per unit area and has unit $J\ m^{-2}$. See [6] entry 377.

121 flux of a beam of particles, *Φ*

$\Phi = dN/dt$, where N is number of particles of a specified type and t is time.
Source: [2] entry 4.218.

Note 1: For a parallel beam, *fluence* rate and flux density are equivalent measures.
Note 2: SI unit: s^{-1}. For a beam of charged particles (ions) the flux is expressed in ampere, *i.e.* $F \times ze$, where z is the charge on a particle and e the elementary charge ($1.602\ 176\ 634 \times 10^{-19}$ C).

122 focused ion beam system, (FIB)

Ion beam system used for machining small regions with sub-micron precision.

Note 1: In general, FIBs use a liquid metal ion source to generate a finely focused ion beam with diameters typically in the range 7 nm to 300 nm and of sufficient *flux*, typically 4 pA to 20 nA, to machine small items for study by *Auger electron spectroscopy*, *secondary-ion mass spectrometry*, or transmission electron microscopy in an economic time. They are also used to manufacture scanning probe microscopy tips, those for atom force microscopy having radii down to 2 nm.

Note 2: FIB-machined *surfaces* can have an ion-damaged surface that needs to be removed.

Source: [2] entry 4.213.

123 fractional sputtering yield

Number of atoms and ions of a particular species sputtered from a sample divided by the total number of atoms and ions sputtered from the sample.

Source: [2] entry 4.446. See also: *fractional ion yield, negative-ion yield, partial sputtering yield, positive-ion yield,* and *total ion yield*.

124 image depth profile

Three-dimensional representation of the spatial distribution of a particular elemental or molecular species, as indicated by emitted *secondary ions* or electrons, as a function of depth or material removed by *sputtering*.

Source: [15].

125 impact energy

Kinetic energy of particles on impact with a sample *surface*.

Note 1: For primary-ion beams in *secondary-ion mass spectrometry* (SIMS), the ion impact energy is given by the difference in electric potential between the ion source and the sample surface multiplied by the charge on the ion. In some SIMS systems, the beam energy is given for the source potential with respect to ground, but the sample potential need not be at ground. The impact energy takes account of any sample potential.

Note 2: Use of the qualifier "impact" indicates that this is the energy of the particles striking the surface.

Source: [2] entry 4.195.

126 implanted areic dose, D_{imp}

Number, N_{imp}, of energetic particles of a specified type incident on a solid within a surface area A and stopped within the solid divided by A. $D_{imp} = N_{imp}/A$.

Note: Particles that are not stopped within the solid are either backscattered or transmitted.

Source: [2] entry 4.176.

127 incidence angle

See: *angle of incidence*.

128 inelastic scattering

Interaction between a moving energetic particle and a second particle or assembly of particles in which the total kinetic energy is not conserved.

Note 1: Kinetic energy is absorbed in solids by various mechanisms, for example inner-shell ionization, *plasmon* and phonon excitation, and *bremsstrahlung* generation. These excitations usually lead to a small change in the direction of the moving particle.

Note 2: In particle collisions, the collision can be elastic, in that the kinetic energy of the particles is conserved, but energy can still be lost by the incident particle. In the scattering of electrons by atoms, the energy lost is usually very small and is often ignored. Where it is not ignored, the scattering is often termed quasi-elastic (see *elastic peak*).

Source: [2] entry 4.244.

129 information depth

Maximum depth, normal to the *surface*, from which useful information is obtained.

Source: [2] entry 4.246, without notes.

130 information radius

Maximum radius of a circular region, in the plane of the *surface*, from which useful information is obtained.

Source: [2] entry 4.247, without notes.

131 instrumental depth resolution

Depth resolution in a sample arising from parameters of the instrument.

Note 1: This concept is used in the secondary-ion mass spectrometry, Auger electron spectroscopy, and X-ray photoelectron spectroscopy.

Note 2: In sputter depth profiling, these parameters involve the system alignment and can include the ion species, energy, and angle of incidence, as well as the option to rotate the sample while sputtering.

Source: [2] entry 4.165.

132 interface

Boundary between two bulk phases having different chemical, elemental, or physical properties.

Source: [2] entry 4.253.

133 ion beam

Directed *flux* of charged atoms or molecules.

Source: [15].

134 ion implantation

Injection of ions into a sample.

Source: [15].

135 Langmuir-Blodgett (LB) film

Film comprising one or more *monolayers* of organic molecules.

Note: The films are transferred from the *surface* of a liquid bath onto solid substrates and many layers can be deposited by repeated immersions. Control of the liquid surface tension during this process allows the molecular density of the monolayers to be controlled.

Source: [2] entry 4.281.

136 lateral resolution
  spatial resolution

Distance, measured either in the plane of the sample *surface* or in a plane at right angles to the axis of the image-forming optics, over which changes in composition can be separately established with confidence.

Note 1: The choice of plane should be stated.

Note 2: In practice, the lateral *resolution* can be realized as either (i) the FWHM (See [6] 61.) of the intensity distribution from a very small emitting point on the sample, or (ii) the distance between the 12 % and 88 % intensity points in a *line scan* across a part of the sample containing a well-defined step function for the signal, relating to the property being resolved. These two values are equivalent for a Gaussian intensity distribution. For other distributions, other parameters might be more appropriate. Often, for a step function, the distance between the 20 % and 80 % intensity points or the 16 % and 84 % intensity points in the line scan is used.

Source: [2] entry 4.385.

Note 3: Lateral or spatial resolution should not be confused with the pixel density in a digital image.

137 line scan

Plot of output signal intensity from a spectrometer, signal intensity from another detector, or processed intensity information from the available software along a line corresponding to a line on the sample *surface*.

Note: The line is most often an *x*- or *y*-linescan from a rectangular *raster*, but, in more sophisticated systems, might be in any arbitrary direction.

Source: [2] entry 4.282.

138 local vacuum level

See: *vacuum level*.

139 matrix factor

Factors, arising from the composition of the matrix, for multiplying the quotient of the measured intensity and the appropriate sensitivity factor in formulae to determine the composition using surface analytical techniques.

Note: In methods such as *Auger electron spectroscopy*, the matrix factor is determined in part by the composition of the sub-surface material and in part by the composition of the *analysis volume* in the sample.

Source: [2] entry 4.298.

140 mean escape depth

Average depth normal to the *surface* from which specified particles or radiations escape.
Source: Modified from [2] entry 4.203, [15].

141 monolayer

Single, closely packed layer of atoms or molecules.

Source: [17] entry II.12.

Note: The term monolayer commonly indicates that all elementary units of the adsorptive or segregated atoms or molecules are in contact with the *surface*, unlike those in *multilayers*.

142 monolayer capacity (chemisorption)

Amount of adsorbate that is needed to occupy all adsorption sites, as determined by the structure of the adsorbent and by the chemical nature of the adsorptive.
Source: [13] p 587.

143 monolayer capacity (physisorption)

Amount of adsorbate which is needed to cover the *surface* with a complete *monolayer* of atoms or molecules in a close-packed array.
Source: [13] p 587.

Note: The type of close packing needs to be stated.

144 multilayer

A system of adjacent layers or *monolayers*.

Note 1: The term bilayer applies to the particular case of a multilayer two monolayers thick.
Note 2: Alternatively, monolayers and multilayers may be termed 'films', provided boundaries can be defined for them.

Source: [17] entry II.13.

Note 3: This term is often applied to solid samples in which the layers are very uniform in thickness and for which the layer thicknesses are in the range 1 nm to 100 nm.

See also: *delta layer*.

145 observed interface width
depth resolution

In *secondary-ion mass spectrometry*, *Auger electron spectroscopy*, and *X-ray photoelectron spectroscopy*, distance over which a change in signal intensity from 16 % to 84 %, or from 84 % to 16 %, is measured at the junction of two dissimilar matrices, the thicknesses of which are more than six times that distance.

Note: The change in signal intensity should be quoted with the observed interface width.

Source: [2] entry 4.254. See also *depth resolution parameter*, *resolution*.

146 partial sputtering yield

Number of atoms and ions of a particular species sputtered from a sample divided by the total number of incident particles.

Source: [2] entry 4.447. See also: *fractional ion yield, fractional sputtering yield, negative-ion yield, positive-ion yield,* and *total ion yield*.

147 peak area

Area under a peak in a spectrum after background removal.

Note: Unit of peak area is unit of ordinate (the ordinate is often *counts* with unit '1') times unit of abscissa (*e.g.* SI: s, J, kg; Common units: eV, u, Da).

Source: [2] entry 4.326, with revised note. See also: *inelastic electron scattering background subtraction*.

148 peak energy

Energy value corresponding to the intensity maximum in a *direct spectrum* or to the intensity minimum (*i.e.* the negative excursion) for a *differential spectrum*.

Note 1: The energy value can relate to the peak envelope for a group of overlapping peaks or to the positions of constituent peaks obtained by *peak synthesis*.

Note 2: For the differential spectrum in *Auger electron spectroscopy* (AES), the *modulation*, or differentiating amplitude should be given.

Note 3: Peak energies for the differential spectrum in AES have greater kinetic energy than those for the direct spectrum.

Source: [2] entry 4.327.

149 peak width

Width of a peak at a defined fraction of the peak height.

Note 1: Any background subtraction method used should be specified.

Note 2: The most common measure of peak width is the full width of the peak at half maximum (FWHM) intensity (See [6] entry 61).

Note 3: For asymmetrical peaks, convenient measures of peak width are the half-widths of each side of the peak at half maximum intensity.

Note 4: 'Peak width' is preferred to the use of 'line width'.

Source: [2] entry 4.331.

150 photoionization cross section

Total ionization *cross section* for an incident photon of a given energy interacting with a material to produce one or more photoelectrons from all sub-shells that are energetically accessible.

Source: [2] entry 4.132. See also: *sub-shell photoionization cross section*.

151 plasmon
    bulk plasmon
    volume plasmon

Excitation of valence-band electrons in a solid in which collective oscillations are generated.

Note 1: Plasmon excitations are often observed as *characteristic energy loss* peaks associated with other peaks in the spectrum, such as those of any elastically scattered *primary electrons*, photoelectron peaks, *Auger electron* peaks, and ionization edges.

Note 2: Plasmons are prominent in some materials and not others.

Note 3: Two types of plasmon are commonly observed: bulk plasmons, associated with material remote from the *surface*, and surface plasmons, associated with material at the surface. When the term plasmon is used without a qualifier, the term refers to the bulk plasmon. Occasionally, *interface* plasmons can be observed that are associated with interfaces. Bulk plasmon energies depend on the electronic structure of the material and are roughly proportional to the square root of valence-band density. Surface plasmon energies are typically between 50 and 90 % of bulk plasmon energies.

Source: [2] entry 4.339.

152 preferential sputtering

Change in equilibrium surface composition of the sample, which can occur when *sputtering* multicomponent samples.

Source: [2] entry 4.443.

153 primary beam

Directed *flux* of *beam particles* or photons incident on a sample.

Source: [2] entry 4.77.

154 projected range

Distance from the *surface* at which an energetic ion or atom comes to rest in the sample, projected along the direction of the beam.

Note 1: Used in energetic-ion analysis, Rutherford backscattering spectrometry, and secondary-ion mass spectrometry.

Note 2: Calculations usually deal with the mean or average projected range for a large number of ions or atoms of the same species and the same energy.

Source: [2] entry 4.352. See also: *range straggling*.

155 radial sectioning

Sample preparation in which a sample is polished by a cylinder in order to expose compositional changes below the original sample *surface*, with the intent that the depth of these layers can be related to the position on the surface created by the cylinder.

Source: [2] entry 4.358.

156 range straggling

Standard deviation of the *projected ranges* of energetic ions or atoms of a given energy.

Source: [2] entry 4.363.

Note: Used in energetic-ion analysis, *Rutherford backscattering spectrometry*, and *secondary-ion mass spectrometry*.

157 raster

Two-dimensional pattern generated by the deflection of a primary beam.

Note: Commonly used rasters cover square or rectangular areas.

Source: [2] entry 4.364.

158 redeposition

Deposition of *sputtered* sample material back onto the sample *surface*.
Source: [2] entry 4.369.

159 relative instrument spectral response function, (RISR)

In *Auger electron spectroscopy* (AES), *secondary-ion mass spectrometry*, and *X-ray photoelectron spectroscopy*, the *spectrometer response function* divided by the response function of a reference instrument, or the average for several such instruments, as a function of energy (AES, XPS, *etc*.) or mass (SIMS).

Note: The RISR can be used to relate spectra from one instrument to spectra from another when using similar excitation sources and geometries.

Source: [2] entry 4.375.

160 relative resolution of a spectrometer

Resolution of a spectrometer at a given energy, mass, or wavelength divided by that energy, mass, or wavelength.

Note 1: The relative resolution of a spectrometer is the reciprocal of the *resolving power of a spectrometer*.
Note 2: It can be convenient to specify the *relative energy resolution* of an *electron spectrometer*, the relative mass resolution of a *mass spectrometer*, or the relative wavelength resolution of an optical spectrometer.
Note 3: In practice, the relative resolution of a spectrometer can be deduced using a source with an emission line of known width, usually chosen to be as narrow as possible.
Note 4: Designs of spectrometer generally maintain the resolution either to be constant throughout the spectrum or to be proportional to the energy, mass, or wavelength being scanned. For the former, the term resolution is useful, whereas, for the latter, the relative resolution or resolving power is more useful.
Note 5: The relative resolution is often expressed as a percentage.

Source: [2] entry 4.376.

161 relative sputtering rate

Sputtering rate of a sample divided by the sputtering rate of a reference sample sputtered under the same conditions.
Source: [2] entry 4.377.

162 resolution (of a spectrometer)

Contribution of the spectrometer to the measured full width at half maximum (See: [6] entry 75) intensities of spectral peaks above their local backgrounds.

Note 1: It can be convenient to specify the *energy resolution* of an *electron spectrometer* or the wavelength resolution of an optical spectrometer.

Note 2: In practice, the spectrometer resolution can be deduced using a source with an emission line of known width, usually chosen to be as narrow as possible.

Note 3: Designs of spectrometer generally maintain the resolution either to be constant throughout the spectrum or to be proportional to the energy, mass, or wavelength being scanned. For the former, the resolution is a useful term, whereas, for the latter, the relative resolution and resolving power are more useful.

See *relative resolution*, *resolving power*.

163 resolving power (of a spectrometer)

Energy, mass, or wavelength divided by the *resolution* of a spectrometer at that energy, mass, or wavelength.

Note 1: The resolving power of a spectrometer is the reciprocal of the relative resolution of a spectrometer.

Note 2: It can be convenient to specify the energy-resolving power of an *electron spectrometer*, the mass-resolving power of a *mass spectrometer*, or the wavelength-resolving power of an optical spectrometer.

Note 3: In practice, the spectrometer resolving power can be deduced using a source with an emission line of known width, usually chosen to be as narrow as possible.

Note 4: Designs of spectrometer generally maintain the resolution either to be constant throughout the spectrum or to be proportional to the energy, mass, or wavelength being scanned. For the former, the resolution is a useful term whereas, for the latter, the relative resolution and resolving power are more useful.

Source: [2] entry 4.388. See also: *relative resolution*.

164 sample bias

Electric potential applied to the whole or part of the sample, referenced to the electric potential of the sample holder.

Source: [2] entry 4.391. See *sample voltage*.

165 sample charging

Change in the electrical potential in the sample or on the sample *surface* caused by particle or photon bombardment.

Source: [2] entry 4.392.

166 sample voltage

Electric potential difference of the sample referenced to ground.

Note 1: The sample voltage can be pulsed or constant, depending on the type of instrument.

Note 2: For insulators, the sample voltage is assumed to be the same as that of the sample holder if an effective charge neutralizing device is used.

Source: Modified from [2] entry 4.393. See *sample bias*.

167 self-assembled monolayer, (SAM)

Film, one molecule thick, in an ordered assembly on a *surface*.

Source: Modified from [2] entry 4.413.

Example: A monolayer of an alkane thiol on gold [18].

168 solid angle of analyser

Solid angle allowing particles or photons to be transmitted from a point on the sample to the detector.
Source: [2] entry 4.22.

169 spatial resolution

See: *lateral resolution*.

170 specific surface area, a_s, a, s

Surface area of a material divided by mass of the material.
Source: [16] p 77.

171 spectrometer response function

Number of particles detected with a *spectrometer* divided by the number of such particles per solid angle and per interval of the dispersing parameter available for measurement as a function of the dispersing parameter.
Source: [2] entry 4.433 without notes. See also: *spectrometer transmission function*.

172 spectrometer transmission function
analyser transmission function

Number of particles transmitted by the analyser divided by the number of such particles per solid angle and per interval of the dispersing parameter (*e.g.* energy, mass, or wavelength) available for measurement as a function of the dispersing parameter.
Source: [2] entry 4.434, without notes. See also: *spectrometer response function*.

173 spin coating

Coating of a thin layer of a soluble material (organic or inorganic) deposited from solution, or solid particles from suspension, under the action of high-speed rotation on a flat substrate.
Note 1: Rotation speeds of about 4000 revolutions per minute are commonly used, producing films generally thinner than 100 nm.
Note 2: Some users place a drop of solution in the centre and some flood the whole sample, prior to the high-speed rotation that removes the solvent.
Source: Modified from [2] entry 4.438.

174 sputter depth profile, (SDP)

Compositional *depth profile* obtained when the surface composition is measured while material is removed by *sputtering*.
Note: In some analytical methods, such as *secondary ion mass spectrometry*, the sputtering is often accomplished by the *ion beam* used for analysis, but in other methods an ion beam might need to be added.
Source: [2] entry 4.440.

175 sputtered particles

See: *sputtering*.

176 sputtering

Process in which microscopic particles of a solid material are ejected from its *surface* after the material is bombarded by energetic particles of a plasma or gas.

Source: [19].

Note: The ejected particles are termed 'sputtered particles'.

177 sputtering rate

Amount, mass, or number of entities of sample material removed, as a result of particle bombardment, per unit time.

Source: Modified from [2] entry 4.444. See also: *erosion rate*.

Note: SI unit: mol s^{-1}, kg s^{-1}, s^{-1}.

178 sputtering yield

Number of atoms and ions sputtered from a sample divided by the total number of incident primary particles.

Source: [2] entry 4.445.

179 standard vacuum level

Electric potential 4.500 eV above the Fermi level.

Note: The Fermi level is an absolute level to which electron kinetic energies can be accurately referenced. Historically, in *Auger electron spectroscopy*, the electron energies have not been referenced to the Fermi level but, instead, have been referenced to the instrument *vacuum level*. This level varies from instrument to instrument and does not provide a consistent reference level. However, most reported *Auger electron* kinetic energies have been referenced to the vacuum level, and most analysts are familiar with the variations that occur from one instrument to another for energies referenced in this way. By convention, the standard vacuum level is defined, as above, to be a consistent reference level close to the value for typical instrument vacuum levels. Energies referenced to the standard vacuum level are consistent and are within approximately 1 eV of those referenced to individual instrument vacuum levels.

Source: [2] entry 4.485.

180 steady-state sputtering

State of the *sputtering* process in which important operational and analytical parameters are unchanging over a meaningful timescale.

Note: Generally, steady state and stoichiometric sputtering are equivalent but, in profiling dilute *delta layers* in semiconductors, for example, the sputtering can be at a steady state while the constituents being studied are not being sputtered in their stoichiometric ratio.

Source: [2] entry 4.449. See also: *stoichiometric sputtering*.

181 steady-state surface composition sputtering
  equilibrium surface composition sputtering

Steady-state surface composition produced by *sputtering* a homogeneous sample under non-varying conditions.

Source: [2] entry 4.442.

182 stoichiometric sputtering

State of the *sputtering* process in which the relative amounts of the elemental components sputtered from a sample are equal to their stoichiometry within the sample.

Note: For most homogeneous materials, stoichiometric sputtering is attained after the sputter removal of a few nanometres from the surface.

Source: [2] entry 4.450. See also: *steady-state sputtering*.

183 surface

Boundary between two phases.

Note: It is recommended that, for the purpose of surface analysis, a distinction be made between 'surface' in general, 'physical surface', and 'experimental surface': Surface — the 'outer portion' of a sample of undefined depth; to be used in general discussions of the outside regions of the sample. Physical Surface — that atomic layer of a sample that, if the sample were placed in a vacuum, is the layer 'in contact with' the vacuum; the outermost atomic layer of a sample. Experimental Surface — that portion of the sample with which there is significant interaction with the particles or radiation used for excitation. It is the volume of sample required for analysis or the volume corresponding to the escape for the emitted radiation or particle, whichever is larger.

Source: [20] p 2243. See also *interface*.

184 surface concentration, Γ

Amount of an adsorbed species divided by the area of the adsorbing *surface*. $\Gamma = n/A$.

Note: SI unit: mol m^{-2}.

Source: [16] p 48.

185 surface contamination

Material, generally unwanted, on the sample *surface* that either is not characteristic of that sample and any process investigated or has arisen from exposure of the sample to particular environments other than those relevant for the original surface or the process to be studied.

Note: Common surface contaminants are hydrocarbons and water. Local reactions with these and the environment can lead to a wide range of oxidation and other products.

Source: [2] entry 4.459.

186 surface coverage, θ

Number of adsorbed molecules on a surface (N) divided by the number of molecules in a filled monolayer on that surface (N_m). $\theta = N/N_m$.

Source: [16] p 77.

187 surface energy

See: *areic surface energy*.

188 surface excess amount, n^σ

For an interface, the difference between the amount of component actually present in the system and that which would be present (in a reference system) if the bulk concentration in the adjoining phases were maintained up to a chosen geometrical dividing surface (Gibbs dividing surface).

Note: For a solid/liquid interface in which no component of the liquid phase penetrates into the solid, the surface excess (or adsorption) of component *i* is defined as: $n_i^g = n_i - V^1 c_i^1$, where n_i is the total amount of *i* in the system, V^1 is the volume of an arbitrarily chosen amount of bulk liquid (in the framework of the so-called algebraic method), and c_i^1 is its bulk concentration in the liquid.

Source: [21] p 969, [16] p 77.

189 surface excess concentration, Γ

Surface excess (n^σ) of a component divided by the area of the dividing *surface* or *interface* (A_s). $\Gamma = n^\sigma / A_s$.

Source: [21] p 970, [16] p 77.

190 surface map

Two- or three-dimensional representation of the sample *surface* where the information at each point in the representation, given by a brightness or colour or as a length in a third dimension, is related to the output signal from a detector or processed intensity information from the available software.

Source: [2] entry 4.289, without notes. See also: *chemical map, elemental map*.

191 surface plasmon

Collective motion of electrons on an interface of two phases which have different permittivity, of which one must have electrical conductivity to sustain the collective motion.

Note 1: Metals such as silver and gold are well known examples of materials exhibiting surface plasmon behaviour.

Note 2: Collective motion of electrons is induced by an injection of energetic particles, for example photons, electrons, ions, or alpha particles.

Source: Modified from [2] entry 4.462.

192 surface segregation

Partitioning of a species from the bulk of a material to the *surface* as a result of kinetic or thermodynamic effects.

Source: [2] entry 4.463.

193 surface tension, γ, σ

Work required to increase a surface area divided by that area.

Note 1: When two phases are studied, surface tension is often called 'interfacial tension'.

Source: [22] p 995.

Note 2: $\gamma = (\partial G / \partial A_{\rm s})_{T,p,n_i}$.
Note 3: SI unit: N m^{-1}, J m^{-2}.

Source: [16] p 77.

194 surfactant

  surface active agent

Substance which lowers the surface tension of the medium in which it is dissolved, and/or the interfacial tension with other phases, and, accordingly, the adsorbed amount at the liquid/vapour and/or at other interfaces is positive.

Source [13] p 611.

Note 1: In practice, the liquid is usually water or a water-based medium. Emulsifiers, detergents, and dispersing agents are examples of surfactants.
Note 2: In many cases, surfactant molecules have a hydrophilic or polar group at one end and a lipophilic or oleophilic group at the other.

195 take-off angle

Angle between the trajectory of a particle as it leaves a *surface* and the local or average surface plane.

Note 1: The particular surface plane needs to be specified.
Note 2: The take-off angle is the complement of the *angle of emission*.
Note 3: In the past, 'take-off angle' has sometimes been used erroneously to mean *angle of emission*.

Source: [2] entry 4.24.

196 thermionic work function, *W*

Parameter describing the apparent *work function* of a solid that controls the electronic current density, J, emitted from a conductor at temperature T. $W = -kT\ln{(J/AT^2)}$, where k is the Boltzmann constant and A is the Richardson constant.

Note 1: For polycrystalline solids, the thermionic work function will be close to the minimum work function of the crystallites present.
Note 2: Richardson constant, $A = (4\pi m_{\rm e}k^2e)/h^3 \approx 1.202 \times 10^6$ A m^{-2} K^{-2} where $m_{\rm e}$ is the mass of the electron, e the elementary charge, and h is the Planck constant.

Source: [2] entry 7.34. See also: *work function*, *photoelectric work function*.

197 thin film

Layer of material, typically less than 100 nm thick, deposited or grown on a substrate.

Source: [15].

Note: Films thinner than 10 nm are often called ultrathin films.

Source: [2] entry 4.471.

198 topographic contrast

Contrast in a *surface map* or image arising from the topography of the sample *surface*.

Note 1: Topographic effects can modify the interaction between the primary beam and the sample, making the interpretation of electron or ion yield data more complex than otherwise.

Note 2: Topographic contrast can change after ion *sputtering*.

Source: [2] entry 4.474.

199 total ion yield

Number of ions of both signs sputtered from a sample divided by the number of incident particles.

Source: [2] entry 4.492. See also: *fractional ion yield*, *fractional sputtering yield*, *negative-ion yield*, *partial ion yield*, *partial sputtering yield*, and *positive-ion yield*.

200 vacuum level, E_{VAC}
   local vacuum level

Energy level of an electron positioned at rest just outside a solid, *i.e.* with zero kinetic energy with respect to the sample surface.

Note 1: 'Just outside' has also been written as "a few nanometers" [23], and is taken as a distance where there is no effect of image forces but that is sufficient for the electron to experience the full impact of the surface dipole.

Note 2: The vacuum level depends on the nature of the surface; for example, it is different between surface crystal planes Si[001] and Si[111].

Source: [24]. See also: [23].

201 vacuum level at infinity, $E_{VAC}(\infty)$

Electric potential of the vacuum at a point in space.

Source: [15].

Note 1: In electron spectroscopy, the point in space is taken at a sufficiently large distance outside the sample, such that electric fields caused by different *work functions* of different parts of the *surface* are zero or extremely small.

Note 2: This level is not experimentally accessible. See [24].

See also: *vacuum level*.

202 vertical profile

See: *depth profile*.

203 volume plasmon

See: *plasmon*.

204 volume yield

Volume sputtered from a sample divided by number of incident particles.

Note: Volume yield is useful for expressing the amount sputtered in organic layers where molecules can be easily fragmented and values of the molecular *sputtering yield* can be much more variable between samples than the volume yield.

See also: *fractional ion yield*, *fractional sputtering yield*, *negative-ion yield*, *partial sputtering yield*, *positive-ion yield*.

205 work function, ϕ_0, *W*

Energy difference of an electron in a solid between the *Fermi level* and that of an electron positioned at rest just outside a solid (*vacuum level*).

Source: [24]. See also: [23].

Note 1: The work functions of the different crystal facets of a single crystal will, in general, differ from one another. These work functions will also change with the state of cleanness of the crystal surfaces.

Note 2: A polycrystalline surface will exhibit an average work function which will depend on the types of exposed constituent single-crystal facets and their areas.

Source: [2] entry 4.487.

Note 3: SI unit: J. Common unit electron volt, eV, where 1 eV = $1.602\ 176\ 634 \times 10^{-19}$ J.

See also: *photoelectric work function*, *thermionic work function*.

206 X-ray linewidth

Energy width of the principal characteristic X-ray line.

Note 1: In *X-ray photoelectron spectroscopy* the X-ray linewidth usually refers to that of the X-ray source.
Note 2: X-ray linewidth contributes to the photoelectron *peak widths*.

Source: [2] entry 4.489.

207 X-ray monochromator

Device used to eliminate photons of energies other than those in a narrow energy or wavelength band.

Note: For *X-ray photoelectron spectroscopy* using Al X-rays, the monochromator is usually aligned close to the Al Kα_1 energy.

Source: [2] entry 4.490.

3.2 Electron Spectroscopy

208 adventitious carbon referencing

In *X-ray photoelectron spectroscopy*, measurement of the *charging potential* of a particular sample from a comparison of the experimentally measured C 1s *binding energy*, arising from adsorbed hydrocarbons on the sample, with a standard binding energy value.

Note 1: A nominal value of 285.0 eV is often used for the binding energy of the relevant C 1s peak, although some analysts prefer specific values in the range 284.6 eV to 285.2 eV, depending on the nature of the substrate. This method does not determine the true charging potential, since the true binding energy of the adsorbed hydrocarbons is not known.

Note 2: Different sample charging potentials can occur on different areas on the *surface*, or at different depths, arising, for example, from sample inhomogeneities or non-uniform intensity of the incident-radiation *flux*.

Source: [2] entry 4.4. See also: *Fermi level referencing*.

209 asymmetry parameter, β

In *X-ray photoelectron spectroscopy* factor which characterizes the intensity distribution, $L(\gamma)$, of photoelectrons ejected by X-rays from isolated atoms at an angle γ from the incident X-ray direction. In the dipole approximation, $L(\gamma) = 1 + \frac{1}{2}\beta[3(\sin^2\gamma)/2 - 1]$

Note: This formula relates to gases and is modified by the effects of *elastic scattering* when applied to solids. At the *magic angle*, $L(\gamma) = 1$.

Source: Modified from [2] entry 4.30.

210 Auger electron

Secondary electron ejected from an atom as a form of energy release (as opposed to energy release more typically in the form of photon emission), following the ejection of a core shell electron and the resulting transition of an electron from a higher *energy level* into the vacancy.

Source: [6] entry 341.

Note 1: Auger electrons can lose energy by *inelastic scattering* as they pass through matter. Measured Auger electron spectra are therefore generally composed of a peak structure of unscattered Auger electrons superimposed on top of a background. In this way, no assumption is made about the physical origin of the background signal (Note modified from [2] entry 4.37).

Note 2: Auger electrons can change their direction of propagation by *elastic scattering* as they pass through matter.

See also: *Auger transition.*

211 Auger electron spectrum

Plot of *intensity* of *Auger electrons* as a function of the electron kinetic energy, usually as part of the energy distribution of detected electrons.

Note 1: When excited by incident electrons, the energy distribution of detected electrons, often measured between 0 eV and 2500 eV, contains Auger electrons, *backscattered* (primary) *electrons*, and *secondary electrons*. The entire distribution is sometimes referred to as an Auger electron spectrum.

Note 2: The Auger electron spectrum can be presented in either *direct spectrum* or *differential spectrum* formats.

Source: [2] entry 4.38.

212 Auger electron yield

Probability that an atom with a vacancy in a particular inner shell will relax by emitting an *Auger electron*.

Source: Modified from [15].

213 Auger parameter

Kinetic energy of a narrow *Auger electron* peak in a spectrum minus the kinetic energy of the most intense *X-ray photoelectron* peak from the same element.

Note 1: The value of the Auger parameter depends on the energy of the X-rays, which therefore needs to be specified.

Note 2: The Auger parameter is sometimes called the *final state* Auger parameter (see *initial state Auger parameter*).

Note 3: The Auger parameter is useful for separating chemical states for samples in which charging causes uncertainty in the *binding energy* measurement or in which the binding energy shift is inadequate to identify the chemical state.

Note 4: The Auger parameter is useful for evaluating the *relaxation energy* of the ionized matrix atom associated with the generation of a *core hole* for those *Auger transitions* between core levels, which have similar *chemical shifts*.

Source: [2] entry 4.41. See also: *modified Auger parameter*.

214 Auger vacancy satellite

Emission of an *Auger electron* in which additional *spectator holes* are present in the *initial state* or the *final state*) for the transition.

Source: [2] entry 4.48.

215 average matrix relative sensitivity factor (in electron spectroscopy), (AMRSF)

Coefficient, proportional to the intensity, calculated for an element in an average matrix, by which the measured intensity for that element is divided in calculations to yield the atomic concentration or atomic fraction of the element present in the sample.

Note: The choice of atomic concentration or atomic fraction should be made clear.

Source: [2] entry 4.416, with deleted notes.

216 backscattered electron

Electron, originating in the incident beam, which is emitted after interaction with the sample.

Note 1: By convention, an electron with energy greater than 50 eV can be considered a backscattered electron.

Note 2: By convention, the incident beam is often called the *primary beam* and the backscattered electrons are often referred to as the backscattered *primary electrons*.

Source: [2] entry 4.58.

217 backscattering correction factor, *R*

In *Auger electron spectroscopy*, factor equal to the total Auger-electron current arising from ionizations in the sample caused by both *primary electrons* and *backscattered electrons* divided by the Auger-electron current arising directly from the primary electrons.

Source: [2] entry 7.2 without notes.

Note: 'Backscattering correction factor' is preferred to the contraction 'backscattering factor'.

218 backscattering fraction, *r*

In *Auger electron spectroscopy*, Auger-electron current arising from ionizations in the sample caused by *backscattered electrons* divided by Auger-electron current arising directly from the *primary electrons*.

Source: [2] entry 7.3, without notes.

219 backscattering yield, η
backscattering coefficient

Number of electrons emitted from the sample with energies greater than 50 eV divided by the number of electrons incident at a given energy and *angle of incidence*.

Source: [2] entry 4.63. See also: *secondary-electron yield*, *total secondary-electron yield*, and *backscattering correction factor*.

220 binding energy

Energy of removing an electron from a given electronic level to the *Fermi level* of a solid or to the *vacuum level* of a free atom or molecule.

Source: [2] entry 4.82. See also: *Fermi level referencing*

221 characteristic electron energy losses

Inelastic scattering of electrons in solids that produces a non-uniform energy loss spectrum determined by the characteristics of the material.

Source: [2] entry 4.95, without notes.

222 charge referencing

Measurement of *charging potential* of a sample in order to correct the measured energies so that those energies correspond to a sample with no surface charge.

Note 1: Charge referencing is often conducted using *adventitious carbon referencing*, using internal carbon referencing or by gold decoration, or by referencing to the substrate when grounded.

Note 2: Different charging potentials can occur on different areas or at different depths in a sample, arising, for example, from sample inhomogeneities or the non-uniform intensity of the incident *flux* of radiation.

Source: [2] entry 4.99 with modified notes.

223 chemical shift (in electron spectroscopy)

Change in *peak energy* arising from a change in the chemical environment of the atom.

Source: [2] entry 4.105.

Note: This term used in electron spectroscopy should not be confused with 'chemical shift in NMR' (See [6] entry 176).

224 chemical state of an atom in electron spectroscopy

State of an atom arising from its chemical interaction with neighbouring atoms in a molecule, compound, solid, liquid, or gas that leads to a characteristic energy or feature observable in electron spectroscopy.

Source: [2] entry 4.107, without notes.

225 chemical state plot
   Wagner plot

In *X-ray photoelectron spectroscopy*, plot of the measured kinetic energy of a sharp *Auger electron* peak *versus* the *binding energy* of a photoelectron peak for the same element.

Note 1: Plots are usually made for a given element that can exist in different chemical states. Such plots are helpful in defining the state for an unknown sample, where measurements of the binding energy alone are inadequate.

Note 2: The binding energy is usually plotted on the abscissa, with values decreasing towards the right.

Source: [2] entry 4.108.

226 differential spectrum (in electron spectroscopy)

Differential of a *direct spectrum* with respect to energy by an analogue electrode *modulation* method or by the numerical differentiation of that spectrum.

Note 1: Used in *Auger electron spectroscopy* and, rarely, in *X-ray photoelectron spectroscopy*.

Note 2: The modulation amplitude (for example in unit eV) or the number of points and the type of differentiating function should be given.

Source: [2] entry 4.171.

227 direct spectrum

Spectrum of intensity of electrons transmitted and detected by a spectrometer with a dispersing energy analyser as a function of energy, E.

Note 1: In retarding field energy analysers, which do not have a dispersing element, the direct spectrum can be obtained from the first differential of the collected current with respect to the retarding energy.

Note 2: By convention, direct spectra in *X-ray photoelectron spectroscopy* are often presented in constant analyser energy mode, in which the spectrum approximates the true spectrum, whereas, in *Auger electron spectroscopy*, spectra are often presented in constant retardation ratio mode, in which the spectrum approximates to E times the true spectrum.

228 dynamic emittance matching

Electron or ion optical method of steering a spectrometer axis to align with the impact area of the primary beam at all points of a *raster* scan on the sample *surface*.

Source: [2] entry 4.184.

229 effective attenuation length

Parameter that, when introduced in place of the *electron inelastic mean free path* into an expression derived for *Auger electron spectroscopy* and *X-ray photoelectron spectroscopy* on the assumption that *elastic scattering* effects are negligible for a given quantitative application, will correct that expression for elastic scattering effects.

Note 1: The effective attenuation length can have different values for different quantitative applications of AES and XPS. However, the most common use of effective attenuation length is in the determination of overlayer-film thicknesses from the measurement of the changes of overlayer and substrate Auger-electron or photoelectron signal intensities after the deposition of a film or as a function of the *emission angle*. For emission angles of up to about 60° (with respect to the surface normal), it is often satisfactory to use a single value of this parameter. For greater emission angles, the effective attenuation length can depend on this angle.

Note 2: Since there are different uses of this term, it is recommended that users specify clearly the particular application and the definition of the parameter for that application (*e.g.* by giving a formula or by providing a reference to a particular source).

Source: [2] entry 4.35.

230 Einstein photoelectric equation

Einstein equation

Equation relating the kinetic energy of an electron, emitted from a conductor illuminated by monochromatic photons, and the photon energy and *work function* of the surface from which the photoelectron is emitted. $\frac{1}{2}m_e v_{max}^2 = h\nu - \phi_0$, where m_e is the mass of an electron, v_{max} the maximum velocity of the emitted electron, h the Planck constant, ν the frequency of the illuminating photons, and ϕ_0 the *photoelectric work function* of the surface.

Source: [2] entry 7.17, with added equation.

231 elastic peak

quasi-elastic peak

Peak in the electron spectrum, produced by quasi-elastically scattered electrons detected by an *electron spectrometer*.

Note 1: All electrons that are scattered by atoms can be elastically scattered in the centre-of-mass frame, but *energy losses* that are typically less than 1 eV might be observed in the laboratory frame. These losses are generally significantly less than the measured energy width of the electrons in a primary-electron beam. Historically, and more generally, the scattering has been called "elastic"; however, the term quasi-elastic is now often used if the small change in energy that occurs on scattering is important.

Note 2: The energy and the energy broadening of the quasi-elastic peak are influenced by the recoil of the scatterer atoms, the energy distribution of the primary (incident) electrons, the scattering geometry, the acceptance geometry, and the response function of the electron spectrometer. The intensity of the elastic peak depends on the electron differential *elastic scattering cross section* and on the *cross section* for *inelastic electron scattering* at the particular *beam energy* of the *primary-electrons* and in the given scattering geometry, including the probability of surface excitations.

Source: [2] entry 4.186. See also: *Elastic peak electron spectroscopy*, *reflection electron energy loss spectroscopy*.

232 electron energy analyser

Measuring instrument [VIM 3.1] for measuring the number of electrons, or an intensity proportional to that number, as a function of the electron kinetic energy.

Note: An electron energy analyser is part of an *electron spectrometer*.

Source: [2] entry 4.187.

233 electron energy loss spectrum

Energy spectrum of electrons from a nominally monoenergetic source emitted after inelastic interactions with the sample, often exhibiting peaks due to specific inelastic loss processes (see *characteristic electron energy losses* and *plasmon*).

Note 1: The electron energy loss spectrum obtained using an incident-electron beam of about the same energy as a peak obtained in *Auger electron spectroscopy* or *X-ray photoelectron spectroscopy* approximates to the energy loss spectrum associated with that peak.

Note 2: The electron energy loss spectrum, measured with an incident-electron beam, is a function of *beam energy*, *angle of incidence* of the beam, *angle of emission*, and the electronic properties of the sample.

Source: [2] entry 4.197.

234 electron inelastic mean free path

Average distance that an electron with a given energy travels between successive inelastic collisions.
Source: [2] entry 4.243.

235 electron retardation

In *Auger electron spectroscopy* and *X-ray photoelectron spectroscopy*, *measurement method* [VIM 2.5] for kinetic energy distribution by retarding the emitted electrons before or within the *electron energy analyser*.
Source: [15].

236 electron spectrometer

Measuring system [VIM 3.2], the essential part of which is an *electron energy analyser*.

Note: The term electron spectrometer can be used either as a synonym for electron energy analyser or to describe a more complex instrument based on an electron energy analyser and additional electron-optical components. Occasionally, the term is used to describe a complete working system with an energy analyser, possible electron-optical components, an electron detector, excitation sources, vacuum pumps, control electronics, and a data-processing system. The meaning will normally be made clear by the context.

Source: [2] entry 4.190.

237 elemental relative sensitivity factor

In *dynamic secondary-ion mass spectrometry*, coefficient for an element by which the measured intensity of a mass peak for that element, divided by the measured intensity of a mass peak for the matrix, is multiplied to yield the atomic concentration of the element present in the sample.

Note 1: The elemental relative sensitivity factor can be obtained by dividing the *relative isotopic sensitivity factor* by the isotope abundance of the detected isotope ion.

Note 2: Matrix terms are strong, and the matrix, bombarding species, incident-ion energy, and *angle of incidence*, as well as the spectrometer operating conditions, all affect relative elemental sensitivity factors significantly.

Source: [2] entry 4.420.

238 extrinsic plasmon

Plasmon excited as an electron travels through a condensed medium.

Note: The probability describing the number of extrinsic plasmons excited by the electron depends on the path length traversed and, for typical applications of Auger-electron spectroscopy and X-ray photoelectron spectroscopy of a homogeneous sample, follows a Poisson distribution for the parameter s/λ, where s is *path length* and λ is *electron inelastic mean free path*.

Source: [2] entry 7.28. See also: *intrinsic plasmon*.

239 Fermi level referencing

Process for establishing the *binding energy* scale for a particular sample by assigning the kinetic energy corresponding to the Fermi level, as determined by analysis of the spectrum obtained from *X-ray photoelectron spectroscopy* or *ultraviolet photoelectron spectroscopy*, as the point of zero binding energy.

Source: [15]. See also: *vacuum level referencing*.

240 final energy state (of an atom)

Energy state of an atom after a particular Auger, X-ray, or photoemission process.

Source: [2] entry 4.215. See also *Auger electron, X-ray photoelectron spectroscopy*, *ultraviolet photoelectron spectroscopy, initial state*.

241 inelastic electron scattering background
inelastic *background*

Intensity distribution in a spectrum for particles originally at one energy but which are emitted at lower energies due to one or more *inelastic scattering* processes.

Note: For *Auger electron spectroscopy* and *X-ray photoelectron spectroscopy*, the inelastic background associated with a particular *Auger electron* or photoelectron peak has been approximated by a measured *electron energy loss spectrum* for which the incident-electron energy is close to the energy of the peak. Simple linear backgrounds have also been used, but these are much less accurate, except for the XPS analysis of insulators.

Source: [2] entry 4.50. See also: *inelastic electron scattering background subtraction, Tougaard background, Shirley background*.

242 inelastic electron scattering background subtraction

Subtraction of a chosen *inelastic electron scattering background* from a measured spectrum in *Auger electron spectroscopy* and *X-ray photoelectron spectroscopy*.

Note: The inelastic background associated with a particular *Auger electron* or photoelectron peak has been approximated by a measured *electron energy loss spectrum* for which the incident-electron energy is close to the energy of the peak.

Source: [2] entry 4.242, with modified Note.

243 inelastic scattering cross section

Cross section for *inelastic scattering* by an electron traversing a material.

Source: [2] entry 4.129. See also: *elastic scattering cross section*.

244 initial energy state (in Auger electron spectroscopy)

Core-hole excited state of an atom prior to *Auger transition* or to X-ray emission.
Source: [2] entry 4.248.

245 initial energy state (in X-ray photoelectron spectroscopy)

Ground state of an atom prior to photoelectron emission.
Source: [2] entry 4.249.

246 initial-state Auger parameter, β

$\beta = 3\,E_B + E_K$, where E_B and E_K are, respectively, the *binding energy* of a photoelectron peak and the Fermi level referenced (see *Fermi level referencing*) kinetic energy of an *Auger electron* peak, each involving the same initial core level of the same element.

Note 1: The initial-state *Auger parameter* is useful for evaluating the change in the atomic core potential contribution to changes in binding energy between two environments, provided the *Auger transition* is between core levels that have similar binding energy shifts.

Note 2: This parameter has no relation to the *asymmetry parameter*, which is also given the symbol β.

Source: [2] entry 4.42. See also: *modified Auger parameter*.

247 interatomic Auger process

Auger transition in which at least one of the final electron vacancies is localized in valence levels or molecular orbitals of atoms adjacent to the atom in which the initial vacancy occurred.

Source: [2] entry 4.45.

248 interface core-level shift

Energy shift observed in core-level photoelectron spectroscopy arising from the changed bonding and/or from the displacements of atoms from their bulk positions near an interface between two materials.

Source: [2] entry 7.24. See also: *surface core-level shift*.

249 intrinsic plasmon

Plasmon excited at the same time as the excitation of a core-level photoelectron or an *Auger electron* associated with the same locality as the excitation of the photoelectron or Auger electron.

Source: [2] entry 7.29. See also: *extrinsic plasmon*.

250 magic angle (in X-ray photoelectron spectroscopy)

In *X-ray photoelectron spectroscopy*, angle at which the spectrometer entrance axis is aligned at 54.7° to the direction of the X-rays at the sample *surface*.

Note: At the magic angle, using the simple dipole theory for the angular distribution of the photoelectrons emitted from an atom irradiated by unpolarized X-rays, it is predicted that the intensity per unit solid angle is the same as the intensity that would be obtained if the scattering were isotropic.

Source: [2] entry 4.15.

251 modified Auger parameter

Sum of the Fermi level referenced (see *Fermi level referencing*) kinetic energy of a narrow *Auger electron* peak in the spectrum and the *binding energy* of the most intense photoelectron peak from the same element.

Note: The modified Auger parameter is the sum of the *Auger parameter* and the energy of the X-rays responsible for the measured photoelectron peak. Unlike the Auger parameter, it does not depend on the energy of the X-rays.

Source: [2] entry 4.43. See also: *initial-state Auger parameter*.

252 pass energy (in electron spectroscopy)

Mean kinetic energy of detected particles in the energy-dispersive portion of an *electron energy analyser*.

Source: [2] entry 4.325.

253 photoelectric effect

Interaction of a photon with bound electrons in atoms, molecules and solids, resulting in the production of one or more photoelectrons.

Source: [2] entry 4.332. See also: *Einstein photoelectric equation*.

254 photoelectric work function, ϕ_0

Minimum photon energy required to liberate an electron from the surface of a conducting solid by absorption of that photon.

Source: [2] entry 7.27, without notes. See also: *work function*, *thermionic work function*.

255 photoelectron X-ray satellite peaks
   satellite peaks

Photoelectron peaks in a spectrum resulting from *photoemission* induced by characteristic minor X-ray lines associated with the X-ray spectrum of the anode material.

Source: [15].
Example: $K\alpha'$, $K\alpha_{3,4}$, $L\alpha_{5,6}$, and $K\beta$ are all minor X-ray lines.

256 photoelectron X-ray satellite subtraction

Removal of *photoelectron X-ray satellite peaks* from a spectrum.

Source: [15].

Note: For unmonochromated Al and Mg X-rays, the satellites usually removed are $K\alpha_{3,4}$ and $K\alpha_{5,6}$. More sophisticated subtraction methods also remove the $K\alpha_2$, $K\alpha'$, and $K\beta$ satellites.

257 photoemission

Emission of electrons from atoms or molecules caused by the *photoelectric effect*.

Source: [15].

258 primary electron

Electron directed at a sample in electron spectroscopy.

Note: Primary electrons are distinguished from *secondary electrons* that are emitted during a measurement.

Source: Modified from [2] entry 4.346.

259 pure-element relative sensitivity factor, (PERSF)

In electron spectroscopy, coefficient, proportional to the intensity measured for a pure sample of an element, by which the measured intensity for that element is divided in calculations to yield the atomic concentration or atomic fraction of the element present in the sample.

Note 1: The choice of atomic concentration or atomic fraction should be made clear.

Note 2: The type of sensitivity factor utilized should be appropriate for the formulae used in the quantification process and for the type of sample analysed, for example homogeneous samples or segregated layers.

Note 3: The source of sensitivity factors should be given to ensure that the correct *matrix factors* or other parameters are used. Matrix factors are significant and should be used with pure-element relative sensitivity factors.

Note 4: Sensitivity factors depend on parameters of the excitation source, the spectrometer, and the orientation of the sample to these parts of the instrument. The numerical values of the sensitivity factors can also depend on the method used to measure the peak intensities.

Source: [2] entry 4.417. See also: *average matrix relative sensitivity factor*.

260 quasi-elastic peak

See: *elastic peak*.

261 relaxation energy (in X-ray photoelectron spectroscopy)

Energy associated with intra-atomic or extra-atomic electronic readjustment to the removal of an atomic electron, so as to minimize the energy of the *final state* of the system.

Source: [15].

262 satellite peaks

See: *photoelectron X-ray satellite peaks*.

263 secondary electron

Electron, generally of low energy, leaving a *surface* as a result of an excitation induced by an incident electron (see: *primary electron*), photon, ion, or neutral particle.

Note: By convention, electrons with energies ≤ 50 eV are considered as secondary electrons unless otherwise specified. Calculations of the energy distribution of the electrons emitted from a surface show that 50 eV is a useful cut-off energy to contain most of the electrons. The cut-off is artificial, and secondary electrons with energies greater than 50 eV usually exist. This convention is not usually observed for glow-discharge spectroscopy.

Source: [2] entry 4.401.

264 secondary-electron yield (in Auger electron spectroscopy), δ
secondary-electron emission coefficient

Number of electrons emitted from a sample with energies less than 50 eV divided by the number of electrons incident at a given energy and *angle of incidence*.

Source: [2] entry 4.403. See also: *secondary electron*.

265 selected-area aperture

Aperture in the electron or ion optical system restricting the detected signal to a small area of the sample *surface*.

Source: [2] entry 4.411.

266 shakeoff

Multi-electron process in which two or more electrons are emitted, partitioning between them the excess kinetic energy.

Note: Shakeoff leads to a continuum background intensity at kinetic energies below that of the parent peak in the electron spectrum. This is in contrast to *shakeup*, which leads to peak structure, also at kinetic energies below that of a parent peak.

Source: [2] entry 4.422.

267 shakeup

Multi-electron process in which an atom is left in an excited state following a photoionization or *Auger electron process*, so that the outgoing electron has a characteristic kinetic energy slightly less than that of the parent photoelectron.

Note: Shakeup peaks are usually observed within 10 eV of the parent peak. However, for gases where the background is low, shakeup peaks have been identified at kinetic energies up to 100 eV less than that of the parent peak.

Source: [2] entry 4.423. See also: *shakeoff*.

268 Shirley background

In *Auger electron spectroscopy* and *X-ray photoelectron spectroscopy*, background calculated to fit the measured spectrum at points at greater and lesser kinetic energy than the peak or peaks of interest, such that the background contribution at a given kinetic energy is in a fixed proportion to the *total peak area* above that background for greater kinetic energies.

Note: Fitting to the background can be made by averaging over a given number of energy channels.

Source: [2] entry 4.54. See also: *Tougaard background*.

269 spectator hole

Electronic configuration of an atom containing an electronic vacancy that can be present during processes, such as *Auger electron* and *X-ray photoelectron emission*, but is not created or destroyed in the process.

Source: Modified from [2] entries 4.429, 4.237 and 4.238.

270 spin orbit splitting

Splitting of p, d, or f levels in an atom arising from the coupling of the spin and orbital angular momentum.

Source: [2] entry 4.439.

271 sub-shell photoionization cross section

Cross section for an incident photon interacting with a material to produce one or more photoelectrons from a given sub-shell.

Note: Photoionization from one sub-shell can lead to *shake-up* or *shakeoff* of electrons from other shells. See *photoionization cross section*.

Source: [2] entry 4.135.

272 surface core-level shift

Energy shift observed in core-level photoelectron spectroscopy arising from the reduced coordination of the surface or near-surface atoms compared to bulk atoms.

Note: Surface core level shifts are often observed for single crystals and nanoparticles and depend on the crystal surface exposed. Shifts can be to lower or higher binding energy, depending on the band structure of the bulk solid. For the outermost atom layer, the shift can be as high as 0.4 eV. In *X-ray photoelectron emission*, the sampling depth is generally many atom layers when photoelectrons are detected with emission angles at, or close to, the surface normal. The shift for the outermost atom layer is thus seen most clearly at near-grazing emission angles. Separate energy shifts can be detected for the second and third atom layers from the surface.

Source: [2] entry 7.31.

273 total secondary-electron yield, σ

Total number of electrons emitted from a sample divided by the total number of electrons incident at a given energy and *angle of incidence*. $\sigma = \delta + \eta$, where δ is the *secondary-electron yield* and η is the *backscattering coefficient*.

Note: The total secondary-electron yield is often simply called the secondary-electron yield. This leads to confusion with the term of that name, which is restricted to secondary electrons with energies less than or equal to 50 eV.

Source: [2] entry 4.405.

274 Tougaard background

In *Auger electron spectroscopy* and *X-ray photoelectron spectroscopy*, intensity distribution of the background due to *inelastic scattering* obtained from the differential *inelastic scattering cross section* with respect to energy loss and the three-dimensional distribution of the emitting atoms in the surface region.

Note 1: A number of classes of atomic distributions can be used together with different differential inelastic scattering cross sections. The atomic distribution and the inelastic scattering cross section should be specified.

Note 2: The Tougaard background is usually calculated to match the measured spectrum over a wide energy range that excludes the peak region and the spectral region extending to approximately 50 eV less kinetic energy than the peaks of interest. The measured spectrum should be corrected for the *spectrometer response function* of the measuring instrument before the calculation of the Tougaard background.

Source: Modified from [2] entry 4.57. See also: *Shirley background*.

275 vacuum level referencing

Method of establishing the kinetic energy scale in which the zero point corresponds to an electron at rest at the *vacuum level*.

Source: [2] entry 4.484. See also: *Fermi level referencing*.

276 valence-band spectrum

X-ray photoelectron energy distribution arising from the excitation of electrons from the valence band of the sample material.

Source: [2] entry 4.486.

277 Wagner plot

See: *chemical state plot*.

3.3 Ion Scattering Spectroscopy

278 aligned incidence spectrum

Backscattering spectrum recorded with the analysing beam aligned with crystallographic axes or planes of the sample that produce channelling.

Source: [15].

279 backscattering spectrum

Plot of backscattering yield *versus* backscattering energy.

Source: [15].

280 beam chopper

Electrostatic or electromagnetic device used to generate pulses of ions from a continuous *ion beam*.

Note: The beam chopper can be used to define the pulse length and hence the mass *resolution* in a *time-of-flight mass spectrometer* and it can also be used to select particular ions in a beam that contains more than one species (Mass resolution is defined in [7] entry 454).

Source: [2] entry 4.109. See also: *beam bunching*.

281 binary elastic scattering peak

In ion-scattering spectrometry, increase in the spectrometer detection system response above the background signal, which can be attributed to the *binary elastic scattering* of an incident ion by a surface atom of a particular mass.

Source: [15].

282 blocking geometry

Experimental arrangement wherein the atom rows or planes of a single-crystal *target* are aligned parallel to a vector from the sample to the detector.

Source: [15].

283 Bohr speed

See: *swift ion*.

284 electronic stopping cross section

Stopping cross section arising from energy transfer to the electrons of the sample.

Note: The maximum of the nuclear stopping cross section occurs at energies of the order of 1 keV per nucleon, whereas that of the electronic stopping cross section occurs at above 100 keV per nucleon. The absolute

value of the electronic stopping cross section maximum is significantly greater than that for the nuclear stopping cross section.

Source: [2] entry 4.452.

285 energy edge

Values of the *backscattering energy* for an element, or for an isotope, that is located at the *surface* of a sample.

Source: [2] entry 4.193.

286 energy, surface approximation

Simplification of calculations involving the energy of an ion passing through a solid sample, where the energy of the ion at the *surface* is used in place of a properly averaged energy.

Source: [15].

Note: This approximation is used to determine the energy at which scattering cross sections (see *elastic scattering cross section*, *inelastic scattering cross section*) or *stopping cross sections*, or both, are evaluated.

287 enhanced elastic cross section

Cross section of an atom for *elastic scattering* that is greater than the *Rutherford cross section* due to partial penetration of a nucleus in the sample by the incident particle.

Source: [2] entry 4.128.

288 experimental scattered-ion intensity

Measured response of the energy filtering and detection system as a consequence of bombarding the sample material with an *ion beam*, usually presented as the ordinate of an *ion-scattering spectrum*.

Source: [2] entry 4.396.

289 ion-scattering spectrometer

Measuring instrument [VIM 3.1] capable of generating a primary beam of principally monoenergetic, singly charged, low-energy ions and determining the energy distribution of the *primary ions* that have been scattered from a solid *surface* through a known angle.

Source: [15].

Note: For applications in surface chemical analysis, the primary ions are commonly of rare-gas atoms with energies in the range 0.1 to 10 keV.

290 ion-scattering spectrum

Plot of the *intensities* of ions, scattered from a sample, as a function of the *scattered-ion energy* divided by the incident-ion energy.

Source: [2] entry 4.267.

291 kinematic factor, *K*

Particle energy after an elastic collision divided by the energy before the collision, in the laboratory frame of reference.

Note: The symbol *K* is often used for the kinematic factor and might have a subscript added in ion-scattering spectrometry or *Rutherford backscattering spectrometry* measurements, denoting the target atom as either, say, K_{Si} or K_{28}. The subscript for atomic mass is preferred, since the isotope is correctly identified.

Source: [2] entry 4.277.

292 nuclear reaction cross section

Cross section at a given *beam energy* and emission direction of the detected product for a particular nuclear reaction per atom.

Note: SI unit m^2. Commonly used unit barn, 1 barn = 10^{-28} m^2.

293 nuclear stopping cross section

Stopping cross section arising from energy transfer to atomic nuclei of the sample.

Note: The maximum of the nuclear stopping cross section occurs at energies of the order of 1 keV per nucleon, whereas that of the electronic stopping cross section occurs at above 100 keV per nucleon. The absolute value of the electronic stopping cross section maximum is significantly greater than that of the nuclear stopping cross section.

Source: [2] entry 4.131.

294 pileup

Counts in a *backscattering spectrum* arising from two or more separate events that occur so closely in time that the signals are not resolved by the detection system and cause counts to be recorded in erroneous channels.

Source: [2] entry 4.336.

295 probe ion

Ion *intentionally* produced by an ion source and directed onto the sample *surface* at a known *angle of incidence* and a known energy.

Source: [2] entry 4.349.

296 random incidence spectrum

Backscattering spectrum recorded with the analysing beam incident on the sample in a direction such as to produce no channelling.

Source: [15].

297 resonance reaction

Nuclear reaction that has a narrow peak in the *nuclear reaction cross section* as a function of energy, the nuclear reaction cross section at the peak being so much larger than the nuclear reaction cross sections at adjacent energies on either side of the peak that essentially all the particles detected from the reaction are due to the peak.

Source: Modified from [15].

298 Rutherford cross section

Elastic scattering cross section calculated using classical mechanics and a Coulomb potential.

Note: The resulting *cross section* formula was first derived by Rutherford.

Source: [2] entry 4.133. See also: *enhanced elastic cross section*, *Rutherford backscattering spectrometry*.

299 scattered-ion energy

Kinetic energy of a *primary ion* after a collision.

Note: Following *binary elastic scattering*, the kinetic energy of the primary or *probe ions*, E_s, is given by $E_s = E_0 [M_0/(M_0 + M_1)]^2 \{\cos\theta + [(M_0/M_1)^2 - \sin^2\theta]^{1/2}\}^2$ where E_0 is the kinetic energy of the incident probe ion prior to scattering; M_0 is the mass of the probe ion; M_1 is the mass of the target atom; θ is the angle between the initial and final velocity vectors for the probe ion, as determined from a common origin in the laboratory coordinate system, expressed as a value between 0° and 180°.

Source: [2] entry 4.394.

300 scattered-ion energy ratio

Scattered-ion energy divided by energy of the incident *probe ion* prior to a collision.

Source: [2] entry 4.395.

301 screening

Response arising from electrons in an atom causing an apparent reduction in the coulomb potential of the nucleus.

Note: In *ion-beam analysis*, when the incident ion is far from the target nucleus, the atom in which the nucleus sits looks neutral to the ion as a result of screening. The screening reduces the *scattering cross section* slightly from the *Rutherford cross section* (about 1 % per 50 increase in the target atomic number for 2 MeV He). The effect becomes more pronounced and increasingly uncertain as the energy decreases and, for *low-energy ion scattering spectrometry*, the cross section is no longer really well-known.

Source: [2] entry 4.398.

302 screening function

Factor by which the *Rutherford cross section* is reduced as a result of *screening* in a given experiment.

Source: [2] entry 4.398.

303 stopping cross section factor

Energy loss of a particle scattered at a given depth in the sample, and detected at a given angle, by the product of the atomic density of the sample atoms and the depth of scattering.

Source: [2] entry 4.453.

304 stopping cross section, $S(E)$

Rate of energy loss of a particle with distance along its trajectory in a sample divided by the atomic density of sample atoms for a sample of infinitesimal thickness.

Note 1: The atomic density is usually taken as the number density, N, but sometimes as the mass density, ρ. The stopping cross section is thus given either by $S(E) \equiv (1/N)\mathrm{d}E/\mathrm{d}x$ or by $S(E) \equiv (1/\rho)\mathrm{d}E/\mathrm{d}x$, where $\mathrm{d}E/\mathrm{d}x$ is the rate of loss of energy E with distance x along the particle trajectory. Note that $\mathrm{d}E/\mathrm{d}x$ is often called the *stopping power*, although it is not in units of power. This inconsistency for the term stopping power leads to its deprecation.

Note 2: SI unit: J m^2 or J m^2 kg^{-1}. Common unit eV m^2 or eV m^2 kg^{-1}.

Source: [2] entry 4.134, with modified notes.

305 stopping power
    stopping force

Rate of *energy loss* of a particle with distance along its trajectory in a sample.

Note 1: Stopping power and stopping force are synonymous terms and are usually represented by $-\mathrm{d}E/\mathrm{d}x$ for a particle of energy E moving in the x-direction. The minus sign makes these terms positive quantities.

Note 2: Stopping power is the official nomenclature of the International Commission on Radiation Units and Measurements (ICRU), but it is recognized that the term does not define a power but a force and so stopping force has been included here as a more precise synonymous term.

Note 3: In older texts, this quantity has also been called "stopping cross section", which is no longer recommended. See Note 1 to *stopping cross section*.

Source: [2] entry 4.455.

306 swift ion

Ion moving with a velocity exceeding the Bohr speed of $c/137$, where c is the velocity of light.

Note: For argon and gold, this criterion requires energies greater than 1 MeV and 5 MeV, respectively.

Source: [2] entry 7.32.

307 system resolution

Energy resolution or *depth resolution* measured in a *backscattering spectrum* for a monoenergetic incident-ion beam.

Source: [2] entry 4.387.

308 target

Sample under investigation.

Source: [2] entry 4.466.

309 theoretical scattered-ion intensity, $I_i(\theta)$

Calculated intensity for *probe ions* scattered into a specified solid angle at a given direction.

Source: [2] entry 4.397, without notes.

310 thin target

In energetic-ion analysis and *Rutherford backscattering spectrometry*, sample whose thickness is sufficiently small that the variation in energy of particles backscattered from atoms of each constitutive element is small with respect to the *system resolution*.

Source: [15].

3.4 Mass spectrometries

311 analyser blanking in secondary-ion mass spectrometry

Action to prevent *secondary ions* from travelling through the *mass spectrometer* and being detected.

Note: This action is usually made by pulsing one of the relevant electrode potentials in *time-of-flight mass spectrometers* to deflect ions of a selected mass range in which intense peaks occur, so that those masses are not detected and thus do not cause unwanted detector saturation.

Source: [2] entry 4.7.

312 beam bunching in secondary-ion mass spectrometry

Reduction in the spread of arrival times of an ion pulse by reduction in the speed of the leading ions or acceleration of those at the trailing edge of the pulse.

Note: This procedure can degrade the optimum focus of the *ion beam*, since different ions experience different fields.

Source: [2] entry 4.66.

313 buncher

Device to shorten the time length of a pulse of ions so that they arrive at a point over a reduced time interval.

Note: The point is usually the sample surface.

Source: [2] entry 7.10.

314 cationized molecule

Ion formed by the association of a cation with a molecule M.
Example: $[M + Na]^+$, $[M + K]^+$, and $[M + NH_4]^+$.
Source: [7] entry 61.

Note 1: Cationization with, for instance, Ag, leads to high yields of some positive ion fragments or *molecular ions*. Each ion has a mass given by the sum of the mass of the parent molecule or fragment and the mass of the added metal atom or atoms. The Ag can be used either as the substrate upon which the molecules are deposited or in the form of a sub-monolayer sputtered onto the molecules already on a *surface*.

Note 2: NH_4^+ can be used as well as metals to cationize molecules.

315 degree of ionization

Number of ions of a species emitted divided by the number of sputtered particles of that species.

Source: [2] entry 4.156.

Note: The use of "ionization coefficient" for degree of ionization is not recommended.

316 dilute limit in secondary-ion mass spectrometry

Atomic fraction or concentration of impurity species in a homogeneous matrix below which the *secondary-ion mass spectrometry* can safely be assumed to be linear with composition.

Source: [2] entry 4.172.

317 disappearance cross section

Cross section for the loss of intensity of an ion signal observed as a result of the bombardment by *primary ions*.

Note 1: The ion signal used is usually that for a large or characteristic fragment of the molecule, such as a cationized ion, protonated ion, or deprotonated ion from the molecule, at a *surface*.
Note 2: Generally, the larger the molecule, the larger the disappearance cross section.
Note 3: It is often assumed that the material being studied is present as a *monolayer*; however, this is an experimentally measured parameter and a value can be obtained irrespective of the precise form of the material under study. The disappearance cross section has practical significance and might or might not be simply related to the damage cross section.

Source: [2] entry 4.125.

318 dual-beam profiling

In *secondary-ion mass spectrometry*, sputter *depth profiling* involving two ion guns.

Note 1: Two similar ion guns can be used in opposite azimuths of the sample to reduce the development of topography.
Note 2: In *time-of-flight mass spectrometer*s, one beam is used with a short on-time for the secondary ion mass spectrometry analysis, while a second is used during the period when the first is off and the mass analysis has been completed in each cycle. The second gun provides the ions for sputter removal of the sample to form the depth profile. This combination allows practical *sputtering rates* to be achieved and the profiling to be optimized separately from the optimization for the SIMS analysis.

Source: [2] entry 4.183.

319 efficiency (in secondary ion mass spectrometry)

Measured yield of an ion species per *primary ion* divided by *disappearance cross section*.

Source: [2] entry 4.185.

320 extraction field

In *secondary-ion mass spectrometry*, electric field above a sample, operational during ion emission from the sample.

Note: The extraction field can be pulsed or constant, depending on the type of instrument.

Source: [2] entry 4.207.

321 extractor voltage (in secondary ion mass spectrometry)

Electric potential, referenced to the sample, of the electrode defining the field above the sample and used to facilitate introduction of emitted ions into the *mass spectrometer*.

Note 1: In pulsed-extraction mode, the extractor voltage will be pulsed to the high value required to extract ions emitted from the sample by the *primary-ion* pulse for at least the time period necessary for the heaviest ion to pass through the extractor electrode and will then be reduced to the extraction bias voltage until the next pulse is required.

Note 2: This voltage, together with the separation distance between the sample and the extractor electrode, defines the *extraction field*.

Source: [2] entry 4.206.

322 fast-atom bombardment secondary ion mass spectrometry (FAB-SIMS)

Secondary ion mass spectrometry in which the *primary-ion* beam is replaced by a fast-atom beam.

Source: [2] entry 4.

323 fractional ion yield

Number of ions of a particular species sputtered from a sample divided by number of particles of that species sputtered from that sample.

Source: [2] entry 4.269. See also: *fractional sputtering yield*, *partial sputtering yield*, and *total ion yield*.

324 fragment ion

Product ion that results from the dissociation of a *precursor ion*.

Source: [7] entry 192.

Note: Fragment ions can dissociate further to form other electrically charged molecular or atomic moieties of successively lower mass.

See also: *metastable ion*.

325 fragmentation reaction (in mass spectrometry)

Reaction of an ion that results in two or more fragments of which at least one is an ion.

Source: [7] entry 191.

Note: The total charge is conserved in fragmentation (See: [2] entry 4.223).

326 g index in G-SIMS

Power for the ratio of mass intensities in two mass spectra measured for two different *primary ion* conditions, used to generate the *G-SIMS* spectrum.

Note 1: The different primary ion conditions can be two, well-separated, energies for the same primary ion or two different primary ions, usually at the same beam energy.

Note 2: A value of 13 has been found to be effective for the g index in generating G-SIMS spectra and a continuous variation between 0 and 40 for analysis.

Source: [2] entry 7.20.

327 G-SIMS with fragmentation pathway mapping, (G-SIMS-FPM)

Development of *G-SIMS* in which the *g index* is varied in order to deduce the linkages between *product ions* and *precursor ion*.

Source: [2] entry 7.19.

328 ion beam ratio

Intensity of analyte ion divided by intensity of matrix ion, both corrected for isotopic abundance.

Source: [2] entry 4.261.

329 liquid-metal ion gun, (LMIG)

Ion gun utilizing a liquid-metal Taylor cone as the source of the *primary ions*.

Note: The Taylor cone generates ion sources of very high brightness. This design enables the gun to provide *beam diameters* in the range 50 nm to 1 µm for ion *beam energies* in the range 5 keV to 30 keV, the smallest diameters generally being at the higher energies.

Source: [2] entry 4.288.

330 *m/z*

deprecated: mass-to-charge ratio
deprecated: thomson

Abbreviation representing the dimensionless quantity formed by dividing the ratio of the mass of an *ion* to the *unified atomic mass unit*, by its *charge number* (regardless of sign). The abbreviation is written in italicized lowercase letters with no spaces.

Note 1: "Mass-to-charge ratio" is deprecated. Mass-to-charge ratio has been used occasionally for the horizontal axis in a plot of a *mass spectrum*, although the quantity measured is not the ion's mass divided by its electric charge. However, *m/z* is recommended as an abbreviation to represent the dimensionless quantity that is used almost universally as the independent variable in a mass spectrum.

Note 2: The term "ratio of mass to charge" should be used for the quantity expressed in kg C^{-1} in SI units.

Note 3: The abbreviation *m/z* should not be used as a variable in a mathematical equation. Instead, the variables *m* (in kg) and *q* (in C) should be used to denote mass and charge.

Note 4: The thomson (Th) unit [25] is deprecated.

Source: [7] entry 356.

331 mass accuracy

Measured mass minus reference value for that mass.

Note: In practice, mass accuracy is expressed as a fractional error. See: *relative mass accuracy*.

Source: [2] entry 4.292.

332 mass spectrometer

Measuring instrument [VIM 3.1] that measures *m/z* values and abundances of gas-phase ions.

Source: [7] entry 318.

333 mass spectrum

Plot of the relative abundances of *ions* forming a beam or other collection as a function of their *m/z* values.

Note: The term is a misnomer because it is *m/z*, rather than mass, that is the independent variable in a *mass spectrum*.

Source: [7] entry 323.

334 metastable background (in secondary-ion mass spectrometry)

Intensity in a *mass spectrum* arising from ions that spontaneously fragment between emission and detection.

Note: In reflectron time-of-flight *mass spectrometer*s, the decay of *metastable ions* leads to broad peaks at a mass dependent on the drift energy and *reflector voltage*. Good design minimizes these background signals.

Source: [2] entry 4.52.

335 metastable ion

Ion formed with internal energy higher than the threshold for dissociation but with a lifetime great enough to allow it to exit the ion source and enter the mass analyser region, where it dissociates before detection.

Source: [7] entry 334.

Note: In general, metastable ions have a lifetime of less than 1 μs. (Source: [2] entry 4.300.)
See also: *metastable background*.

336 molecular fragment

Ion or neutral particle that was part of a larger molecular structure and contains information about that structure.

Source: [2] entry 4.302.

337 molecular image

Image of a *surface* formed from ions characteristic of a particular molecule.

Source: [2] entry 4.303. See also: *static limit*, *surface map*.

338 molecular ion

Ion formed by the removal of one or more electrons from a molecule to form a positive ion or the addition of one or more electrons to a molecule to form a negative ion.

Note 1: Terms "pseudo-molecular ion" and "quasi-molecular ion" should not be used; molecular ion is reserved for the intact ionized molecule with no component added or removed other than electrons.

Source: [7] entry 342.

Note 2: Peaks from protonated and deprotonated molecules are often of greater intensity than the molecular ion (Source: [2] entry 4.304).

339 negative-ion yield

Number of negatively-charged *secondary ions* sputtered from a sample divided by total number of incident primary particles.

Source: [2] entry 4.270. See also: *positive-ion yield, fractional ion yield*, and *total ion yield, sputtering*.

340 nominal mass

Mass of a *molecular ion* or molecule calculated using the isotope mass of the most abundant constituent element isotope of each element rounded to the nearest integer value and multiplied by the number of atoms of each element.

Source: [7] entry 368.

341 partial ion yield
partial ion sputtering yield

Number of ions of a particular species sputtered from a sample divided by the number of incident particles.

Source: [2] entry 4.491. See also: *fractional ion yield, fractional sputtering yield, negative-ion yield, partial sputtering yield, positive-ion yield,* and *total ion yield.*

342 polyatomic fragment

Ion or neutral particle composed of three or more atoms.

Source: [2] entry 4.340.

343 positive-ion yield

Number of positively-charged *secondary ions* sputtered from a sample divided by the total number of incident primary particles.

Source: [2] entry 4.271. See also: *negative-ion yield, fractional ion yield*, and *total ion yield*.

344 precursor ion
progenitor ion

Ion that reacts to form particular *product ions* or undergoes specified neutral losses.

Note 1: The reaction can be of different types, including unimolecular dissociation, ion/molecule reaction, change in charge state, possibly preceded by isomerization.
Note 2: The term 'parent ion' is no longer recommended.

Source: [7] entry 407.

345 primary ion

Ion extracted from a source and directed at a sample.

Source: [2] entry 4.348. See also: *probe ion, secondary ion.*

346 product ion

Ion formed as the product of a reaction involving a particular *precursor ion.*

Note 1: The reaction can be of different types, including unimolecular dissociation to form *fragment ions* or an ion/molecule reaction, or can simply involve a change in the number of charges. Thus, all fragment ions are product ions, but not all product ions are necessarily fragment ions.

Note 2: The term 'daughter ion' is no longer recommended.

Source: [7] entry 412.

347 progenitor ion

See: *precursor ion.*

348 pulse rate (in secondary ion mass spectrometry)

Number of ion pulse cycles per second in *secondary ion mass spectrometry*.

Source: [2] entry 4.354. See also: *repetition rate.*

349 pulse width (in secondary ion mass spectrometry)

Full width at half maximum of the time distribution of the pulse of ions generated by a beam chopper and, optionally, the use of *beam bunching* in *secondary ion mass spectrometry*.

Note: The pulse width is usually measured using the H^+ ion. The velocity of H^+ ions, for a given *extraction field*, is larger than that of other ions. The width in time of the H^+ pulse thus provides a more reliable value for the width of the extraction pulse.

Source: [2] entry 4.355.

350 pulsed extraction field

Extraction *field* around the sample that is pulsed to the working value for extracting ions for the time necessary for operation of a *time-of-flight mass spectrometer*, but is otherwise at a low value.

Note: This is the usual mode in time-of-flight *secondary ion mass spectrometry* systems, either for studying insulators, where *charge neutralization* is established while the extraction field is off, or for *depth profiling* using a second *ion beam* while the extraction field is off.

Source: [2] entry 4.356.

351 reflector voltage

Electric potential set on the reflector electrode of a *reflectron* mass spectrometer with the zero referenced, such that an ion emitted from the sample with an energy numerically equal to the reflector voltage would just be on the point of reflection or transmission by the reflector electrode.

Source: [2] entry 4.373.

352 reflectron

Component of a *time-of-flight mass spectrometer* that uses a static electric field to reverse the direction of travel of the ions and improves mass *resolution* by assuring that ions of the same *m/z* but different translational energy arrive at the detector at the same time.

Source: [7] entry 447.

353 relative isotopic sensitivity factor

In *dynamic secondary-ion mass spectrometry*, coefficient for an element by which the measured intensity for an isotope of that element, divided by the measured intensity for a matrix ion, is multiplied to yield the atomic concentration of that isotope of the element present in the sample.

Note: Matrix terms are strong, and the matrix, bombarding species, incident-ion energy, and *angle of incidence*, as well as the spectrometer operating conditions, all affect relative elemental sensitivity factors significantly.

Source: [2] entry 4.421.

354 relative mass accuracy

Mass accuracy divided by reference mass.

Source: [2] entry 4.293.

355 repetition rate (in secondary ion mass spectrometry)

Rate at which the whole cycle of primary-ion pulse, ion extraction, mass analysis, and removal of slow ions is repeated to build up a *mass spectrum* in a *time-of-flight mass spectrometer*.

Source: [2] entry 4.383.

356 secondary ion

Ion ejected from a sample *surface* as a result of energy and momentum transfer from a *primary ion*.

Source: [2] entry 4.406.

357 secondary-electron yield (in secondary ion mass spectrometry)
secondary-electron emission coefficient

Number of electrons emitted from a sample divided by the number of particles incident upon the sample *surface*.

Note: Secondary-electron yield is sometimes given for a particular type of energetic incident particle such as Ar^+.

Source: [2] entry 4.404.

358 secondary-ion angular distribution

Number of secondary ions as a function of angle of emission.

Source: [2] entry 4.407.

359 secondary-ion energy distribution

Number of *secondary ions* as a function of kinetic energy at a specified collection angle.

Source: [2] entry 4.408.

360 secondary-ion yield

Number of ions sputtered from a sample divided by the number of ions incident with a given mass, energy, charge, and *angle of incidence*.

Source: [2] entry 4.409.

361 shots per pixel in secondary ion mass spectrometry

Number of ion pulses incident at each pixel in an image for one *raster* frame in *secondary ion mass spectrometry*.

Source: [2] entry 4.426.

4.1.1 spike (in secondary-ion mass spectrometry)

Limited region in space and time within which the majority of atoms in an irradiated material are in rapid motion in *secondary ion mass spectrometry*.

Note 1: The term spike is usually applied to the region generated by a single primary particle. In SIMS, this primary particle can often be a *cluster ion*.

Source: [2] entry 4.437.

Note 2: The use of the term 'spike' in SIMS should not be confused with its use in general analytical chemistry (See: [26] entry 2.68).

362 SIMS ion image

Two-dimensional *surface map* of the spatial distribution of the amount of a particular *secondary ion* emitted from within a specific area of the sample in *secondary ion mass spectrometry*.

Source: [2] entry 4.262.

363 static limit (in secondary ion mass spectrometry)

Ion *fluence* above which any significant changes in the spectrum, arising from beam damage, are observed in *secondary ion mass spectrometry*.

Note 1: Classically, a limit of 10^{12} ions per cm^2, or 10^{16} ions per m^2 is taken as the limit not to be exceeded in *static secondary ion mass spectrometry*. This limit is based on one incident ion for each 1000 surface atoms.
Note 2: For imaging, the total molecular signal can be used, and here the limit can be greater and reach 100 times the limit given in Note 1.
Note 3: For large molecules, the damage cross section and *disappearance cross section* are both generally larger than for small molecules, leading to a static limit less than 10^{12} ions per cm^2.

Source: [2] entry 4.448.

364 stop event (in secondary ion mass spectrometry)

Registration of a particle by a time-to-digital converter in *secondary ion mass spectrometry*.

Note: The arrival time for each ion providing a pulse at the detector is registered by the time-to-digital converter (TDC). This is a stop event. TDCs might only record a fixed number of stop events during the time following each *primary-ion* pulse, for example 512 or 1024, other events being lost.

Source: [2] entry 4.451.

365 time-of-flight (TOF) mass spectrometer

Mass spectrometer that separates ions by *m/z* in a field-free region after acceleration through a fixed accelerating potential. Ions of the same initial translational energy and different *m/z* require different times to traverse a given distance in the field-free region.

Source: [7] entry 525.

366 Taylor cone

See: *liquid-metal ion gun*.

367 transformation probability

Probability of a defined charged or neutral species being produced, by consumption of a defined parent atomic or molecular configuration at a *surface*, as a result of *sputtering* in *secondary ion mass spectrometry*.

Source: [2] entry 4.476.

368 ultra-shallow depth profile

Depth profile in *secondary-ion mass spectrometry* where the depth over which significant changes occur is less than 10 nm.

Source: [2] entry 4.479.

369 useful ion yield

In *secondary ion mass spectrometry*, number of ions of a particular isotope detected divided by the number of atoms of the same element sputtered from the sample.

Source: [2] entry 4.272.

370 useful spatial resolution (in secondary ion mass spectrometry)

Image *resolution* in *secondary ion mass spectrometry* obtained in practice.
Note: The image resolution is poorer than the primary-ion *beam diameter* as a result of either the need to maintain the damage level below a limit set by the integrity of the data or the need to record sufficient signal when the sample is being consumed during analysis.

Source: [2] entry 4.482.

3.5 Optical and X-Ray spectroscopy

371 absorption length (in X-ray reflectometry)

Distance over which the transmitted X-ray intensity falls by 1/e, where e is the base of the natural logarithm.
Source: [2] entry 7.1.

372 absorption spectrum

General term for the spectrum of radiation absorbed by a sample.

Note 1: The ordinate quantity may be absorption cross-section, absorption coefficient or absorbance.

Note 2: If the ordinate quantity is the absorbance, but not otherwise, the spectrum may be called an absorbance spectrum.

Source: [6] entry 10.

373 anti-Stokes Raman scattering
anti-Stokes scattering

Raman scattering of electromagnetic radiation in which the scattered radiation has greater energy (greater wavenumber) than the exciting radiation.

Source: [6] entry 496. See also: *Stokes Raman scattering*.

374 beam footprint in X-ray reflectometry

Area on the specimen irradiated by X-rays in *X-ray reflectometry*.

Note 1: In typical commercial equipment, the beam width is 200 μm, so at 0,3° incident angle, the beam footprint is 38 mm long; at 1°, it is 11.5 mm and at zero incidence angle it is infinite. For 100 μm incident beam width, these values are halved.

Note 2: The beam footprint along the beam direction can be reduced by the use of a suitable knife-edge diaphragm mounted in a plane that is normal to the sample surface and whose normal, in turn, aligns with the beam azimuth. The knife-edge is parallel to, and adjusted to be close to, the surface at the point where the X-ray beam centre strikes the sample surface. This closeness limits the footprint size but also reduces the measured signal intensity.

Source: [2] entry 7.5.

375 beam spill-off in X-ray reflectometry

Fraction of the incident X-ray beam in *X-ray reflectometry* missing the specimen.

Source: [2] entry 7.6.

376 complex refractive index, $\hat{n}$
refractive index

Speed of light in a given medium divided by the speed of light in vacuum.

Note 1: $\hat{n} = n + ik$. The real part, n, is usually called the 'refractive index', and is the entire refractive index when no radiation is absorbed. The imaginary part, k, describes absorption.

Note 2: The older literature, and some physics literature today, uses $\hat{n} = n(1 + i\kappa)$, where κ is called the attenuation index. For simplicity, this usage is discouraged.

Source: [6] entry 29.

377 critical angle (in total-reflection X-ray fluorescence spectroscopy)

Glancing angle at which the sample matrix *X-ray fluorescence*, when plotted against the glancing angle, is at the first point of inflection.

Source: [2] entry 4.12.

378 critical angle (in X-ray reflectrometry)

Angle between the incident beam and the specimen surface, as the angle of incidence increases from the total reflection condition, at which the reflectivity is at the first point of inflexion.

Note: In practical cases, the critical angle is often taken as the angle at which the reflected intensity has fallen to 50 % of that in the total external reflection condition. The error here is generally small.

Source: [2] entry 7.12, with deleted note.

379 delayed onset (in an X-ray absorption spectrum)

X-ray energy at which there is a significant increase of absorption and for which the increased absorption occurs at a greater energy than a core-level *binding energy*.

Note: For many elements, there is a significant increase of absorption when the X-ray energy is equal to the electron-binding energy for a sub-shell. A delayed onset occurs for some elements and sub-shells when the corresponding increase of absorption occurs, instead, at an energy larger than the sub-shell binding energy.

Source: [2] entry 4.157.

380 dispersion plane (in X-ray reflectrometry)

Plane containing the source, detector, incident, and specularly reflected X−ray beams in *X-ray reflectrometry*.

Source: [2] entry 7.16.

381 elastic scattering (of light)

See: *Rayleigh scattering*.

382 Rayleigh scattering
　　elastic scattering (of light)

Light scattering in which the incident and scattered radiation has the same frequency.

Source: [6] entry 634.

383 reflectance, *ρ, R*

Spectral intensity (See: [6] entry 129) reflected by the sample divided by spectral intensity incident on the sample.

Note: For non-scattering and non-luminescent samples the sum of *absorptance* (*α*), *transmittance* (*τ*) and *reflectance* (*ρ*) equals one.

Source: [6] entry 112.

384 refractive index

See: *complex refra4ctive index*.

385 scattering vector in X-ray reflectometry, *q*, *Q*

Vector in reciprocal space giving the difference between the scattered and incident wave vectors in *X-ray reflectometry*.

Source: [2] entry 7.30. See also: *X-ray wave vector*.

386 Stokes Raman scattering
  Stokes scattering

Raman scattering of electromagnetic radiation in which the scattered radiation has lesser energy (lesser wavenumber) than the exciting radiation.

Source: [6] entry 648.

387 total reflection of X-rays

Condition where the *glancing angle* for the incident X-rays is at or less than the *critical angle* and the X-rays are either reflected or absorbed in a region very close to the *surface*.

Note: The reflected intensity is close to 100 % of the incident intensity and the transmitted intensity is zero.
Source: [2] entry 4.475.

388 transmission factor
  transmission fraction

See: *transmittance*.

389 transmission spectrum
  transmittance spectrum

General term for the spectrum of transmitted electromagnetic radiation.

Note: The ordinate quantity is usually the fraction of the incident radiation that is transmitted, usually called the percent transmission, with range 0 to 100 %. If the ordinate quantity is the fraction transmitted, *i.e.*, the *transmittance*, the ordinate range is 0 to 1 and the spectrum may be called a transmittance spectrum.
Source: [6] entry 146.

390 transmittance, *T, τ*
  transmission factor
  transmission fraction

Transmitted radiant power at wavenumber $\tilde{v}$ divided by the incident radiant power.

Note 1: For non-scattering, non-luminescent samples, the sum of *absorptance* (*α*), transmittance (*T*), and *reflectance* (*ρ*) equals one.
Note 2: For scattering, non-luminescent samples, the term 'transmission fraction' is usually used instead of transmittance.
Source: [6] entry 147.

391 wave vector in X-ray reflectometry, *k*

Vector in reciprocal space describing the direction of propagation of X-rays and equal in magnitude to $2\pi/\lambda$, where λ is the wavelength of the X-rays.

Note: In different fields of study, the wave vector is taken as $2\pi/\lambda$ or as $1/\lambda$. In *X-ray reflectometry* the former is usually used.

Source: [2] entry 7.36. See *scattering vector in X-ray reflectometry*.

392 X-ray emission spectrum

Spectrum comprising the continuum *Bremsstrahlung* and the most energetic characteristic spectral lines defined by differences in binding energy between electron *energy levels*.
Source: [6] entry 485.

393 X-ray jump ratio

X-ray absorption coefficient at an energy just above an absorption edge divided by that at an energy just below the edge.

Note: X-ray absorption spectra can have complex shapes for X-ray energies in the vicinity of photoionization thresholds, and a well-defined edge is not always observed at the threshold.

Source: [2] entry 4.276.

4 Membership of Sponsoring Body

The membership of IUPAC Analytical Chemistry Division at the time of the project was as follows:
President: Zoltan Mester; **Past President:** Jan Labuda; **Vice President:** Érico Marlon de Moraes Flores; **Secretary:** Takae Takeuchi; **Titular Members:** Medhat A. Al-Ghobashy, Derek Craston, Attila Felinger, Irene Rodriguez Meizoso, Sandra Rondinini, David Shaw. **Associate Members:** Jiri Barek, M. Filomena Camões, Petra Krystek, Hasuck Kim, Ilya Kuselman, M. Clara Magalhães, Tatiana A. Maryutina; **National Representatives:** Boguslaw Buszewski, Mustafa Culha, D. Brynn Hibbert, Hongmei Li, Wandee Luesaiwong, Serigne Amadou Ndiaye, Mariela Pistón Pedreira, Frank Vanhaecke, Winfield Earle Waghorne, Susanne Kristina Wiedmer.

Index of terms

Index of symbols and abbreviations

β	asymmetry parameter
β	initial-state Auger parameter
γ	surface tension
δ	secondary-electron yield
ϕ_0	work *function*
ϕ_0	photoelectric *work function*, flux of a beam of particles
η	backscattering yield
Γ	surface concentrationsurface excess concentration
Γ	surface concentrationsurface excess concentration
θ	surface coverage
ρ	reflectance
σ	cross sectionsurface tensiontotal secondary-electron yield
σ_e	elastic cross section
τ	transmittance
ω	angle of incidence
a	specific surface area
a_s	specific surface area
A_s	area of surface or interface (See: surface excess concentration)
D	areic dose
D_{imp}	implanted areic dose
E_{VAC}	vacuum level
$E_{VAC}(\infty)$	vacuum level at infinity
G	areic dose rate
I_{av}	average beam current
$I_i(\theta)$	theoretical scattered-ion intensity
k	wave vector in X-ray reflectometry
K	kinematic factor
n_σ	surface excess
q	scattering vector in X-ray reflectometry
Q	scattering vector in X-ray reflectometry
r	backscattering fraction
R	backscattering correction factorreflectance
s	specific surface area
$S(\varepsilon)$	stopping cross section
T	transmittance
W	work functionthermionic work function
AES	Auger spectroscopy
AMRSF	average matrix relative sensitivity factor
APECS	Auger photoelectron coincidence spectroscopy
ATR	attenuated total reflection

ATRIRS	attenuated total reflection infrared spectroscopy
CDP	compositional depth profile
DAPCI	desorption atmospheric pressure chemical ionization
DAPPI	desorption atmospheric pressure photoionization
DART	direct analysis in real time
DESI	desorption electrospray ionization
DRAIRS	diffuse reflection-absorption infrared spectroscopy
DRIFTS	diffuse reflectance infrared Fourier transform spectroscopy (See: diffuse reflection-absorption infrared spectroscopy)
DRS	direct recoil spectroscopy
DSIMS	dynamic secondary-ion mass spectrometry
EESI	extractive electrospray ionization
ELDIMS	electrospray laser desorption ionization mass spectrometry
EPES	elastic peak electron spectroscopy
ERD	elastic recoil detection (See: direct recoil spectroscopy)
ERDA	elastic recoil detection analysis (See: direct recoil spectroscopy)
ESCA	electron spectroscopy for chemical analysis (See: X-ray photoelectron spectroscopy)
EXAFS	extended X-ray absorption fine structure spectroscopy
FAB	fast atom bombardment
FIB	focused ion beam system
GISAXS	grazing-incidence small-angle X-ray scattering analysis
G-SIMS-FPM	G-SIMS with fragmentation pathway mapping
IBA	ion beam analysis
IRRAS	infrared reflection-absorption spectroscopy (See: reflection-absorption infrared spectroscopy)
IRS	internal reflection spectroscopy (See: attenuated total reflection spectroscopy)
LAESI	laser ablation electrospray ionization
LB	Langmuir-Blodgett
LEIS(S)	low-energy ion scattering spectrometry
LMIG	liquid-metal ion gun
MALDESI	matrix-assisted laser desorption electrospray ionization
MALDI	matrix-assisted laser desorption/ionization mass spectrometry
MS	mass spectrometry
NSOM	near-field scanning optical microscopy (See: scanning near-field optical microscopy)
PADI	plasma assisted desorption ionization
PERSF	pure-element relative sensitivity factor
PIXE	particle-induced X-ray emission analysis
MEIS(S)	medium-energy ion scattering spectrometry
NEXAFS	Near-edge extended X-ray absorption fine structure spectroscopy (See: X-ray absorption near-edge spectroscopy)
RAIRS	reflection-absorption infrared spectroscopy
RBS	Rutherford backscattering spectrometry
REELS	reflection electron energy loss spectroscopy
RISR	relative instrument spectral response function
SALDI	surface-assisted laser desorption/ionization
SAM	self-assembled monolayer
SDP	sputter depth profile
SEIRAS	surface-enhanced infrared spectroscopy
SERS	surface-enhanced Raman spectroscopy
SERRS	surface-enhanced resonant Raman spectroscopy
SEXAFS	surface extended X-ray absorption fine structure spectroscopy
SFGS	sum frequency generation spectroscopy
SHG	second harmonic generation
SIMS	secondary-ion mass spectrometry
SNOM	scanning near-field optical microscopy
SRXAS	synchrotron radiation small-angle X-ray scattering (See: small-angle X-ray scattering)
SSIMS	static secondary-ion mass spectrometry
TDC	time-to-digital converter (See: stop event)
TERS	tip enhanced Raman spectroscopy
TOF	time-of-flight

TXRF	total reflection X-ray fluorescence spectroscopy
UPS	ultraviolet photoelectron spectroscopy
VSFS	vibrational sum frequency spectroscopy (See: sum frequency generation spectroscopy)
WAXS	wide-angle X-ray scattering (See: small-angle X-ray scattering)
XAFS	X-ray absorption fine structure spectroscopy
XANES	X-ray absorption near-edge spectroscopy
XPS	X-ray photoelectron spectroscopy
XRR	X-ray reflectometry
XSW	X-ray standing waves

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