~~Recommendation~~: Glossary of Methods and Terms used in Surface Chemical Analysis

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Glossary of Methods and Terms used in Surface Chemical Analysis ~~(IUPAC Recommendations 2019)~~

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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.

Keywords: Surface chemical analysis; Electron Spectroscopy of surfaces, Ion spectroscopy of surfaces, Photon spectroscopy of surfaces, terminology

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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 which yield atomic and molecular information but does not include methods which 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 covers mainly spectroscopic techniques while Part 2 includes some surface spectroscopies which have been used in the scanning probe mode. The present Recommendations 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 accommodation in layout of minor edits, 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 sections 2 and 3 a term printed in italics in a definition or a note is defined in another entry in this section of the Glossary.

To avoid unnecceary duplication where a term is already defined in the recent "Glossary of Methods and Terms used in Analytical Spectroscopy (IUPAC Recommendations 20xx)" we do not repeat it here but cross reference.

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]

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 synchrotron 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.

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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. Spectra conventionally 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 mono-energetic 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*.

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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*.

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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: By a suitable choice of angle of scattering, the scattered primary ions can be removed from the spectrum.

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*.

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9 **ion beam analysis, (IBA)**

Measurement method [VIM 2.5] to elucidate 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 or *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 is involved.

Source: [2] entry 3.11.

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

Measurement method [VIM 2.5] to elucidate 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 or *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 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 or *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 so that enhanced signal quality and visibility are 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.

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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 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 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*.

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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 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 analyze 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 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 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 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

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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 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 1: 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 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 analyzed.

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 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.

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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 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 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 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

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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 abundance of ionized entities emitted from a sample in air as a result of the bombardment by a focused plasma.

Note 2: The energy of the plasma ions is very low.

Note 3: The beam atoms usually used are helium, nitrogen, air, or argon.

Note 4: 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], and 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 analyzed by mass spectrometry.

Note: SIMS is, by convention, generally classified as dynamic, in which the material surface layers are continually removed as they are being measured, and 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.

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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 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, i.e. for almost all powdered samples.

Note 2: ATRIRS has particular application in 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 which is 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].

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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 1: 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 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 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 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 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 of the surface or for particles on the surface for lengths scales between several nm and several hundred nm.

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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 of the specimen, the scattered intensity falling outside the specular condition (see *specular X-ray reflectometry*).

Note 1: Imperfections generating diffuse XRR include surface and interface roughnesses, film defects, and inhomogeneities. By modelling, quantitative estimates can be made of these.

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: May be employed with polarization modulation to minimize background

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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 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 reflectrometry**

Mode of *X-ray reflectrometry* in which the angle between the detected beam and the sample surface, and the incident beam and the sample surface, are equal. See also *off-specular X-ray reflectrometry*.

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

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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 1: 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 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.

54 **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.

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Source: Modified from [6] entry 654.

55 surface-enhanced resonant Raman spectroscopy, (SERRS)

Measurement method [VIM 2.5] of *surface-enhanced Raman spectroscopy* (SERS) by which the Raman spectrum is significantly enhanced when the conditions occur 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.

56 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 give 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

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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 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 1: 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.

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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, 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.

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, and 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.

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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**

Relation 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}.

$\theta_{\mathrm{B}} = K_{\mathrm{eq}}^{\mathrm{B}} p_{\mathrm{B}} / (1 + K_{\mathrm{eq}}^{\mathrm{B}} p_{\mathrm{B}})$.

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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.

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74 **angle lapping**

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

Note 1: 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 referred to the sample surface.

77 **areic dose rate**, G

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

Note: 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.

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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. The total amount of particle radiation impacting the *surface* has been taken by some to be dose, and the amount divided by the area of the surface to be dose by others. 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 1: 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.

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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.

$$S_{\mathrm{AB}}(\varepsilon) = xS_{\mathrm{A}}(\varepsilon) + yS_{\mathrm{B}}(\varepsilon)$$

where $S_{\mathrm{AB}}(\varepsilon)$ is the stopping cross section of the compound $\mathrm{A}_x\mathrm{B}_y$, and $S_{\mathrm{A}}(\varepsilon)$ and $S_{\mathrm{B}}(\varepsilon)$ 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*.

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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: 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.

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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.

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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*.

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103 **delta layer**

Layer of discrete composition, one atom thick, formed during 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 which 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.

Example: 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

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measured for a step change in composition, care shall 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*.

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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.

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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 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* $F = \mathrm{d}N/\mathrm{d}A$ where N is number of particles and A is area.

Note 1: For a scanned parallel beam, the fluence can be referred 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 $\mathrm{J\ m}^{-2}$. See [6] entry 377.

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121 **flux of a beam of particles**, Φ

$\Phi = \mathrm{d}N/\mathrm{d}t$ 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 electronic charge ($1.602176634 \times 10^{-19}$ 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 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.

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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 which 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 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*.

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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 by repeated immersions many layers can be deposited. 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.

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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.

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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 which 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.

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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: Monolayers and multilayers may be alternatively named '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 16 % to 84 %, or 84 % to 16 %, change in signal intensity 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 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*

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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

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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 1: 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.

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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.

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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 sputtering rate of a reference sample sputtered under the same conditions.

Source: [2] entry 4.377.

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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.

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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 analyzer**

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

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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 as 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 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,

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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 which, if the sample were placed in a vacuum, is the layer 'in contact with' the vacuum; the outermost

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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* which 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: $n_i^\sigma = n_i - V^l c_i^l$ where n_i is the total amount of i in the system, V^l is the volume of an arbitrarily chosen amount of bulk liquid (in the framework of the so-called algebraic method) and c_i^l is its bulk concentration in the liquid.

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

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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*.

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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: $\gamma = \left(\partial G/\partial A_s\right)_{T,p,n_i}$.

Note 3: SI unit: N m^{-1}, J m^{-2}.

Source: [16] p 77.

194 **surfactant**
surface active agent

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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. $W = -kT\ln\left(J/AT^2\right)$, 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, $A = \left(4\pi m_e k^2 e\right)/h^3 \approx 1.202\times10^6$ A m^{-2} K^{-2} where m_e and e are the mass and charge of the electron, respectively, 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.

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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 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 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.

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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 × 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*

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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: $L(\gamma) = 1 + ½\beta\left[3\left(\sin^2\gamma\right)/2 - 1\right]$

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 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.

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Note 2: 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*.

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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 1: 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

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as 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 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.

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Note 1: Charge referencing is often conducted using *adventitious carbon referencing*, using internal carbon referencing or by gold decoration, or 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 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 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.

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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 which, 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 measurement of the changes of overlayer and substrate Auger-electron or photoelectron signal intensities after 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 kinetic energy of an electron, emitted from a conductor illuminated by monochromatic photons, and photon energy and *work function* of the surface from which the photoelectron is emitted. $\frac{1}{2} m_\mathrm{e} v_\mathrm{max}^2 = h\nu - \phi_0$, where m_e is the mass of an electron, v_max the maximum velocity of the emitted electron, h the Planck constant, ν

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1
2
3 the frequency of the illuminating photons, and ϕ_0 the *photoelectric work function* of the
4
5 surface.
6
7 Source: [2] entry 7.17, with added equation.
8
9 231 **elastic peak**
10 quasi-elastic peak
11
12 Peak in the electron spectrum, produced by quasi-elastically scattered electrons
13 detected by an *electron spectrometer*.
14
15 Note 1: All electrons that are scattered by atoms can be elastically scattered in the
16 centre-of-mass frame, but *energy losses* that are typically less than 1 eV
17 might be observed in the laboratory frame. These losses are generally
18 significantly less than the measured energy width of the electrons in a
19 primary-electron beam. Historically, and more generally, the scattering has
20 been called "elastic"; however, the term quasi-elastic is now often used if the
21 small change in energy that occurs on scattering is important.
22
23 Note 2: The energy and the energy broadening of the quasi-elastic peak are
24 influenced by the recoil of the scatterer atoms, the energy distribution of the
25 primary (incident) electrons, the scattering geometry, the acceptance
26 geometry, and the response function of the electron spectrometer. The
27 intensity of the elastic peak depends on the electron differential *elastic*
28 *scattering cross section* and on the *cross section* for *inelastic electron*
29
30 *scattering* at the particular *beam energy* of the *primary-electrons* and in the
31 given scattering geometry, including the probability of surface excitations.
32
33 Source: [2] entry 4.186. See also: *Elastic peak electron spectroscopy*, *reflection electron*
34
35 *energy loss spectroscopy*.
36
37 232 **electron energy analyser**
38
39 *Measuring instrument* [VIM 3.1] for measuring the number of electrons, or an intensity
40 proportional to that number, as a function of the electron kinetic energy.
41
42 Note: An electron energy analyser is part of an *electron spectrometer*.
43
44 Source: [2] entry 4.187.
45
46 233 **electron energy loss spectrum**
47
48 Energy spectrum of electrons from a nominally monoenergetic source emitted after
49 inelastic interactions with the sample, often exhibiting peaks due to specific inelastic
50 loss processes (see *characteristic electron energy losses* and *plasmon*).
51
52 Note 1: The electron energy loss spectrum obtained using an incident-electron beam
53 of about the same energy as a peak obtained in *Auger electron spectroscopy*
54 or *X-ray photoelectron spectroscopy* approximates to the energy loss
55 spectrum associated with that peak.
56
57 Note 2: The electron energy loss spectrum, measured with an incident-electron beam,
58 is a function of *beam energy*, *angle of incidence* of the beam, *angle of*
59 *emission*, and the electronic properties of the sample.
60

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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

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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.

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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, providing 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*.

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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].

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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.*

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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 1: 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 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.

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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 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.

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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 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 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 excitation of electrons from the

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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 *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*.

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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

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commonly of rare-gas atoms with energies in the range 0.1 keV 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 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 for 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.

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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

$$E_s = E_0\left[M_0/(M_0 + M_1)\right]^2\left\{\cos\theta + \left[\left(M_0/M_1\right)^2 - \sin^2\theta\right]^{½}\right\}^2$$

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.

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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.

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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].

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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

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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.

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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

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3 sample and used to facilitate introduction of emitted ions into the *mass spectrometer*.
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5 Note 1: In pulsed-extraction mode, the extractor voltage will be pulsed to the high
6 value required to extract ions emitted from the sample by the *primary-ion*
7 pulse for at least the time period necessary for the heaviest ion to pass
8 through the extractor electrode and will then be reduced to the extraction
9 bias voltage until the next pulse is required.
10
11 Note 2: This voltage, together with the separation distance between the sample and
12 the extractor electrode, defines the *extraction field* .
13
14 Source: [2] entry 4.206.
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17 322 **fast-atom bombardment secondary ion mass spectrometry, (FAB-SIMS)**
18
19 *Secondary ion mass spectrometry* in which the *primary-ion* beam is replaced by a fast-
20 atom beam.
21
22 Source: [2] entry 4.
23
24 323 **fractional ion yield**
25
26 Number of ions of a particular species sputtered from a sample divided by number of
27 particles of that species sputtered from that sample.
28
29 Source: [2] entry 4.269. See also: *fractional sputtering yield*, *partial sputtering yield*, and
30 *total ion yield*.
31
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33 324 **fragment ion**
34
35 *Product ion* that results from the dissociation of a *precursor ion*.
36
37 Source: [7] entry 192.
38 Note: Fragment ions can dissociate further to form other electrically charged
39 molecular or atomic moieties of successively lower mass.
40
41 See also: *metastable ion*.
42
43 325 **fragmentation reaction (in mass spectrometry)**
44
45 Reaction of an ion that results in two or more fragments of which at least one is an ion.
46
47 Source: [7] entry 191.
48 Note: The total charge is conserved in fragmentation. (See: [2] entry 4.223).
49
50 326 **g index in G-SIMS**
51
52 Power for the ratio of mass intensities in two mass spectra measured for two different
53 *primary ion* conditions, used to generate the *G-SIMS* spectrum.
54
55 Note 1: The different primary ion conditions can be two, well-separated, energies for
56 the same primary ion or two different primary ions usually at the same beam
57 energy.
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59 Note 2: A value of 13 has been found to be effective for the g index in generating G-
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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 (SI unit kg C^{-1}). 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.

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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.

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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 molecular ions 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 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 total number of incident primary particles.

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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*, an ion/molecule reaction, or 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.

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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*

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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 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 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.

4.4.1 **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*.

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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*.

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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* for which 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 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 reflectrometry)**

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.

Note2: If the ordinate quantity is the absorbance, but not otherwise, the spectrum may be called an absorbance spectrum.

Source: [6] entry 10.

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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 reflectrometry**

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

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 reflectrometry**

Fraction of the incident X-ray beam in *X-ray reflectrometry* 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 speed of light in vacuum.

Note 1: $\hat{n} = n + \mathrm{i}k$. 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 $\hat{n} = n(1+ \mathrm{i}\kappa)$ 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.

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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.

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384 **refractive index**

See: *complex refractive index.*

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

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

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 $\tilde{\nu}$ divided by incident radiant power.

Note 1: For non-scattering, non-luminescent samples the sum of *absorptance* (α),

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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 reflectrometry, 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 reflectrometry*.

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 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 concentration*

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1
2
3
4 Γ *surface excess concentration*
5 θ *surface coverage*
6
7 ρ *reflectance*
8 σ *cross section*
9
10 σ *surface tension*
11 σ *total secondary-electron yield*
12
13 σ_e *elastic cross section*
14 τ *transmittance*
15
16 ω *angle of incidence*
17
18
19 a *specific surface area*
20 a_s *specific surface area*
21
22 A_s area of surface or interface (See: *surface excess concentration*)
23 D *areic dose*
24
25 D_{imp} *implanted areic dose*
26 E_{VAC} *vacuum level*
27
28 $E_{VAC}(\infty)$ *vacuum level at infinity*
29 G *areic dose rate*
30
31 I_{av} *average beam current*
32 $I_i(\theta)$ *theoretical scattered-ion intensity*
33
34 k *wave vector in X-ray reflectrometry*
35 K *kinematic factor*
36
37 n^{σ} *surface excess*
38 q *scattering vector in X-ray reflectrometry*
39
40 Q *scattering vector in X-ray reflectrometry*
41 r *backscattering fraction*
42
43 R *backscattering correction factor*
44 R *reflectance*
45
46 s *specific surface area*
47 $S(E)$ *stopping cross section*
48
49 T *transmittance*
50 W *work function*
51
52 W *thermionic work function*
53
54
55 AES *Auger spectroscopy*
56 AMRSF *average matrix relative sensitivity factor*
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58 APECS *Auger photoelectron coincidence spectroscopy*
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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*

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1
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4 *microscopy*)
5 PADI *plasma assisted desorption ionization*
6
7 PERSF *pure-element relative sensitivity factor*
8 PIXE *particle-induced X-ray emission analysis*
9
10 MEIS(S) *medium-energy ion scattering spectrometry*
11 NEXAFS Near-edge extended X-ray absorption fine structure spectroscopy (See: *X-*
12
13 *ray absorption near-edge spectroscopy*)
14 RAIRS *reflection-absorption infrared spectroscopy*
15
16 RBS *Rutherford backscattering spectrometry*
17 REELS *reflection electron energy loss spectroscopy*
18
19 RISR *relative instrument spectral response function*
20 SALDI *surface-assisted laser desorption/ionization*
21
22 SAM *self-assembled monolayer*
23 SDP *sputter depth profile*
24
25 SEIRAS *surface-enhanced infrared spectroscopy*
26 SERS *surface-enhanced Raman spectroscopy*
27
28 SERRS *surface-enhanced resonant Raman spectroscopy*
29 SEXAFS *surface extended X-ray absorption fine structure spectroscopy*
30
31 SFGS *sum frequency generation spectroscopy*
32 SHG *second harmonic generation*
33
34 SIMS *secondary-ion mass spectrometry*
35 SNOM *scanning near-field optical microscopy*
36
37 SRXAS synchrotron radiation small-angle X-ray scattering (See: *small-angle X-*
38 *ray scattering*)
39
40 SSIMS *static secondary-ion mass spectrometry*
41 TDC time-to-digital converter (See: *stop event*)
42
43 TERS *tip enhanced Raman spectroscopy*
44 TOF *time-of-flight*
45
46 TXRF *total reflection X-ray fluorescence spectroscopy*
47 UPS *ultraviolet photoelectron spectroscopy*
48
49 VSFS vibrational sum frequency spectroscopy (See: *sum frequency generation*
50 *spectroscopy*)
51
52 WAXS wide-angle X-ray scattering (See: *small-angle X-ray scattering*)
53 XAFS *X-ray absorption fine structure spectroscopy*
54
55 XANES *X-ray absorption near-edge spectroscopy*
56 XPS *X-ray photoelectron spectroscopy*
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58 XRR *X-ray reflectometry*
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XSW *X-ray standing waves*

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