
**Surface chemical analysis —
Vocabulary —**

**Part 1:
General terms and terms used in
spectroscopy**

iTeh STANDARD PREVIEW
Analyse chimique des surfaces — Vocabulaire —
(standards.iteh.ai) Partie 1: Termes généraux et termes utilisés en spectroscopie

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ISO copyright office
Case postale 56 • CH-1211 Geneva 20
Tel. + 41 22 749 01 11
Fax + 41 22 749 09 47
E-mail copyright@iso.org
Web www.iso.org

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Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

Attention is drawn to the possibility that some of the elements of this document may be the subject of patent rights. ISO shall not be held responsible for identifying any or all such patent rights. Details of any patent rights identified during the development of the document will be in the Introduction and/or on the ISO list of patent declarations received (see www.iso.org/patents).

Any trade name used in this document is information given for the convenience of users and does not constitute an endorsement.

For an explanation on the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the WTO principles in the Technical Barriers to Trade (TBT) see the following URL: Foreword - Supplementary information

The committee responsible for this document is ISO/TC 201, *Surface chemical analysis*, Subcommittee SC 1, *Terminology*.

This second edition cancels and replaces the first edition (ISO 18115-1:2010), which has been technically revised.

ISO 18115 consists of the following parts, under the general title *Surface chemical analysis — Vocabulary*:

- *Part 1: General terms and terms used in spectroscopy*
- *Part 2: Terms used in scanning-probe microscopy*

Introduction

Surface chemical analysis is an important area which involves interactions between people with different backgrounds and from different fields. Those conducting surface chemical analysis might be materials scientists, chemists, or physicists and might have a background that is primarily experimental or primarily theoretical. Those making use of the surface chemical data extend beyond this group into other disciplines.

With the present techniques of surface chemical analysis, compositional information is obtained for regions close to a surface (generally within 20 nm) and composition-versus-depth information is obtained with surface analytical techniques as surface layers are removed. The surface analytical terms covered in this part of ISO 18115 extend from the techniques of electron spectroscopy and mass spectrometry to optical spectrometry and X-ray analysis. The terms covered in ISO 18115-2 relate to scanning-probe microscopy. Concepts for these techniques derive from disciplines as widely ranging as nuclear physics and radiation science to physical chemistry and optics.

The wide range of disciplines and the individualities of national usages have led to different meanings being attributed to particular terms and, again, different terms being used to describe the same concept. To avoid the consequent misunderstandings and to facilitate the exchange of information, it is essential to clarify the concepts, to establish the correct terms for use, and to establish their definitions.

The terms and definitions in this International Standard have been prepared in conformance with the principles and style defined in ISO 1087-1:2000 and ISO 10241:1992. Essential aspects of these standards appear in 2.1 to 2.3. This part of ISO 18115 comprises the 78 abbreviations and 590 definitions of the combined ISO 18115-1:2010 and Amendment 1 to ISO 18115-1:2010. Corrections have been made to terms 4.61, backscattering factor, and 4.480, unified atomic mass unit that appeared in ISO 18115-1:2010.

The terms are given in alphabetical order, classified under [Clauses 3](#), [4](#), and [5](#) from the former International Standard with corrections and [Clauses 6](#), [7](#), and [8](#) from Amendment 1:

- [Clause 3](#): Definitions of the surface analysis methods;
- [Clause 4](#): Definitions of terms for surface analysis;
- [Clause 5](#): Definitions of terms for multivariate analysis;
- [Clause 6](#): Definitions of supplementary terms for the surface analysis methods;
- [Clause 7](#): Definitions of supplementary terms for surface analysis;
- [Clause 8](#): Definitions of supplementary terms for multivariate analysis.

Additional terms, important for surface analysis, are given in an extract from IEC 60050-111 in [Annex A](#).

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Surface chemical analysis — Vocabulary —

Part 1: General terms and terms used in spectroscopy

0 Scope

This part of ISO 18115 defines terms for surface chemical analysis. It covers general terms and those used in spectroscopy while ISO 18115-2 covers terms used in scanning-probe microscopy.

1 Abbreviated terms

AC	alternating current
AES	Auger electron spectroscopy
AMRSF	average matrix relative sensitivity factor
ANN	artificial neural network
APECS	Auger photoelectron coincidence spectroscopy
ARAES	angle-resolved Auger electron spectroscopy
AREPES	angle-resolved elastic peak electron spectroscopy
ARXPS	angle-resolved X-ray photoelectron spectroscopy
CDP	compositional depth profile
CRM	certified reference material
DA/DFA	discriminant analysis/discriminant function analysis
DAPCI	desorption atmospheric pressure chemical ionization
DAPPI	desorption atmospheric pressure photoionization
DART	direct analysis in real time
DC	direct current
DESI	desorption electrospray ionization
DRS	direct recoil spectroscopy
eV	electron volts
EELS	electron energy loss spectroscopy
EESI	extractive electrospray ionization
EIA	energetic-ion analysis
ELDI	electrospray enhanced laser desorption mass spectrometry

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EPES	elastic peak electron spectroscopy
EPMA	electron probe microanalysis
ERD	elastic recoil detection
ERDA	elastic recoil detection analysis
ESCA	electron spectroscopy for chemical analysis
EXAFS	extended X-ray absorption fine structure spectroscopy
FABMS	fast atom bombardment mass spectrometry
FIB	focused ion beam system
FWHM	full width at half maximum
GDMS	glow discharge mass spectrometry
GDOES	glow discharge optical emission spectrometry
GDS	glow discharge spectrometry
GISAXS	grazing-incidence small-angle X-ray scattering
HSA	hemispherical sector analyser
IBA	ion beam analysis
ISS	ion-scattering spectrometry
LAESI	laser ablation electrospray ionization
LB	Langmuir-Blodgett
LDI	laser desorption ionization
LEIS(S)	low-energy ion scattering spectrometry
LMIG	liquid-metal ion gun
LMIS	liquid-metal ion source
MAF analysis	maximum autocorrelation factor analysis
MALDI	matrix-assisted laser desorption/ionization mass spectrometry
MALDESI	matrix-assisted laser desorption electrospray ionization
MCR	multivariate curve resolution
MEIS(S)	medium-energy ion scattering spectrometry
MVA	multivariate analysis
NEXAFS	near-edge extended X-ray absorption fine structure spectroscopy
PADI	plasma-assisted desorption ionization
PCA	principal-component analysis
PERSF	pure-element relative sensitivity factor

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PIXE	particle-induced X-ray emission
PLS	partial least squares
RBS	Rutherford backscattering spectrometry
REELS	reflection electron energy loss spectroscopy
RISR	relative instrument spectral response function
rf	radio-frequency
RM	reference material
RSF	relative sensitivity factor
SALDI	surface-assisted laser desorption/ionization
SAM	self-assembled monolayer
SAXS	small-angle X-ray scattering
SDP	sputter depth profile
SEM	scanning electron microscope
SEP	surface excitation parameter
SEXAFS	surface extended X-ray absorption fine structure spectroscopy
SIMS	secondary-ion mass spectrometry
SNMS	sputtered neutral mass spectrometry
SSA	spherical sector analyser
TOF or ToF	time of flight
TXRF	total-reflection X-ray fluorescence spectroscopy
UPS	ultraviolet photoelectron spectroscopy
XAFS	X-ray absorption fine structure spectroscopy
XANES	X-ray absorption near-edge spectroscopy
XPS	X-ray photoelectron spectroscopy
XRR	X-ray reflectometry
XSW	X-ray standing waves

2 Format

2.1 Use of terms printed *italic* in definitions

A term printed in *italics* in a definition or a note is defined in another entry in this part of ISO 18115. However, the term is printed in *italics* only the first time it occurs in each entry.

2.2 Non-preferred and deprecated terms

A term listed lightface is non-preferred or deprecated. The preferred term is listed boldface.

2.3 Subject fields

Where a term designates several concepts, it is necessary to indicate the subject field to which each concept belongs. The field is shown lightface, between angle brackets, preceding the definition, on the same line.

3 Definitions of the surface analysis methods

3.1

Auger electron spectroscopy

AES

method in which an *electron spectrometer* (4.190) is used to measure the energy distribution of *Auger electrons* (4.37) emitted from a *surface* (4.458)

Note 1 to entry: 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* (4.211) but, where an electron beam is used, the reference can either be the Fermi level or the *vacuum level* (4.483). Spectra, conventionally, can be presented in the *direct* (4.173) or *differential* (4.171) forms.

3.2

desorption electrospray ionization

DESI

method in which a mass spectrometer is used to measure the mass-to-charge quotient 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 to entry: 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 to entry: DESI is one of the few surface analysis methods designed to analyse materials without exposure to vacuum. It is used for complex molecules, organic molecules, and biomolecules. *In vivo* analysis is claimed to be possible.

3.3

dynamic SIMS

SIMS (3.17) in which the material *surface* (4.458) is sputtered at a sufficiently rapid rate that the original surface cannot be regarded as undamaged during the analysis

Note 1 to entry: Dynamic SIMS is often simply termed SIMS.

Note 2 to entry: The ion *areic dose* (4.175) during measurement is usually more than 10^{16} ions/m².

3.4

elastic peak electron spectroscopy

EPES

method in which an *electron spectrometer* (4.190) is used to measure the energy, intensity, and/or energy broadening distribution of quasi-elastically scattered electrons from a solid or liquid *surface* (4.458)

Note 1 to entry: See *recoil effect* (4.366) and *reflection electron energy loss spectroscopy (REELS)* (3.16).

Note 2 to entry: An electron beam in the energy range 100 eV to 3 keV is often used for this kind of spectroscopy.

Note 3 to entry: In general, electron sources with energy spreads that are less than 1 eV are required to provide adequate information.

Note 4 to entry: EPES is often an auxiliary method of *AES* (3.1) and *REELS* (3.16), providing information on the composition of the surface layer. EPES is suitable for the experimental determination of the *inelastic mean free path* (4.243), the electron *differential elastic scattering cross section* (4.127), and the *surface excitation parameter* (4.461).

3.5

DEPRECATED: electron spectroscopy for chemical analysis
 DEPRECATED: ESCA
 method encompassing both *AES* (3.1) and *XPS* (3.23)

Note 1 to entry: The term ESCA has fallen out of use as, in practice, it was only used to describe situations more clearly defined by the term X-ray photoelectron spectroscopy (XPS). Since 1980, the latter term has been preferred.

3.6**fast atom bombardment mass spectrometry****FABMS**

DEPRECATED: FAB

method in which a mass spectrometer is used to measure the mass-to-charge quotient and abundance of *secondary ions* (4.406) emitted from a sample as a result of the bombardment by fast neutral atoms

3.7**G-SIMS**

variant of *static SIMS* (3.20) 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 to entry: As with static SIMS, the ion *areic dose* (4.175) during measurement is restricted to less than 10^{16} ions/m² to an extent that depends on both the material of the sample and the size of the *molecular fragments* (4.302) being analysed.

Note 2 to entry: The G-SIMS spectrum enables the mass of whole molecules on the *surface* (4.458) to be determined more readily than in static SIMS.

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

3.8**glow discharge mass spectrometry****GDMS**

method in which a mass spectrometer is used to measure the mass-to-charge quotient and abundance of ions from a *glow discharge* (4.228) generated at a *surface* (4.458)

3.9**glow discharge optical emission spectrometry****GDOES**

method in which an optical emission spectrometer is used to measure the wavelength and intensity of light emitted from a *glow discharge* (4.228) generated at a *surface* (4.458)

3.10**glow discharge spectrometry****GDS**

method in which a spectrometer is used to measure relevant intensities emitted from a *glow discharge* (4.228) generated at a *surface* (4.458)

Note 1 to entry: This is a general term that encompasses *GDOES* (3.9) and *GDMS* (3.8).

3.11**ion beam analysis****IBA**

method designed to elucidate composition and structure of the near-surface atomic layers of a solid material, in which principally monoenergetic, singly charged *probe ions* (4.349) scattered from the *surface* (4.458) are detected and recorded as a function of their energy or *angle of scattering* (4.18), or both

Note 1 to entry: *LEIS(S)* (3.12), *MEIS(S)* (3.13), and *RBS* (3.15) 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.

3.12

low-energy ion scattering spectrometry

LEIS(S)

method designed to elucidate composition and structure of the very outermost atomic layers of a solid material, in which principally monoenergetic, singly charged *probe ions* (4.349) scattered from the *surface* (4.458) are detected and recorded as a function of their energy or *angle of scattering* (4.18), or both

Note 1 to entry: LEIS(S) is a form of *IBA* (3.11) in which the probe ions, typically He or Ne, have energies in the range 0,1 keV to 10 keV.

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

3.13

medium-energy ion scattering spectrometry

MEIS(S)

method designed to elucidate composition and structure of the outermost atomic layers of a solid material, in which principally monoenergetic, singly charged *probe ions* (4.349) scattered from the *surface* (4.458) are detected and recorded as a function of their energy or *angle of scattering* (4.18), or both

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

Note 2 to entry: By using *channelling* (4.94) 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 to entry: In some cases, an angle-sensitive detector is used that allows extensive structure and *depth profile* (4.350) information to be obtained.

Note 4 to entry: The acronym usually has only one "S".
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3.14

matrix-assisted laser desorption/ionization mass spectrometry

MALDI

method in which a *time of flight* (4.473) mass spectrometer is used to measure the *mass-to-charge ratio* (4.296) and abundance of ions emitted, as a result of a short pulse of laser illumination, from a sample whose analyte is contained in an ion-assisting matrix

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

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

3.15

Rutherford backscattering spectrometry

RBS

method designed to elucidate composition and structure of layers at the *surface* (4.458) of a solid material, in which principally monoenergetic, singly charged *probe ions* (4.349) scattered from the surface with a *Rutherford cross section* (4.133) are detected and recorded as a function of their energy or *angle of scattering* (4.18), or both

Note 1 to entry: RBS is a form of *IBA* (3.11) 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 to entry: By using *channelling* (4.94) 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.

3.16 reflection electron energy loss spectroscopy REELS

method in which an *electron spectrometer* (4.190) 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* (4.197)

Note 1 to entry: See *elastic peak electron spectroscopy* (3.4) (EPES)

3.17 secondary-ion mass spectrometry SIMS

method in which a mass spectrometer is used to measure the mass-to-charge quotient and abundance of *secondary ions* (4.406) emitted from a sample as a result of bombardment by energetic ions

Note 1 to entry: See *dynamic SIMS* (3.3), *static SIMS* (3.20), and *G-SIMS* (3.7).

Note 2 to entry: 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* (4.175) during measurement is restricted to less than 10^{16} ions/m² in order to retain the *surface* (4.458) in an essentially undamaged state.

3.18 small-angle X-ray scattering SAXS

method in which the elastically scattered intensity of X-rays is measured for small-angle deflections

Note 1 to entry: The angular scattering is usually measured within the range $0,1^\circ$ 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 to entry: 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 to entry: The X-ray source can be a synchrotron, in which case the term *synchrotron radiation* (4.465) small-angle X-ray scattering (SRXAS) is occasionally encountered.

3.19 sputtered neutral mass spectrometry SNMS

method in which a mass spectrometer is used to measure the mass-to-charge quotient and abundance of secondary ionized neutral species emitted from a sample as a result of particle bombardment

Note 1 to entry: The neutral species can be detected by using *plasma* (4.337), electron, or photon-ionization methods.

3.20 static SIMS

SIMS (3.17) in which the material *surface* (4.458) is sputtered at a sufficiently low rate that the original surface is insignificantly damaged during the analysis

Note 1 to entry: See dynamic *SIMS* (3.3).

Note 2 to entry: The ion *areic dose* (4.175) during measurement is restricted to less than 10^{16} ions/m² to an extent that depends on both the material of the sample and the size of the *molecular fragments* (4.302) being analysed.

3.21 total reflection X-ray fluorescence spectroscopy TXRF

method in which an X-ray spectrometer is used to measure the energy distribution of *fluorescence* (4.219) X-rays emitted from a *surface* (4.458) irradiated by primary X-rays under the condition of *total reflection* (4.475)

3.22

ultraviolet photoelectron spectroscopy

UPS

method in which an *electron spectrometer* (4.190) is used to measure the energy distribution of photoelectrons emitted from a *surface* (4.458) irradiated by ultraviolet photons

Note 1 to entry: 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* (4.465) is used.

3.23

X-ray photoelectron spectroscopy

XPS

method in which an *electron spectrometer* (4.190) is used to measure the energy distribution of photoelectrons and *Auger electrons* (4.37) emitted from a *surface* (4.458) irradiated by X-ray photons

Note 1 to entry: X-ray sources in common use are unmonochromated Al K α and Mg K α X-rays at 1 486,6 eV, and 1 253,6 eV, respectively. Modern instruments also use monochromated Al K α X-rays. Some instruments make use of various X-ray sources with other *anodes* (4.27) or of *synchrotron radiation* (4.465).

4 Definitions of terms for surface analysis

4.1

absorption coefficient, linear

linear **attenuation coefficient**

4.2

absorption coefficient, mass

attenuation coefficient, mass

<TXRF, XPS> quantity μ/ρ in the expression, $(\mu/\rho)\Delta(\rho x)$, for the fraction of a parallel beam of specified particles or radiation removed in passing through a thin layer of mass thickness $\Delta(\rho x)$ of a substance in the limit as $\Delta(\rho x)$ approaches zero, where $\Delta(\rho x)$ is measured in the direction of the beam

Note 1 to entry: See *attenuation length* (4.34).

Note 2 to entry: The mass density of the substance is ρ and x is the distance in the direction of the beam.

Note 3 to entry: The intensity or number of particles in the beam decays as $\exp(-\mu x)$ with the distance x .

Note 4 to entry: The mass attenuation (absorption) coefficient is the quotient of the linear attenuation (absorption) coefficient by the mass density of the substance.

4.3

abundance sensitivity

<GDMS> ratio of the maximum ion current recorded at a mass m to the ion current arising from the same species recorded at an adjacent mass ($m \pm 1$)

[SOURCE: IUPAC]

4.4

adventitious carbon referencing

<XPS> determining the *charging potential* (4.103) of a particular sample from a comparison of the experimentally determined C 1s *binding energy* (4.82), arising from adsorbed hydrocarbons on the sample, with a standard binding energy value

Note 1 to entry: See *Fermi level referencing* (4.212) and *internal carbon referencing* (4.257).

Note 2 to entry: 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* (4.103) since the true binding energy of the adsorbed hydrocarbons is not known.

Note 3 to entry: Different *sample charging* (4.392) potentials can occur on different areas on the *surface* (4.458), or at different depths, arising, for example, from sample inhomogeneities or non-uniform intensity of the incident-radiation *flux* (4.221).

4.5 afterglow

<GDS> luminescence of the decaying *plasma* (4.337) present in a *glow discharge* (4.228) device after complete cessation of the sustaining discharge power

4.6 altered layer

<particle bombardment> 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 to entry: For silicon bombarded by 4 keV O₂⁺ at near-normal incidence, after *sputtering* (4.441) for a sufficient time to reach a steady state, the *surface* (4.458) is converted to stoichiometric SiO₂ 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* (4.352).

Note 2 to entry: The *depth resolution* (4.164) in *SIMS* (3.17) can be greater or smaller than the altered-layer thickness, depending on the analyte and bombarding-ion species.

4.7 analyser blanking

<SIMS> action to prevent *secondary ions* (4.406) from travelling through the mass spectrometer and being detected

Note 1 to entry: This action is usually made by pulsing one of the relevant electrode potentials in *time of flight* (4.473) mass spectrometers to deflections of a selected mass range in which intense peaks occur, so that those masses are not detected and thus do not cause unwanted detector saturation.

4.8 analysis area

<sample> two-dimensional region of a sample *surface* (4.458) measured in the plane of that surface from which the entire analytical signal or a specified percentage of that signal is detected

4.9 analysis area

<spectrometer> two-dimensional region of a sample *surface* (4.458) 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 percentage of that signal is detected

4.10 analysis volume

<sample> three-dimensional region of a sample from which the entire analysis signal or a specified percentage of that signal is detected

4.11 analysis volume

<spectrometer> three-dimensional region within the spectrometer from which the entire analytical signal or a specified percentage of that signal can be detected

4.12 angle, critical

<TXRF> *glancing angle* (4.13) at which the sample matrix X-ray *fluorescence* (4.219), when plotted against the glancing angle, is at the first point of inflection

4.13 angle, glancing

angle between the incident beam and the average surface plane

Note 1 to entry: The *angle of incidence* (4.17) and the glancing angle are complementary.