

BS ISO 18115-1:2013



BSI Standards Publication

Surface chemical analysis — Vocabulary

Part 1: General terms and terms used in
spectroscopy

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National foreword

This British Standard is the UK implementation of ISO 18115-1:2013. It supersedes BS ISO 18115-1:2010 which is withdrawn.

The UK participation in its preparation was entrusted to Technical Committee CII/60, Surface chemical analysis.

A list of organizations represented on this committee can be obtained on request to its secretary.

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**Surface chemical analysis —
Vocabulary —**

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

Analyse chimique des surfaces — Vocabulaire —

Partie 1: Termes généraux et termes utilisés en spectroscopie



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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](#).

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

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

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”.

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° 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 deflect ions of a selected mass range in which intense peaks occur, so that those masses are not detected and thus do not cause unwanted detector saturation.

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.

4.14

angle lapping

sample preparation in which a sample is mechanically polished at an angle to the original *surface* ([4.458](#))

Note 1 to entry: See *ball catering* ([4.64](#)) and *radial sectioning* ([4.358](#)).

Note 2 to entry: This angle can often be less than 1° so that depth information with respect to the original surface is transformed to lateral information.

4.15

angle, magic

<XPS> angle at which the spectrometer entrance axis is aligned at 54,7° to the direction of the X-rays at the sample *surface* ([4.458](#))

Note 1 to entry: 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.

4.16

angle of emission

emission angle

angle between the trajectory of a particle or photon as it leaves a *surface* ([4.458](#)), and the local or average surface normal

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

4.17

angle of incidence

incidence angle

angle between the incident beam and the local or average surface normal

Note 1 to entry: The particular surface normal, such as the surface normal to an elementary portion of a rough *surface* ([4.458](#)) or the normal to the average surface plane, needs to be specified.

4.18

angle of scattering

scattering angle

angle between the direction of the incident particle or photon and the direction that the particle or photon is travelling after scattering

4.19

angle-resolved AES

ARAES

angle-dependent AES

procedure in which *Auger electron* ([4.37](#)) intensities are measured as a function of the *angle of emission* ([4.16](#))

4.20

angle-resolved EPES

AREPES

<EPES> method involving *EPES* ([3.4](#)) measurements as a function of the *scattering angle* ([4.18](#))

4.21

angle-resolved XPS

ARXPS

angle-dependent XPS

procedure in which X-ray photoelectron intensities are measured as a function of the *angle of emission* ([4.16](#))

Note 1 to entry: This procedure is often used to obtain information on the distribution with depth of different elements or compounds in a layer approximately 5 nm thick at the *surface* ([4.458](#)).

4.22

angle, solid, of analyser

solid angle of analyser that will transmit particles or photons from a point on the sample to the detector

Note 1 to entry: See *analyser transmission function* ([4.434](#)).

4.23

angle, solid, of detector

<EIA, RBS> solid angle intercepted by the detector from an origin at the centre of the beam spot

4.24

angle, take-off

angle between the trajectory of a particle as it leaves a *surface* ([4.458](#)) and the local or average surface plane

Note 1 to entry: The particular surface plane needs to be specified.

Note 2 to entry: The take-off angle is the complement of the *angle of emission* ([4.16](#)).

Note 3 to entry: In the past, take-off angle has sometimes been used erroneously to mean angle of emission.

4.25

anion

negatively charged ion

Note 1 to entry: See *cation* ([4.92](#)).

4.26

anode

<GDS, DC operation> more positively charged electrode in a *glow discharge* ([4.228](#)) device

Note 1 to entry: See *cathode* ([4.88](#)) <GDS, DC operation>.

4.27

anode

<GDS, rf operation> electrode that is more positively charged over a large fraction of the rf cycle in a radio-frequency-powered *glow discharge* ([4.228](#)) device

Note 1 to entry: See *cathode* ([4.89](#)) <GDS, rf operation>.

Note 2 to entry: The rf power applied to a typical rf glow discharge device that is used for surface chemical analysis is sinusoidal and bipolar, with a time-averaged electric potential of zero relative to ground potential. The reason that the anode is not more positively charged over the entire rf cycle is that the magnitude of the *DC bias* ([4.145](#)) is usually slightly less than one-half of the applied rf peak-to-peak potential.

Note 3 to entry: The precise fraction of the rf cycle over which the anode is more positively charged depends upon the source geometry and other factors.

4.28

anode glow

<GDS> thin luminous region of a *glow discharge* ([4.228](#)) immediately adjacent to the *anode* ([4.27](#))

Note 1 to entry: See *cathode layer* ([4.91](#)), *negative glow* ([4.314](#)), and *positive column* ([4.342](#)).

Note 2 to entry: The anode glow may not be noticeable in a glow discharge used for surface chemical analysis.

4.29

aperture, contrast

aperture, in an ion or electron optical system, designed to reduce unwanted *background signal* ([4.56](#))

Note 1 to entry: This aperture can also govern the spatial resolution and other properties of the system.

4.30 asymmetry parameter

β

<XPS> factor (5.5) which characterizes the intensity distribution, $L(\gamma)$, of photoelectrons ejected by unpolarized X-rays from isolated atoms in a direction γ from the incident X-ray direction in accordance with

$$L(\gamma) = 1 + \frac{1}{2}\beta \left[\frac{3}{2}(\sin^2 \gamma) - 1 \right]$$

Note 1 to entry: This formula relates to gases and is modified by the effects of *elastic scattering* (4.80) when applied to solids. At the *magic angle* (4.15), $L(\gamma) = 1$.

4.31 DEPRECATED: atomic mass unit

see Note 3 to “*unified atomic mass unit* (4.480)”

Note 1 to entry: See *unified atomic mass unit* (4.480).

4.32 atomic mixing

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

Note 1 to entry: See *cascade mixing* (4.87), *collision cascade* (4.114), *ion-beam-induced mass transport* (4.260), *knock-on* (4.279), and *recoil implantation* (4.279).

4.33 attenuation coefficient

quantity μ in the expression $\mu\Delta x$ for the fraction of a parallel beam of specified particles or radiation removed in passing through a thin layer Δx of a substance in the limit as Δx approaches zero, where Δx is measured in the direction of the beam

Note 1 to entry: See *attenuation length* (4.34) and *mass absorption coefficient* (4.2).

Note 2 to entry: The intensity or number of particles in the beam decays as $\exp(-\mu/x)$ with the distance x .

Note 3 to entry: Attenuation coefficient is often used in place of *linear attenuation coefficient* (4.1) and is used in EPMA. Both are the reciprocal of *attenuation length* (4.34) which is used in AES (3.1) and XPS (3.23).

4.34 attenuation length

quantity l in the expression $\Delta x/l$ for the fraction of a parallel beam of specified particles or radiation removed in passing through a thin layer Δx of a substance in the limit as Δx approaches zero, where Δx is measured in the direction of the beam

Note 1 to entry: See *attenuation coefficient* (4.33), *decay length* (4.150), *effective attenuation length* (4.35), *electroninelastic mean free path* (4.243), *linear absorption coefficient* (4.1), and *mass absorption coefficient* (4.2).

Note 2 to entry: The intensity or number of particles in the beam decays as $\exp(-x/l)$ with the distance x .

Note 3 to entry: For electrons in solids, the behaviour only approximates to an exponential decay due to the effects of *elastic scattering* (4.80). Nevertheless, for some measurement conditions in AES (3.1) and XPS (3.23), the *signal intensity* (4.252) can depend approximately exponentially on path length, but the exponential constant (the parameter l) will then normally be different from the corresponding inelastic mean free path. Where that approximation is valid, the term *effective attenuation length* is used.

4.35 attenuation length, effective

<AES, XPS> parameter which, when introduced in place of the *inelastic mean free path* (4.243) into an expression derived for AES (3.1) and XPS (3.23) on the assumption that *elastic scattering* (4.80) effects are negligible for a given quantitative application, will correct that expression for elastic scattering effects

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

Note 2 to entry: 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* (4.16). 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 larger emission angles, the effective attenuation length can depend on this angle.

Note 3 to entry: 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).

4.36

Auger de-excitation

process in which the excess energy of an excited atom or ion is given up by the *Auger process* (4.44)

Note 1 to entry: See *Auger neutralization* (4.40).

Note 2 to entry: The Auger process can involve energy levels in neighbouring atoms and lead to ejection of an electron into the vacuum. This electron's energy can then usefully be characteristic of a surface atom with which a metastable probe atom (e.g. He) is in close proximity.

4.37

Auger electron

electron emitted from atoms in the *Auger process* (4.44)

Note 1 to entry: See *Auger transition* (4.46).

Note 2 to entry: Auger electrons can lose energy by *inelastic scattering* (4.244) as they pass through matter. Measured Auger electron spectra are therefore generally composed of a peak structure of unscattered Auger electrons superimposed on a background of inelastically scattered Auger electrons with intensities extending to lower kinetic energies, and on backgrounds arising from other processes.

Note 3 to entry: Auger electrons can change their direction of propagation by *elastic scattering* (4.80) as they pass through matter.

4.38

Auger electron spectrum

plot of the *Auger electron* (4.37) intensity as a function of the electron *kinetic energy* (4.278), usually as part of the energy distribution of detected electrons

Note 1 to entry: When excited by incident electrons, the energy distribution of detected electrons, often measured between 0 eV and 2 500 eV, contains Auger electrons, *backscattered* (primary) *electrons* (4.58) and *secondary electrons* (4.402). The entire distribution is sometimes referred to as an Auger electron spectrum.

Note 2 to entry: The Auger electron spectrum can be presented in either the *direct spectrum* (4.173) or *differential spectrum* (4.171) formats.

4.39

Auger electron yield

probability that an atom with a vacancy in a particular inner shell will relax by an *Auger process* (4.44)

[SOURCE: ASTM E673-03]

4.40

Auger neutralization

<ion at a surface> 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 to entry: The ejected electron can be emitted into the vacuum.

4.41

Auger parameter

<XPS> *kinetic energy* (4.278) of a narrow *Auger electron* (4.37) peak in a spectrum minus the kinetic energy of the most intense photoelectron peak from the same element

Note 1 to entry: See initial-state *Auger parameter* (4.42) and *modified Auger parameter* (4.43).

Note 2 to entry: The value of the Auger parameter depends on the energy of the X-rays, which therefore needs to be specified.

Note 3 to entry: The Auger parameter is sometimes called the *final state* (4.215) Auger parameter.

Note 4 to entry: The Auger parameter is useful for separating chemical states for samples in which charging causes uncertainty in the *binding energy* (4.82) measurement or in which the binding energy shift is inadequate to identify the chemical state.

Note 5 to entry: The Auger parameter is useful for evaluating the *relaxation energy* (4.380) of the ionized matrix atom associated with the generation of a core *hole* (4.237) for those *Auger transitions* (4.46) between core levels which have similar *chemical shifts* (4.105).

4.42

Auger parameter, initial-state

<XPS> β , where $\beta = 3E_B + E_K$ and where E_B and E_K are, respectively, the *binding energy* (4.82) of a photoelectron peak and the *Fermi level* (4.211) referenced *kinetic energy* (4.278) of an *Auger electron* (4.37) peak, each involving the same initial core level of the same element

Note 1 to entry: See *Auger parameter* (4.41) and *Auger parameter, modified* (4.43).

Note 2 to entry: 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* (4.46) is between core levels that have similar binding energy shifts.

Note 3 to entry: This parameter has no relation to the *asymmetry parameter* (4.30) which is also given the symbol β .

4.43

Auger parameter, modified

<XPS> sum of the *Fermi level* (4.211) referenced *kinetic energy* (4.278) of a narrow *Auger electron* (4.37) peak in the spectrum and the *binding energy* (4.82) of the most intense photoelectron peak from the same element

Note 1 to entry: See *Auger parameter* (4.41) and *initial-state Auger parameter* (4.42).

Note 2 to entry: 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.

4.44

Auger process

relaxation (4.378), by electron emission, of an atom with a vacancy in an inner electron shell

[SOURCE: ASTM E673-03]

Note 1 to entry: See *Auger de-excitation* (4.36), *Auger electron* (4.37), and *Auger transition* (4.46).

Note 2 to entry: The emitted electrons have characteristic energies, defined by the *Auger transition* (4.46).

4.45

Auger process, interatomic

Auger transition (4.46) 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

4.46**Auger transition**

Auger process (4.44) involving designated electron shells or sub-shells

Note 1 to entry: The three shells involved in the Auger process are designated by three letters. The first letter designates the shell containing the initial vacancy and the last two letters designate the shells containing electron vacancies left by the Auger process (for example, KLL or LMN). When a valence electron is involved, the letter V is used (for example, LMV or KVV). When a particular sub-shell involved is known, this can also be indicated (for example, KL₁L₂). Coupling terms can also be added, where known, to indicate the final atomic state (for example, L₃M_{4,5}M_{4,5}¹D).

Note 2 to entry: More complicated Auger processes (such as multiple initial ionizations and additional electronic excitations) can be designated by separating the initial and *final states* (4.215) by a hyphen (for example, LL-VV, or K-VVV).

Note 3 to entry: When an Auger process involves an electron from the same principal shell as the initial vacancy (for example, L₁L₂M), it is referred to as a *Coster-Kronig transition* (4.119). If all electrons are from the same principal shell (for example, M₁M₂M₃) the process is called a *superCoster-Kronig transition* (4.457).

4.47**Auger transition rate**

quotient of the probability for an *Auger process* (4.44) by time

4.48**Auger vacancy satellite**

Auger transition (4.46) in which additional *spectator holes* (4.429) are present in the *initial state* (4.248, 4.249) or the *final state* (4.215) for the transition

4.49**background equivalent concentration**

<GDS> concentration of an element in a sample that would produce, in the absence of the background, a *signal intensity* (4.252) equivalent to the measured background intensity

Note 1 to entry: In *GDS* (3.10), results are often expressed in mass fractions and so the background equivalent concentration is usually expressed in these units.

4.50**background, inelastic**

intensity distribution in the spectrum for particles originally at one energy but which are emitted at lower energies due to one or more *inelastic scattering* (4.244) processes

Note 1 to entry: See *inelastic electron scattering background subtraction* (4.242), *Shirley background* (4.54), *Sickafus background* (4.55), and *Tougaard background* (4.57).

Note 2 to entry: For *AES* (3.1) and *XPS* (3.23), the inelastic background associated with a particular *Auger electron* (4.37) or photoelectron peak has been approximated by a measured *electron energy loss spectrum* (4.197) for which the incident-electron energy is close to the energy of the peak. The Tougaard background is also used. A simpler, but less accurate, inelastic background function is the Shirley background. Simple linear backgrounds have also been used, but these are much less accurate except for the XPS analysis of insulators.

4.51**background, instrumental**

intensity contribution, generally unwanted, arising from non-ideal behaviour of one or more parts of the instrument

4.52**background, metastable**

<SIMS> intensity in the *mass spectrum* (4.295) arising from ions that spontaneously fragment between emission and detection

Note 1 to entry: In reflectron time-of-flight mass spectrometers, the decay of *metastable ions* (4.300) leads to broad peaks at a mass dependent on the drift energy and *reflector voltage* (4.373). Good design minimizes these *background signals* (4.56).

4.53

background, relative standard deviation of the

quotient of the standard deviation characterizing the *noise* (4.315) in the *background signal* (4.56) by the intensity of the background signal

4.54

background, Shirley

<AES, XPS> background calculated to fit the measured spectrum at points at higher and lower *kinetic energy* (4.278) 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* (4.326) above that background for higher kinetic energies

Note 1 to entry: See *Tougaard background* (4.57).

Note 2 to entry: The fitting to the background can be made by averaging over a given number of energy channels.

4.55

background, Sickafus

<AES, XPS> single-term power law background designed to describe the intensity of the *secondary electron* (4.402) cascade as a function of electron emission *kinetic energy* (4.278)

Note 1 to entry: The measured secondary-electron cascade, for correction application of the Sickafus background, should be the experimentally observed spectrum corrected for the *spectrometer response function* (4.433) of the measuring instrument.

Note 2 to entry: The spectrum shape, for a Sickafus background $B_s(E)$, is given by

$$B_s(E) \propto E^{-m}$$

where E is the electron emission kinetic energy and m is a number in the range 1 to 2.

4.56

background signal

signal present at a particular position, energy, mass or wavelength due to processes or sources other than those of primary interest

Note 1 to entry: See *Shirley background* (4.54), *Sickafus background* (4.55), and *Tougaard background* (4.57).

4.57

background, Tougaard

<AES, XPS> intensity distribution obtained from a model for the differential *inelastic scattering cross section* (4.129) with respect to *energy loss* (4.196) and the three-dimensional distribution of the emitting atoms in the surface region

Note 1 to entry: See *Shirley background* (4.54).

Note 2 to entry: 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 3 to entry: 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* (4.278) than the peaks of interest. The measured spectrum should be corrected for the *spectrometer response function* (4.433) of the measuring instrument before calculation of the Tougaard background.

4.58

backscattered electron

<AES, EELS, EPMA> electron, originating in the incident beam, which is emitted after interaction with the sample

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

Note 2 to entry: By convention, the incident beam is often called the *primary beam* (4.77) and the backscattered electrons are often referred to as the backscattered *primary electrons* (4.346).

4.59

backscattering coefficient

backscattering yield

<EIA, RBS> quotient of the number of detected particles in an interval of *backscattering energy* (4.60) by that interval and by the number of incident ions

4.60

backscattering energy

energy of a particle from the *primary beam* (4.77) after it has undergone a backscattering collision and escaped from the sample

4.61

DEPRECATED: backscattering factor

<AES>*backscattering correction factor* (7.2) or *backscattering fraction* (7.3)

Note 1 to entry: This term, although in common usage, is ambiguous and is replaced by *backscattering correction factor* (7.2) or *backscattering fraction* (7.3). It is deprecated since the two replacement terms, although related, have different values.

4.62

backscattering spectrum

<EIA, RBS> plot of *backscattering yield* (4.59) versus *backscattering energy* (4.60)

[SOURCE: ASTM E673-03]

4.63

backscattering yield

backscattering coefficient

η

<AES, EPMA> ratio of the total number of electrons emitted from the sample with energies greater than 50 eV to the total number of electrons incident at a given energy and *angle of incidence* (4.17)

Note 1 to entry: See *secondary-electron yield* (4.403), *total secondary-electron yield* (4.405), and *backscattering factor* (4.61).

4.64

ball cratering

procedure in which the sample is abraded by a sphere in order to expose compositional changes in layers below the original *surface* (4.458) with the intent that the depth of those layers can be related to the lateral position in the crater created by the abrasion

Note 1 to entry: See *angle lapping* (4.14) and *radial sectioning* (4.358).

4.65

beam blanking

electrostatic or electromagnetic process designed to prevent any *beam particles* (4.76) from impacting the sample

Note 1 to entry: See *beam bunching* (4.66) and *beam chopper* (4.109).

Note 2 to entry: For pulsed *ion beams* (4.259), the beam is usually deflected into a beam collector from which no particles can reach the sample and where the process of *sputtering* (4.441) causes minimal effect on nearby components of the ion optical system. Typically, in time of flight static SIMS systems, a beam of between 0,2 pA and 2 pA might be on for between 0,6 ns and 30 ns and off for around 100 μ s, with 10 000 repetitions per second.

4.66

beam bunching

<SIMS> 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 1 to entry: See *beam blanking* ([4.65](#)) and *beam chopper* ([4.109](#)).

Note 2 to entry: This procedure can degrade the optimum focus of the *ion beam* ([4.259](#)) since different ions experience different fields.

4.67

beam convergence angle

angular interval containing all or a specified fraction of the beam in the space prior to or at the focal plane

Note 1 to entry: See *beam divergence angle* ([4.74](#)).

Note 2 to entry: Where the beam is symmetrical, the full or semi-angle can be used. The particular measure of angle needs to be stated.

4.68

beam current

I

quotient of dQ by dt , where dQ is the quantity of electric charge of a specified polarity in the beam passing in the time interval dt

$$I = dQ / dt$$

Note 1 to entry: See *pulse beam current* ([4.72](#)) and *average beam current* ([4.69](#)).

Note 2 to entry: For beams in which the current varies with time, the instantaneous and time-averaged beam currents will generally differ. For a pulsed beam, the current when the beam is on might or might not be equal to the DC, or unpulsed, beam current.

4.69

beam current, average

quotient of Q by t , where Q is the quantity of electric charge of a specified polarity in the beam passing in the time interval t

Note 1 to entry: For beams in which the instantaneous current varies periodically with time, the time interval t is an integral number of periods.

4.70

beam current density

J

<for a parallel beam of charged particles> quotient of dI by dA , where dI is the element of *beam current* ([4.68](#)) incident on an area dA at right angles to the direction of the beam

$$J = dI / dA$$

Note 1 to entry: See *fluence* ([4.217](#)), *flux* ([4.221](#)), and *dose* ([4.174](#)).

Note 2 to entry: For a convergent or divergent beam, the area dA is replaced by a small sphere of cross-sectional area dA .

4.71

beam current, integrated

total electric charge transported in the beam over a specified time

4.72

beam current, pulse

quotient of Q by t_p where Q is the quantity of electric charge of a specified polarity in the beam passing during the period t_p in which the pulse is on

4.73

beam diameter

<for a particle beam of circular cross section> full width of the beam at half maximum intensity measured in a plane normal to the beam direction

[SOURCE: ASTM E673-03]

Note 1 to entry: The beam diameter is usually specified at a given point in space, such as the position of the sample.

4.74

beam divergence angle

angular interval containing all or a specified fraction of the beam in the space after the focal plane

Note 1 to entry: See *beam convergence angle* (4.67).

Note 2 to entry: Where the beam is symmetrical, the full or semi-angle can be used. The particular measure of angle needs to be stated.

4.75

beam energy

kinetic energy (4.278) of the *beam particles* (4.76)

Note 1 to entry: See *impact energy* (4.195) and *incident particle energy* (4.241).

Note 2 to entry: The energy is usually given in electron volts.

Note 3 to entry: The beam energy is often taken to be the particle energy on impact at the sample *surface* (4.458). However, where a sample is at a potential other than ground, the *impact energy* (4.195) of the particles can differ from the beam energy as delivered by an electron or ion gun to the sample environment. In this case, use of the term impact energy avoids confusion.

4.76

beam particle

electron, positron, ion, atomic, molecular, or cluster species contained in the incident beam

4.77

beam, primary

directed *flux* (4.221) of particles or photons incident on a sample

4.78

beam profile

spatial distribution of the beam *flux* (4.221) in a plane normal to the beam axis

4.79

DEPRECATED: beam source energy

see *beam energy* (4.75)

4.80

binary elastic scattering

elastic scattering

collision between a moving particle and a second particle in which the total *kinetic energy* (4.278) and the total momentum are conserved

Note 1 to entry: See *inelastic scattering* (4.244).

Note 2 to entry: In elastic scattering interactions, the moving particle can be deflected through angles of up to 180°.

4.81

binary elastic scattering peak

<ISS> increase in the spectrometer detection system response above the background level which can be attributed to *binary elastic scattering* (4.80) of an incident ion by a surface atom of a particular mass

[SOURCE: ASTM E673-03]

4.82

binding energy

energy that shall be expended in removing an electron from a given electronic level to the *Fermi level* (4.211) of a solid or to the *vacuum level* (4.483) of a free atom or molecule

4.83

blocking geometry

<EIA, RBS> experimental arrangement wherein the atom rows or planes of a single-crystal *target* (4.466) are aligned parallel to a vector from the sample to the detector

[SOURCE: ASTM E673-03]

4.84

bond cleavage

bond scission

breakage of a molecular bond

Note 1 to entry: This breakage can lead to two fragments that might or might not be charged, or to a single rearranged product.

Note 2 to entry: For α - and β -cleavage, see Reference [2] or [3].

4.85

Bragg's rule

empirical rule formulated by W.H. Bragg and R. Kleeman that states that the *stopping cross section* (4.134) 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, that is,

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

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

[SOURCE: ASTM E673-03, modified]

4.86

bremsstrahlung

<EPMA, XPS> photon radiation emitted from a material due to the deceleration of incident electrons within that material

Note 1 to entry: The bremsstrahlung radiation has a continuous spectral distribution up to the energy of the incident electrons.

Note 2 to entry: In *XPS* (3.23), the bremsstrahlung from a conventional X-ray source with an Al or Mg *anode* (4.27) leads to a continuous photoelectron background. This radiation might also photoionize inner shells, which would be energetically impossible with characteristic Al $K\alpha$ or Mg $K\alpha$ X-rays. As a result, *Auger electron* (4.37) features can appear at negative *binding energy* (4.82) values and, in addition, the intensities of other Auger electron features can be greater than if the inner shell vacancies had been created only by the *characteristic X-rays* (4.96). The bremsstrahlung-excited Auger electron features can be helpful in determining the various *Auger parameters* (4.41) needed to identify chemical states.

4.87

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

Note 1 to entry: See *atomic mixing* (4.32), *collision cascade* (4.114), *knock-on* (4.279), and *recoil implantation* (4.279).

Note 2 to entry: If atomic mixing and knock-on effects are not significant, the measured *sputter depth profile* (4.440) of a *delta layer* (4.158) will be asymmetric on account of cascade mixing since the *surface* (4.458) moves through the sample as it is sputtered. The initial internal profile produced will be Gaussian, however, until significant delta material has been lost through the sample surface.

Note 3 to entry: If cascade mixing is the only significant mixing process, the centroid of the measured distribution will lie at the true delta position (after any shift in the depth scale arising from pre-equilibrium effects has been corrected).

Note 4 to entry: In the *dilute limit* (4.172), the measured *depth profile* (4.350) for the delta layer will have an exponential tail because any internal atom has an equal probability of being moved deeper or shallower and there is thus an indefinitely persistent but decaying concentration in the near-surface region. The presence of this tail often leads to the belief that there is a directional *knock-on* (4.279) process at work. True knock-on effects have rarely if ever been observed, however, and are probably not significant as causes of sputter profile distortion.

4.88

cathode

<GDS, DC operation> more negatively charged electrode in a *glow discharge* (4.228) device

Note 1 to entry: See *anode* (4.26) <GDS, DC operation>.

4.89

cathode

<GDS, rf operation> electrode that is more negatively charged over a large fraction of the rf cycle in a radio-frequency-powered *glow discharge* (4.228) device

Note 1 to entry: See *anode* (4.27) <GDS, rf operation>.

Note 2 to entry: The rf power applied to a typical rf glow discharge device that is used for surface chemical analysis is sinusoidal and bipolar, with a time-averaged electric potential of zero relative to ground potential. The reason that the cathode is not more negatively charged over the entire rf cycle is that the magnitude of the *DC bias* (4.145) is usually slightly less than one-half of the applied rf peak-to-peak potential.

Note 3 to entry: The precise fraction of the rf cycle over which the cathode is more negatively charged depends upon the source geometry and other factors.

4.90

cathode fall

fall potential

DEPRECATED: cathode drop

<GDS> electric potential difference between the *cathode* (4.88), (4.89) surface and the *negative glow* (4.314)

Note 1 to entry: In direct-current *glow discharge spectrometry* (3.10) typically used for surface chemical analysis, the cathode fall is usually in the range 200 V to 2 000 V, with the cathode surface being more negative. In an rf glow discharge, the cathode fall is time-varying, with a peak-to-peak value normally in the range 500 V to 2 000 V.

4.91

cathode layer

<GDS> thin luminous region of *glow discharge* (4.228) between the *Aston dark space* (4.141) and the *cathode dark space* (4.142)

Note 1 to entry: See *negative glow* (4.314), *positive column* (4.342), and *anode glow* (4.28).

Note 2 to entry: The cathode layer may not be noticeable in a glow discharge used for surface chemical analysis.

4.92

cation

positively charged ion

Note 1 to entry: See *anion* (4.25) and *cationized ion* (4.93).

4.93

cationized ion

positively charged ion resulting from a neutral molecule combining with a *cation* (4.92), usually a metal ion

Note 1 to entry: Cationization with, for instance, Ag leads to high yields of some positive ion fragments or *molecular ions* (4.304). 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* (4.458).

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

4.94 channelling

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

Note 1 to entry: In *IBA* (3.11), for ion or atom motion aligned with the strings of atoms of a single crystal, the part of the beam that strikes the first atom of a string will scatter (giving a “surface peak”), but the rest of the beam can go through the “empty” spaces of the crystal without direct scattering. The small-angle collisions that the fast particles have with the channel walls mostly focus the beam into the channels. Thus, the channelling yield can be as low as 1 % of the full, non-aligned, yield. Channelling is sensitive to off-lattice-site atoms and can be used to evaluate strain as well as amorphous overlayers and depth distributions of point defects (direct scattering centres), provided that the number of these atoms or defects is comparable to the channelling yield. It is also sensitive to line defects, which often do not have a large direct scattering effect but can cause substantial subsequent dechannelling deeper in the crystal. In these cases, the point defect concentrations have to be greater than about 1 atomic % and the dislocation densities greater than about $10^{11}/\text{cm}^2$.

4.95 characteristic electron energy losses

inelastic scattering (4.244) of electrons in solids that produces a non-uniform *energy loss spectrum* (4.197) determined by the characteristics of the material

Note 1 to entry: See *plasmon* (4.339) and *surface plasmon* (4.462).

Note 2 to entry: The most probable characteristic losses arise from excitation of valence electrons. For some solids (for example, non-transition metals), inelastic scattering is dominated by plasmon excitations. For other solids, the inelastic scattering might be due to a combination of plasmon excitation and single valence-electron excitations, and these excitations might not be distinguishable. Inelastic scattering can also occur through the excitation of core level electrons when this is energetically possible.

Note 3 to entry: The characteristic energy losses are most prominent in the energy loss range 0 eV to 100 eV.

Note 4 to entry: Characteristic electron energy loss peaks are often observed in association with other peaks in a spectrum [e.g. *Auger electron* (4.37) peaks, photoelectron peaks, and the peak arising from *elastic scattering* (4.80) of *primary electrons* (4.346)].

4.96 characteristic X-rays

photons emitted by ionized atoms and having a particular distribution in energy and intensity which is characteristic of the atomic number and chemical environment of the atom

[SOURCE: ASTM E673-03]

Note 1 to entry: In *XPS* (3.23), the term is applied to the X-ray source used to excite photoelectrons in the sample.

Note 2 to entry: In EPMA, characteristic X-rays emitted from the sample are detected and analysed to give information on the composition of the sample.

4.97 charge modification

alteration of the amount or the distribution of charge at a sample *surface* (4.458)

4.98 charge neutralization

DEPRECATED: charge compensation

DEPRECATED: charge stabilization

maintenance at a fixed potential, usually near neutrality, of the *surface* (4.458) of a non-conducting or poorly conducting sample material under bombardment by primary particles or photons

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

4.99

charge referencing

<AES, XPS> method by which the *charging potential* (4.103) of a sample is determined in order to correct the measured energies so that those energies correspond to a sample with no surface charge

Note 1 to entry: Charge referencing is often conducted using *adventitious carbon referencing* (4.4), using *internal carbon referencing* (4.257) or by *gold decoration* (4.234).

Note 2 to entry: 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* (4.221) of radiation.

4.100

charge transfer

charge exchange

<GDS> transfer of charge from an atom, molecule or ion to another atom, molecule or ion

4.101

charge transfer, asymmetric

charge exchange, asymmetric

<GDS> *charge transfer* (4.100) between an atom, molecule or ion and another atom, molecule or ion of a different *chemical species* (4.106)

Note 1 to entry: For example, $\text{Ar}^+ + \text{M} \rightarrow \text{Ar} + \text{M}^{*+}$, where M is often a transition metal in GDS (3.10) applications and M^{*+} is in an electronically excited, ionic state.

Note 2 to entry: Generally, asymmetric charge transfer is less efficient than *symmetric charge transfer* (4.102), owing to the effects of energy overlap and quantum-mechanical considerations on reaction *cross sections* (4.123).

4.102

charge transfer, symmetric

charge exchange, symmetric

<GDS> *charge transfer* (4.100) between an atom, molecule or ion and another atom, molecule or ion of the same *chemical species* (4.106)

Note 1 to entry: For example, $\text{Ar}^+ + \text{Ar} \rightarrow \text{Ar} + \text{Ar}^+$. This reaction is believed to be an efficient mechanism in the *cathode dark space* (4.142) of an analytical *glow discharge* (4.228), resulting in a large population of fast Ar atoms directed toward the sample *surface* (4.458). These fast Ar atoms can contribute significantly to sample *sputtering* (4.441).

4.103

charging potential

electrical potential of the surface region of an insulating sample, caused by irradiation

Note 1 to entry: 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* (4.221) of radiation.

Note 2 to entry: The surface and bulk potentials can differ, for example as a result of band bending, *interface* (4.253) dipoles and charge centres.

4.104

chemical effects

<AES, EELS, EPMA, XPS> changes in the shape of a measured spectrum, or in the peak energy for an element, arising from chemical bonding

4.105

chemical shift

<AES, EELS, EPMA, XPS> change in *peak energy* (4.327) arising from a change in the chemical environment of the atom

4.106

chemical species

atom, molecule, ion, or functional group

4.107

chemical state of an atom

<AES, EELS, UPS, XPS> 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

Note 1 to entry: Examples of features observed are satellite peaks, shifts in the peak energy positions, changes in the *lineshape* (4.284), and changes in the *characteristic electron energy losses* (4.95) spectra at lower *kinetic energies* (4.278) than the photoelectron or *Auger electron* (4.37) peaks.

Note 2 to entry: A full description of chemical state is denoted by the complete set of electronic states and the electron configuration in the core of the atom providing the signal, as well as the electronic and physical structure (including charge distribution, density of electronic states, and electronic configuration) local to this atom.

Note 3 to entry: The chemical state of a selected atom is determined by its interaction (e.g. chemical-bonding ionicity or covalency) with nearby atoms, most importantly its nearest neighbours. It is determined by the oxidation number of an atom in a compound, by the coordination (mostly by its stereo structure and coordination number) and by the differences in the kinds of element in the position of the first-nearest neighbour, second-nearest neighbour, and so on. These all affect the effective charge and spin state of the selected atom.

Note 4 to entry: Different or distinguishable sets of chemical properties (different chemical states) of a *chemical species* (4.106) can occur as a consequence of differing valence-band electronic structures, including charge distributions and electronic configurations, localized on the given chemical species. In *XPS* (3.23), the term chemical state is mostly used for characterizing measured binding energies, Auger electron kinetic energies, and *Auger parameters* (4.41) with different oxidation states of a given element in different chemical compounds, e.g. the Cr III oxidation state in Cr₂O₃ and Cr(OH)₃. In *AES* (3.1), the term chemical state is often used to characterize the shape of the *Auger electronspectrum* (4.38) for the atoms of an element in different chemical environments, e.g. the shape of the carbon Auger electron spectrum for graphite and for various carbides. Differences in the chemical properties of a chemical species in various environments can result in differences in the respective peak energies, satellite structures, lineshapes, or *energy loss* (4.196) features in the corresponding Auger or photoelectron spectra.

Note 5 to entry: The quantum theory of atoms in molecules defines an atom in a molecule or crystal as a bounded region of real space, an open quantum system. However, there is no wave function for the atom; they are only for the total system. Hence, there is no state designation for the atom, only for the total system. What physics provides are expectation values of all the observables, measurable or otherwise, for the bound atom. In this sense, its state is defined within the total system by the net charge and energy of the atom and how changes of charge and energy are reflected in the observed (e.g. Auger or photoelectron) spectra.

4.108

chemical-state plot

Wagner plot

<XPS> plot of the measured *kinetic energy* (4.278) of a sharp *Auger electron* (4.37) peak versus the *binding energy* (4.82) of a photoelectron peak for the same element

Note 1 to entry: 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 to entry: The binding energy is usually plotted on the abscissa with values decreasing towards the right.

4.109

chopper, beam

<SIMS> electrostatic or electromagnetic device used to generate pulses of ions from a continuous *ion beam* (4.259)

Note 1 to entry: See *beam blanking* (4.65) and *beam bunching* (4.66).

Note 2 to entry: The beam chopper can be used to define the pulse length and hence the mass resolution in a *time of flight* (4.473) mass spectrometer and it can also be used to select particular ions in a beam that contains more than one species.

4.110

chromatic aberration

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

4.111

cluster ion

ion composed of many atoms or *chemical species* ([4.106](#))

Note 1 to entry: The cluster can have a positive or negative charge.

Note 2 to entry: Cluster ions are used for primary-ion sources with enhanced properties compared with those of monatomic ions. Examples of such sources are Au_3^+ , Au_5^+ , Bi_3^+ , Bi_5^+ , C_{60}^+ , H_3O^+ , $(\text{H}_2\text{O})_n$, $[\text{Os}_3(\text{CO})_{12}]^+$, and SF_5^+ .

4.112

cluster SIMS

<SIMS> *SIMS* ([3.17](#)) but utilizing a *primary beam* ([4.77](#)) composed of *cluster ions* ([4.111](#))

Note 1 to entry: Cluster ion sources are often used in *static SIMS* ([3.20](#)) to enhance molecular signals and in *dynamic SIMS* ([3.3](#)) to enhance *depth resolution* ([4.164](#)).

4.113

collective motion

<SIMS, sputtering> movement of a number of atoms or molecules at the same time and in the same region

4.114

collision cascade

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

[SOURCE: ASTM E673-03]

Note 1 to entry: See *atomic mixing* ([4.32](#)), *cascade mixing* ([4.87](#)), *knock-on* ([4.279](#)), and *recoil implantation* ([4.279](#)).

4.115

compositional depth profile

CDP

chemical or atomic composition measured as a function of distance normal to the *surface* ([4.458](#))

4.116

constant ΔE mode

constant analyser energy mode

CAE mode

fixed analyser transmission mode

FAT mode

mode of *electron energy analyser* ([4.187](#)) operation that varies the *electron retardation* ([4.189](#)) but keeps the *pass energy* ([4.325](#)) constant in the energy-dispersive portion of the analyser

Note 1 to entry: This mode is often used in *XPS* ([3.23](#)) to maintain a high and constant *energy resolution* ([4.384](#)) throughout the spectrum. In this case, the analyser transmission usually falls with increasing *kinetic energy* ([4.278](#)) of the analysed electrons.

4.117

constant $\Delta E/E$ mode

constant retardation ratio mode

CRR mode

fixed retardation ratio mode

FRR mode

mode of *electron energy analyser* ([4.187](#)) operation that varies the retarding potential so that the *pass energy* ([4.325](#)) in the energy-dispersive portion of the analyser is a constant fraction of the original *vacuum level* ([4.483](#)) referenced *kinetic energy* ([4.278](#))

Note 1 to entry: This mode is often used in *AES* ([3.1](#)) to improve the *signal-to-noise ratio* ([4.427](#)) for high-energy emitted electrons at the expense of spectral resolution. In this case, the analyser transmission usually rises with increasing kinetic energy of the analysed electrons as a result of the increased energy width accepted.

4.118

cooperative uplifting

collective motion ([4.113](#)) of atoms or molecules under an atom or molecule at a *surface* ([4.458](#)), causing its desorption

4.119

Coster-Kronig transition

Auger process ([4.44](#)) involving an electron from the same principal shell as the initial vacancy

Note 1 to entry: See *Auger transition* ([4.46](#)) and *super Coster-Kronig transition* ([4.457](#)).

EXAMPLE $L_1L_2M_5; M_1M_2N_5$.

4.120

counts

total number of pulses recorded by a detector system in a defined time interval

Note 1 to entry: The counts can be representative, one-for-one with the particles being detected (in the absence of *dead time* ([4.146](#)) losses in the counting measurement) in which case they follow Poissonian statistics (unless other *noise* ([4.315](#)) 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 to entry: In multidetector systems, the apportion of counts into relevant channels of the spectrum can lead to changes from the expected Poissonian statistics in each channel since the counts in neighbouring channels can be partly correlated.

4.121

crater depth

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

Note 1 to entry: The crater is generally formed by ion bombardment in *sputter depth profiling* ([4.440](#)) and, in this case, can be different from the thickness of sample material removed by *sputtering* ([4.441](#)) due to dilation of the *altered layer* ([4.6](#)).

Note 2 to entry: 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.

4.122

crater edge effect

occurrence of signals from the crater edge which often originate from depths shallower than the central region of the crater formed in *depth profiling* ([4.163](#))

4.123**cross section**

<for a specified target entity and for a specified reaction or process produced by incident charged or uncharged particles of specified type and energy> quotient of the probability of reaction or process for the target entity by the incident-particle *fluence* (4.218)

Note 1 to entry: Cross sections are often expressed as an area per target entity (atom, molecule, etc.) for the relevant process.

Note 2 to entry: A cross section of σ per atom for the removal of particles from a given state in a beam will lead to a reduction dN in the number N of particles in that state in a distance dx , given by the relationship:

$$dN = N\sigma n dx$$

where n is the density of atoms traversed by the beam.

Integration leads to the relationship

$$N = N_0 \exp(-n\sigma x)$$

where N_0 is the value of N at the origin of x .

4.124**cross section, damage**

cross section (4.123) for the change in the number of particular entities considered to be a result of damage caused by bombardment by defined ions, electrons, or photons

Note 1 to entry: See *cross section, disappearance* (4.125).

Note 2 to entry: The particular entities can, for example, be specific molecules on a *surface* (4.458), specific observed ion fragments, atoms in a given chemical state, or polymer cross-linking as inferred from spectral data.

Note 3 to entry: Generally, the larger the entity, the larger the damage cross section.

Note 4 to entry: As a result of the break-up of larger entities, the observed entity can increase or decrease in intensity.

Note 5 to entry: Cross sections are often expressed as an area per target entity (atom, molecule, etc.) for the relevant process.

Note 6 to entry: Either as a result of the damage or as a result of electron or ion *sputtering* (4.441), the damaged material can be removed from the sample. For bulk samples, this can reduce any change in the relevant signal observed. For *monolayer* (4.307) samples, such sputtering can increase any change in the relevant signal observed. *Preferential sputtering* (4.443) can also change the relevant signal observed.

Note 7 to entry: A cross section of σ per atom for the removal of entities from a given state on a surface will lead to a reduction dN in the number N of entities in that state in a time dt given by the relation:

$$dN = N J \sigma dt$$

where J is the primary-ion or electron *dose* (4.174) rate density.

Integration leads to the relation

$$N = N_0 \exp(-J \sigma t)$$