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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.

International Standards are drafted in accordance with the rules given in the ISO/IEC Directives, Part 2.

The main task of technical committees is to prepare International Standards. Draft International Standards adopted by the technical committees are circulated to the member bodies for voting. Publication as an International Standard requires approval by at least 75 % of the member bodies casting a vote.

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.

ISO 18115-1 was prepared by Technical Committee ISO/TC 201, *Surface chemical analysis*, Subcommittee SC 1, *Terminology*.

Together with Part 2 (see below), it cancels and replaces ISO 18115:2001, which has been split into two parts and at the same time technically revised. The two parts also incorporate the Amendments ISO 18115:2001/Amd.1:2006 and ISO 18115:2001/Amd.2:2007.

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 Part 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 the two parts of ISO 18115 have been prepared in conformance with the principles and style defined in ISO 1087-1:2000, *Terminology work — Vocabulary — Part 1: Theory and application*, and ISO 10241:1992, *International terminology standards — Preparation and layout*. Essential aspects of these standards appear in Subclauses 3.1 to 3.3. The terms are given in alphabetical order, classified under three headings:

Clause 4: Definitions of the surface analysis methods.

Clause 5: Definitions of terms for surface analysis.

Clause 6: Definitions of terms for multivariate analysis.

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

A single alphabetical index to this part of ISO 18115 is given after the Bibliography. To help users, a second index is provided for the terms in Part 2 covering scanning-probe microscopy. To assist retrieval, compound terms can be found in the indexes in both natural and reverse word order.

This part of ISO 18115 contains new terms in addition to those previously published in ISO 18115:2001, *Surface chemical analysis — Vocabulary*, ISO 18115:2001/Amd.1 and those sections of ISO 18115:2001/Amd.2 that did not involve scanning-probe microscopy. Those terms in ISO 18115:2001/Amd.2 that did involve scanning-probe microscopy now appear in ISO 18115-2.

Surface chemical analysis — Vocabulary —

Part 1:
General terms and terms used in spectroscopy

1 Scope

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

2 Abbreviations

AES	Auger electron spectroscopy
AMRSF	average matrix relative sensitivity factor
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
dc	direct current
DESI	desorption electrospray ionization
eV	electron volts
EELS	electron energy loss spectroscopy
EIA	energetic-ion analysis
EPES	elastic peak electron spectroscopy
EPMA	electron probe microanalysis
ESCA	electron spectroscopy for chemical analysis
FABMS	fast atom bombardment mass spectrometry
FIB	focussed ion beam system

FWHM	full width at half maximum
GDMS	glow discharge mass spectrometry
GDOES	glow discharge optical emission spectrometry
GDS	glow discharge spectrometry
HSA	hemispherical sector analyser
IBA	ion beam analysis
ISS	ion-scattering spectrometry
LB	Langmuir-Blodgett
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
MCR	multivariate curve resolution
MEIS(S)	medium-energy ion scattering spectrometry
MVA	multivariate analysis
PCA	principal-component analysis
PERSF	pure-element relative sensitivity factor
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
SAM	self-assembled monolayer
SAXS	small-angle X-ray scattering
SDP	sputter depth profile
SEM	scanning electron microscope
SEP	surface excitation parameter

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	ultra-violet photoelectron spectroscopy
XPS	X-ray photoelectron spectroscopy

3 Format

3.1 Use of terms printed boldface in definitions

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

3.2 Non-preferred and deprecated terms

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

3.3 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.

4 Definitions of the surface analysis methods

4.1
Auger electron spectroscopy
AES
a method in which an **electron spectrometer** is used to measure the energy distribution of **Auger electrons** emitted from a **surface**

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

4.2
desorption electrospray ionization
DESI
a 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 Water and methanol are often used as the solvents to create the droplets. Acids and alkalis are added to control the solution pH.

NOTE 2 DESI is one of the few surface analysis methods designed to analyse materials without exposure to vacuum. It is used for complex molecules, organic molecules and biomolecules. *In vivo* analysis is claimed to be possible.

4.3
dynamic SIMS
SIMS in which the material **surface** is sputtered at a sufficiently rapid rate that the original surface cannot be regarded as undamaged during the analysis

NOTE 1 Dynamic SIMS is often simply termed SIMS.

NOTE 2 The ion **areic dose** during measurement is usually more than 10^{16} ions/m^2.

4.4
elastic peak electron spectroscopy
EPES
a method in which an **electron spectrometer** is used to measure the energy, intensity and/or energy broadening distribution of quasi-elastically scattered electrons from a solid or liquid **surface**

cf. **recoil effect**, **reflected electron energy loss spectroscopy**, **REELS**

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

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

NOTE 3 EPES is often an auxiliary method of **AES** and **REELS**, providing information on the composition of the surface layer. EPES is suitable for the experimental determination of the **inelastic mean free path**, the electron **differential elastic scattering cross section** and the **surface excitation parameter**.

4.5
electron spectroscopy for chemical analysis (deprecated)
ESCA (deprecated)
a method encompassing both **AES** and **XPS**

NOTE 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.

4.6
fast atom bombardment mass spectrometry
FABMS
FAB (deprecated)
a method in which a mass spectrometer is used to measure the mass-to-charge quotient and abundance of **secondary ions** emitted from a sample as a result of the bombardment by fast neutral atoms

4.7
G-SIMS
variant of **static SIMS** in which the intensities for each mass in two spectra from the same area, recorded with different beam energies or different bombarding ions, are ratioed to each other and the result is used to scale one of the spectra to generate a new spectrum

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

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

NOTE 3 The “G” in G-SIMS originally indicated the gentleness of the process generated.

4.8
glow discharge mass spectrometry
GDMS
a method in which a mass spectrometer is used to measure the mass-to-charge quotient and abundance of ions from a **glow discharge** generated at a **surface**

4.9
glow discharge optical emission spectrometry
GDOES
a method in which an optical emission spectrometer is used to measure the wavelength and intensity of light emitted from a **glow discharge** generated at a **surface**

4.10
glow discharge spectrometry
GDS
a method in which a spectrometer is used to measure relevant intensities emitted from a **glow discharge** generated at a **surface**

NOTE This is a general term that encompasses **GDOES** and **GDMS**.

4.11
ion beam analysis
IBA
a 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** scattered from the **surface** are detected and recorded as a function of their energy or **angle of scattering**, or both

NOTE **LEIS(S)**, **MEIS(S)** and **RBS** 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.

4.12
low-energy ion scattering spectrometry
LEIS(S)
a 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** scattered from the **surface** are detected and recorded as a function of their energy or **angle of scattering**, or both

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

NOTE 2 The acronym usually has only one “S”.

4.13
medium-energy ion scattering spectrometry
MEIS(S)
a method, designed to elucidate composition and structure of the outermost atomic layers of a solid material, in which principally monoenergetic, singly charged **probe ions** scattered from the **surface** are detected and recorded as a function of their energy or **angle of scattering**, or both

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

NOTE 2 By using **channelling** and aligning the incident-ion beam along a crystal axis, the scattering from the substrate may 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 may be further suppressed, improving the signal quality and visibility for amorphous overlayers to a high level.

NOTE 3 In some cases, an angle-sensitive detector is used that allows extensive structure and **depth profile** information to be obtained.

NOTE 4 The acronym usually has only one “S”.

4.14
matrix-assisted laser desorption/ionization mass spectrometry
MALDI
a method in which a time-of-flight mass spectrometer is used to measure the **mass-to-charge ratio** 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 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 MALDI is used to analyse non-volatile polar biological and organic macromolecules as well as polymers to masses of over 3 000 kDa.

4.15
Rutherford backscattering spectrometry
RBS
a method, designed to elucidate composition and structure of layers at the **surface** of a solid material, in which principally monoenergetic, singly charged **probe ions** scattered from the surface with a **Rutherford cross section** are detected and recorded as a function of their energy or **angle of scattering**, or both

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

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

4.16
reflection electron energy loss spectroscopy
REELS
a method in which an **electron spectrometer** is used to measure the energy distribution of electrons quasi-elastically scattered by atoms at or in a surface layer and the associated **electron energy loss spectrum**

cf. **elastic peak electron spectroscopy**, **EPES**

4.17
secondary-ion mass spectrometry
SIMS
a method in which a mass spectrometer is used to measure the mass-to-charge quotient and abundance of **secondary ions** emitted from a sample as a result of bombardment by energetic ions

cf. **dynamic SIMS**, **static SIMS**, **G-SIMS**

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

4.18
small-angle X-ray scattering
SAXS
a method in which the elastically scattered intensity of X-rays is measured for small-angle deflections

NOTE 1 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 Wide-angle X-ray scattering (WAXS) is an analogous technique, similar to X-ray crystallography, in which scattering at larger angles, which is sensitive to periodicity on smaller length scales, is measured.

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

4.19
sputtered neutral mass spectrometry
SNMS
a 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 The neutral species may be detected by using **plasma**, electron or photon ionization methods.

4.20
static SIMS
SIMS in which the material **surface** is sputtered at a sufficiently low rate that the original surface is insignificantly damaged during the analysis

cf. **dynamic SIMS**

NOTE The ion **areic dose** during measurement is restricted to less than 10^{16} ions/m^2 to an extent that depends on both the material of the sample and the size of the **molecular fragments** being analysed.

4.21
total reflection X-ray fluorescence spectroscopy
TXRF
a method in which an X-ray spectrometer is used to measure the energy distribution of **fluorescence** X-rays emitted from a **surface** irradiated by primary X-rays under the condition of **total reflection**

4.22
ultra-violet photoelectron spectroscopy
UPS
a method in which an **electron spectrometer** is used to measure the energy distribution of photoelectrons emitted from a **surface** irradiated by ultra-violet photons

NOTE Ultra-violet sources in common use include various types of discharges that can generate the resonance lines of various gases (e.g. the He I and He II emission lines at energies of 21,2 eV and 40,8 eV, respectively). For variable energies, **synchrotron radiation** is used.

4.23
X-ray photoelectron spectroscopy
XPS
a method in which an **electron spectrometer** is used to measure the energy distribution of photoelectrons and **Auger electrons** emitted from a **surface** irradiated by X-ray photons

NOTE X-ray sources in common use are unmonochromated Al Kα and Mg Kα X-rays at 1 486,6 eV and 1 253,6 eV, respectively. Modern instruments also use monochromated Al Kα X-rays. Some instruments make use of various X-ray sources with other **anodes** or of **synchrotron radiation**.

5 Definitions of terms for surface analysis

5.1
absorption coefficient, linear
linear **attenuation coefficient**

5.2
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

cf. **attenuation length**

NOTE 1 The mass density of the substance is ρ and x is the distance in the direction of the beam.

NOTE 2 The intensity or number of particles in the beam decays as $\exp(-\mu x)$ with the distance x.

NOTE 3 The mass attenuation (absorption) coefficient is the quotient of the linear attenuation (absorption) coefficient by the mass density of the substance.

5.3
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 ($m \pm 1$)

[IUPAC[3]]

5.4
adventitious carbon referencing
⟨XPS⟩ determining the **charging potential** of a particular sample from a comparison of the experimentally determined C 1s **binding energy**, arising from adsorbed hydrocarbons on the sample, with a standard binding energy value

cf. **Fermi level referencing, internal carbon referencing**

NOTE 1 A nominal value of 285,0 eV is often used for the binding energy of the relevant C 1s peak, although some analysts prefer specific values in the range 284,6 eV to 285,2 eV, depending on the nature of the substrate. This method does not determine the true **charging potential** since the true binding energy of the adsorbed hydrocarbons is not known.

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

5.5
afterglow
⟨GDS⟩ luminescence of the decaying **plasma** present in a **glow discharge** device after complete cessation of the sustaining discharge power

5.6
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 For silicon bombarded by 4 keV O_2^+ at near-normal incidence, after **sputtering** for a sufficient time to reach a steady state, the **surface** is converted to stoichiometric SiO_2 to a depth of around 15 nm with lower oxygen concentrations at greater depths. At 2 keV, this is reduced to 7 nm, these thicknesses being approximately twice the **projected range**.

NOTE 2 The **depth resolution** in **SIMS** may be greater or smaller than the altered-layer thickness, depending on the analyte and bombarding-ion species.

5.7
analyser blanking
⟨SIMS⟩ action to prevent **secondary ions** from travelling through the mass spectrometer and being detected

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

5.8
analysis area
⟨sample⟩ two-dimensional region of a sample **surface** measured in the plane of that surface from which the entire analytical signal or a specified percentage of that signal is detected

5.9
analysis area
⟨spectrometer⟩ two-dimensional region of a sample **surface** at the analytical point but set in the plane at right angles to the spectrometer axis from which the entire analytical signal or a specified percentage of that signal is detected

5.10
analysis volume
⟨sample⟩ three-dimensional region of a sample from which the entire analysis signal or a specified percentage of that signal is detected

5.11
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

5.12
angle, critical
⟨TXRF⟩ **glancing angle** at which the sample matrix X-ray **fluorescence**, when plotted against the glancing angle, is at the first point of inflection

5.13
angle, glancing
angle between the incident beam and the average surface plane

NOTE **Angle of incidence** and glancing angle are complementary.

5.14
angle lapping
sample preparation in which a sample is mechanically polished at an angle to the original **surface**

cf. **ball cratering**, **radial sectioning**

NOTE This angle may often be less than 1° so that depth information with respect to the original surface is transformed to lateral information.

5.15
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**

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

5.16
angle of emission
emission angle
angle between the trajectory of a particle or photon as it leaves a **surface** and the local or average surface normal

NOTE The particular surface normal needs to be specified.

5.17
angle of incidence
incidence angle
angle between the incident beam and the local or average surface normal

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

5.18
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

5.19
angle-resolved AES
ARAES
angle-dependent AES
a procedure in which **Auger electron** intensities are measured as a function of the **angle of emission**

5.20
angle-resolved EPES
AREPES
⟨EPES⟩ a method involving **EPES** measurements as a function of the **scattering angle**

5.21
angle-resolved XPS
ARXPS
angle-dependent XPS
a procedure in which X-ray photoelectron intensities are measured as a function of the **angle of emission**

NOTE 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**.

5.22
angle, solid, of analyser
solid angle of analyser that will transmit particles or photons from a point on the sample to the detector

cf. **analyser transmission function**

5.23
angle, solid, of detector
⟨EIA, RBS⟩ solid angle intercepted by the detector from an origin at the centre of the **beam spot**

5.24
angle, take-off
angle between the trajectory of a particle as it leaves a **surface** and the local or average surface plane

NOTE 1 The particular surface plane needs to be specified.

NOTE 2 Take-off angle is the complement of **angle of emission**.

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

5.25
anion
negatively charged ion

cf. **cation**

5.26
anode
⟨GDS, dc operation⟩ more positively charged electrode in a **glow discharge** device

cf. **cathode** ⟨GDS, dc operation⟩

5.27
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** device

cf. **cathode** ⟨GDS, rf operation⟩

NOTE 1 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** is usually slightly less than one-half of the applied rf peak-to-peak potential.

NOTE 2 The precise fraction of the rf cycle over which the anode is more positively charged depends upon the source geometry and other factors.

5.28
anode glow
⟨GDS⟩ thin luminous region of a **glow discharge** immediately adjacent to the **anode**

cf. **cathode layer**, **negative glow** and **positive column**

NOTE The anode glow may not be noticeable in a glow discharge used for surface chemical analysis.

5.29
aperture, contrast
aperture, in an ion or electron optical system, designed to reduce unwanted **background signal**

NOTE This aperture can also govern the spatial resolution and other properties of the system.

5.30
asymmetry parameter
β
⟨XPS⟩ **factor** 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

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

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

5.31
atomic mass unit (deprecated)
See Note 3 to "**unified atomic mass unit**".

cf. **unified atomic mass unit**

5.32
atomic mixing
migration of sample atoms due to energy transfer with incident particles in the surface region

cf. **cascade mixing**, **collision cascade**, **ion-beam-induced mass transport**, **knock-on**, **recoil implantation**

5.33
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

cf. **attenuation length**, **mass absorption coefficient**

NOTE 1 The intensity or number of particles in the beam decays as $\exp(-\mu/x)$ with the distance x.

NOTE 2 Attenuation coefficient is often used in place of **linear attenuation coefficient** and is used in EPMA. Both are the reciprocal of **attenuation length** which is used in **AES** and **XPS**.

5.34
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

cf. **attenuation coefficient**, **decay length**, **effective attenuation length**, **electron inelastic mean free path**, **linear absorption coefficient**, **mass absorption coefficient**

NOTE 1 The intensity or number of particles in the beam decays as $\exp(-x/l)$ with the distance x.

NOTE 2 For electrons in solids, the behaviour only approximates to an exponential decay due to the effects of **elastic scattering**. Nevertheless, for some measurement conditions in **AES** and **XPS**, the **signal intensity** may 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.

5.35
attenuation length, effective
⟨AES, XPS⟩ parameter which, when introduced in place of the **inelastic mean free path** into an expression derived for **AES** and **XPS** on the assumption that **elastic scattering** effects are negligible for a given quantitative application, will correct that expression for elastic scattering effects

cf. **attenuation length**

NOTE 1 The effective attenuation length may 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 **emission angle**. For emission angles of up to about 60° (with respect to the surface normal), it is often satisfactory to use a single value of this parameter. For larger emission angles, the effective attenuation length can depend on this angle.

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

5.36
Auger de-excitation
process in which the excess energy of an excited atom or ion is given up by the **Auger process**

cf. **Auger neutralization**

NOTE 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.

5.37
Auger electron
electron emitted from atoms in the **Auger process**

cf. **Auger transition**

NOTE 1 Auger electrons can lose energy by **inelastic scattering** as they pass through matter. Measured Auger electron spectra are therefore generally composed of a peak structure of unscattered Auger electrons superimposed on a background of inelastically scattered Auger electrons with intensities extending to lower kinetic energies, and on backgrounds arising from other processes.

NOTE 2 Auger electrons may change their direction of propagation by **elastic scattering** as they pass through matter.

5.38
Auger electron spectrum
plot of the **Auger electron** intensity as a function of the electron **kinetic energy**, usually as part of the energy distribution of detected electrons

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

NOTE 2 The Auger electron spectrum may be presented in either the **direct spectrum** or **differential spectrum** formats.

5.39
Auger electron yield
probability that an atom with a vacancy in a particular inner shell will relax by an **Auger process**

[ASTM E673-03[1]]

5.40
Auger neutralization
⟨ion at a surface⟩ a process in which an electron, tunnelling from the conduction band of a solid, neutralizes an incoming ion and an electron is ejected from a surface atom

NOTE The ejected electron may be emitted into the vacuum.

5.41
Auger parameter
⟨XPS⟩ **kinetic energy** of a narrow **Auger electron** peak in a spectrum minus the kinetic energy of the most intense photoelectron peak from the same element

cf. **initial-state Auger parameter**, **modified Auger parameter**

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

NOTE 2 The Auger parameter is sometimes called the **final-state** Auger parameter.

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

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

5.42
Auger parameter, initial-state
⟨XPS⟩ β, where $\beta = 3E_B + E_K$ and where E_B and E_K are, respectively, the **binding energy** of a photoelectron peak and the **Fermi level** referenced **kinetic energy** of an **Auger electron** peak, each involving the same initial core level of the same element

cf. **Auger parameter**, **modified Auger parameter**

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

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

5.43
Auger parameter, modified
〈XPS〉 sum of the **Fermi level** referenced **kinetic energy** of a narrow **Auger electron** peak in the spectrum and the **binding energy** of the most intense photoelectron peak from the same element

cf. **Auger parameter**, **initial-state Auger parameter**

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

5.44
Auger process
relaxation, by electron emission, of an atom with a vacancy in an inner electron shell

[ASTM E673-03[1]]

cf. **Auger de-excitation**, **Auger electron**, **Auger transition**

NOTE The emitted electrons have characteristic energies, defined by the Auger transition.

5.45
Auger process, interatomic
Auger transition in which at least one of the final electron vacancies is localized in valence levels or molecular orbitals of atoms adjacent to the atom in which the initial vacancy occurred

5.46
Auger transition
Auger process involving designated electron shells or sub-shells

NOTE 1 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, KL_1L_2). Coupling terms can also be added, where known, to indicate the final atomic state (for example, $L_3M_{4,5}M_{4,5}$;^{1}D).

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

NOTE 3 When an Auger process involves an electron from the same principal shell as the initial vacancy (for example, L_1L_2M), it is referred to as a **Coster-Kronig transition**. If all electrons are from the same principal shell (for example, $M_1M_2M_3$) the process is called a **super Coster-Kronig transition**.

5.47
Auger transition rate
quotient of the probability for an **Auger process** by time

5.48
Auger vacancy satellite
Auger transition in which additional **spectator holes** are present in the **initial state** or the **final state** for the transition

5.49
background equivalent concentration
〈GDS〉 **concentration** of an element in a sample that would produce, in the absence of the background, a **signal intensity** equivalent to the measured background intensity

NOTE In **GDS**, results are often expressed in mass fractions and so the background equivalent concentration is usually expressed in these units.

5.50
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** processes

cf. **inelastic scattering background subtraction**, **Shirley background**, **Sickafus background**, **Tougaard background**

NOTE For **AES** and **XPS**, the inelastic background associated with a particular **Auger electron** or photoelectron peak has been approximated by a measured **electron energy loss spectrum** for which the incident-electron energy is close to the energy of the peak. 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.

5.51
background, instrumental
intensity contribution, generally unwanted, arising from non-ideal behaviour of one or more parts of the instrument

5.52
background, metastable
⟨SIMS⟩ intensity in the **mass spectrum** arising from ions that spontaneously fragment between emission and detection

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

5.53
background, relative standard deviation of the
quotient of the standard deviation characterizing the **noise** in the **background signal** by the intensity of the background signal

5.54
background, Shirley
⟨AES, XPS⟩ background calculated to fit the measured spectrum at points at higher and lower **kinetic energy** than the peak or peaks of interest such that the background contribution at a given kinetic energy is in a fixed proportion to the total **peak area** above that background for higher kinetic energies

cf. **Tougaard background**

NOTE The fitting to the background may be made by averaging over a given number of energy channels.

5.55
background, Sickafus
⟨AES, XPS⟩ single-term power law background designed to describe the intensity of the **secondary-electron** cascade as a function of electron emission **kinetic energy**

NOTE 1 The measured secondary-electron cascade, for correction application of the Sickafus background, should be the experimentally observed spectrum corrected for the **spectrometer response function** of the measuring instrument.

NOTE 2 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.

5.56
background signal
signal present at a particular position, energy, mass or wavelength due to processes or sources other than those of primary interest

cf. **Shirley background**, **Sickafus background**, **Tougaard background**

5.57
background, Tougaard
⟨AES, XPS⟩ intensity distribution obtained from a model for the differential **inelastic scattering cross section** with respect to **energy loss** and the three-dimensional distribution of the emitting atoms in the surface region

cf. **Shirley background**

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

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

5.58
backscattered electron
⟨AES, EELS, EPMA⟩ electron, originating in the incident beam, which is emitted after interaction with the sample

NOTE 1 By convention, an electron with energy greater than 50 eV may be considered as a backscattered electron.

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

5.59
backscattering coefficient
backscattering yield
⟨EIA, RBS⟩ quotient of the number of detected particles in an interval of **backscattering energy** by that interval and by the number of incident ions

5.60
backscattering energy
energy of a particle from the **primary beam** after it has undergone a backscattering collision and escaped from the sample

5.61
backscattering factor
⟨AES⟩ **factor** defining the fractional increase in the **Auger electron** current due to additional ionizations in the sample caused by **backscattered electrons** above that arising directly from the **primary electrons**

NOTE Different usages exist; the factor is commonly the fractional increase r, as defined above, and sometimes unity plus that fractional increase, R $(= 1 + r)$. The latter usage is deprecated. For clarity, the particular usage needs to be defined.

5.62
backscattering spectrum
⟨EIA, RBS⟩ plot of **backscattering yield** versus **backscattering energy**

[ASTM E673-03[1]]

5.63
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**

cf. **secondary-electron yield**, **total secondary-electron yield**, **backscattering factor**

5.64
ball cratering
a procedure in which the sample is abraded by a sphere in order to expose compositional changes in layers below the original **surface** with the intent that the depth of those layers can be related to the lateral position in the crater created by the abrasion

cf. **angle lapping**, **radial sectioning**

5.65
beam blanking
electrostatic or electromagnetic process designed to prevent any **beam particles** from impacting the sample

cf. **beam bunching**, **beam chopper**

NOTE For pulsed **ion beams**, the beam is usually deflected into a beam collector from which no particles can reach the sample and where the process of **sputtering** 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 µs, with 10 000 repetitions per second.

5.66
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

cf. **beam blanking**, **beam chopper**

NOTE This procedure may degrade the optimum focus of the **ion beam** since different ions experience different fields.

5.67
beam convergence angle
angular interval containing all or a specified fraction of the beam in the space prior to or at the focal plane

cf. **beam divergence angle**

NOTE Where the beam is symmetrical, the full or semi-angle may be used. The particular measure of angle needs to be stated.

5.68
beam current
I
quotient of $\mathrm{d}Q$ by $\mathrm{d}t$, where $\mathrm{d}Q$ is the quantity of electric charge of a specified polarity in the beam passing in the time interval $\mathrm{d}t$

$$I = \mathrm{d}Q/\mathrm{d}t$$

cf. **pulse beam current**, **average beam current**

NOTE 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.

5.69
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 For beams in which the instantaneous current varies periodically with time, the time interval t is an integral number of periods.

5.70
beam current density
J
⟨for a parallel beam of charged particles⟩ quotient of $\mathrm{d}I$ by $\mathrm{d}A$, where $\mathrm{d}I$ is the element of **beam current** incident on an area $\mathrm{d}A$ at right angles to the direction of the beam

$$J = \mathrm{d}I/\mathrm{d}A$$

cf. **fluence**, **flux**, **dose**

NOTE For a convergent or divergent beam, the area $\mathrm{d}A$ is replaced by a small sphere of cross-sectional area $\mathrm{d}A$.

5.71
beam current, integrated
total electric charge transported in the beam over a specified time

5.72
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

5.73
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

[ASTM E673-03[1]]

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

5.74
beam divergence angle
angular interval containing all or a specified fraction of the beam in the space after the focal plane

cf. **beam convergence angle**

NOTE Where the beam is symmetrical, the full or semi-angle may be used. The particular measure of angle needs to be stated.

5.75
beam energy
kinetic energy of the **beam particles**

cf. **impact energy**, **incident-particle energy**

NOTE 1 The energy is usually given in electron volts.

NOTE 2 The beam energy is often taken to be the particle energy on impact at the sample **surface**. However, where a sample is at a potential other than ground, the **impact energy** of the particles may 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.

5.76
beam particle
electron, positron, ion, atomic, molecular or cluster species contained in the incident beam

5.77
beam, primary
directed **flux** of particles or photons incident on a sample

5.78
beam profile
spatial distribution of the beam **flux** in a plane normal to the beam axis

5.79
beam source energy (deprecated)
See **beam energy**.

5.80
binary elastic scattering
elastic scattering
collision between a moving particle and a second particle in which the total **kinetic energy** and the total momentum are conserved

cf. **inelastic scattering**

NOTE In elastic scattering interactions, the moving particle may be deflected through angles of up to 180°.

5.81
binary elastic scattering peak
⟨ISS⟩ increase in the spectrometer detection system response above the background level which can be attributed to **binary elastic scattering** of an incident ion by a surface atom of a particular mass

[ASTM E673-03[1]]

5.82
binding energy
energy that must be expended in removing an electron from a given electronic level to the **Fermi level** of a solid or to the **vacuum level** of a free atom or molecule

5.83
blocking geometry
⟨EIA, RBS⟩ experimental arrangement wherein the atom rows or planes of a single-crystal **target** are aligned parallel to a vector from the sample to the detector

[ASTM E673-03[1]]

5.84
bond cleavage
bond scission
breakage of a molecular bond

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

NOTE 2 For α- and β-cleavage, see Reference [2] or [3].

5.85
Bragg's rule
empirical rule formulated by W.H. Bragg and R. Kleeman that states that the **stopping cross section** of a compound sample is equal to the sum of the products of the elemental stopping cross sections for each constituent and its atomic fraction, that is,

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

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

[Adapted from ASTM E673-03[1]]

5.86
bremsstrahlung
⟨EPMA, XPS⟩ photon radiation emitted from a material due to the deceleration of incident electrons within that material

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

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

5.87
cascade mixing
a diffusion-like process in which atoms of material are moved randomly by energy deposited by incident particles slowing down in the sample surface region

cf. **atomic mixing**, **collision cascade**, **knock-on**, **recoil implantation**

NOTE 1 If atomic mixing and knock-on effects are not significant, the measured **sputter depth profile** of a **delta layer** will be asymmetric on account of cascade mixing since the **surface** 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 2 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 3 In the **dilute limit**, the measured **depth profile** 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** 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.

5.88
cathode
⟨GDS, dc operation⟩ more negatively charged electrode in a **glow discharge** device

cf. **anode** ⟨GDS, dc operation⟩

5.89
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** device

cf. **anode** ⟨GDS, rf operation⟩

NOTE 1 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** is usually slightly less than one-half of the applied rf peak-to-peak potential.

NOTE 2 The precise fraction of the rf cycle over which the cathode is more negatively charged depends upon the source geometry and other factors.

5.90
cathode fall
fall potential
cathode drop (deprecated)
⟨GDS⟩ electric potential difference between the **cathode** surface and the **negative glow**

NOTE In direct-current **glow discharge spectrometry** 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.

5.91
cathode layer
⟨GDS⟩ thin luminous region of **glow discharge** between the **Aston dark space** and the **cathode dark space**

cf. **negative glow**, **positive column**, **anode glow**

NOTE The cathode layer may not be noticeable in a glow discharge used for surface chemical analysis.

5.92
cation
positively charged ion

cf. **anion**, **cationized ion**

5.93
cationized ion
positively charged ion resulting from a neutral molecule combining with a **cation**, usually a metal ion

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

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

5.94
channelling
preferential motion of energetic particles along the crystal axes of a crystalline solid as the particles move through the sample

NOTE In **IBA**, 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 $10^{11}/cm^2$.

5.95
characteristic electron energy losses
inelastic scattering of electrons in solids that produces a non-uniform **energy loss spectrum** determined by the characteristics of the material

cf. **plasmon**, **surface plasmon**

NOTE 1 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 2 The characteristic energy losses are most prominent in the energy loss range 0 eV to 100 eV.

NOTE 3 Characteristic electron energy loss peaks are often observed in association with other peaks in a spectrum (e.g. **Auger electron** peaks, photoelectron peaks, and the peak arising from **elastic scattering** of **primary electrons**).

5.96
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

[ASTM E673-03[1]]

NOTE 1 In **XPS**, the term is applied to the X-ray source used to excite photoelectrons in the sample.

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

5.97
charge modification
alteration of the amount or the distribution of charge at a sample **surface**

5.98
charge neutralization
charge compensation (deprecated)
charge stabilization (deprecated)
maintenance at a fixed potential, usually near neutrality, of the **surface** of a non-conducting or poorly conducting sample material under bombardment by primary particles or photons

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

5.99
charge referencing
⟨AES, XPS⟩ a method by which the **charging potential** 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 Charge referencing is often conducted using **adventitious carbon referencing**, using **internal carbon referencing** or by **gold decoration**.

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

5.100
charge transfer
charge exchange
⟨GDS⟩ transfer of charge from an atom, molecule or ion to another atom, molecule or ion

5.101
charge transfer, asymmetric
charge exchange, asymmetric
⟨GDS⟩ **charge transfer** between an atom, molecule or ion and another atom, molecule or ion of a different **chemical species**

NOTE 1 For example, $Ar^+ + M \rightarrow Ar + M^{+*}$, where M is often a transition metal in **GDS** applications and M^{+*} is in an electronically excited, ionic state.

NOTE 2 Generally, asymmetric charge transfer is less efficient than **symmetric charge transfer**, owing to the effects of energy overlap and quantum-mechanical considerations on reaction **cross sections**.

5.102
charge transfer, symmetric
charge exchange, symmetric
⟨GDS⟩ **charge transfer** between an atom, molecule or ion and another atom, molecule or ion of the same **chemical species**

NOTE For example, $Ar^+ + Ar \rightarrow Ar + Ar^+$. This reaction is believed to be an efficient mechanism in the **cathode dark space** of an analytical **glow discharge**, resulting in a large population of fast Ar atoms directed toward the sample **surface**. These fast Ar atoms may contribute significantly to sample **sputtering**.

5.103
charging potential
electrical potential of the surface region of an insulating sample, caused by irradiation

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

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

5.104
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

5.105
chemical shift
⟨AES, EELS, EMPA, XPS⟩ change in **peak energy** arising from a change in the chemical environment of the atom

5.106
chemical species
atom, molecule, ion or functional group

5.107
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 Examples of features observed are satellite peaks, shifts in the peak energy positions, changes in the **lineshape** and changes in the **characteristic electron energy loss** spectra at lower **kinetic energies** than the photoelectron or **Auger electron** peaks.

NOTE 2 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 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 Different or distinguishable sets of chemical properties (different chemical states) of a **chemical species** 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**, the term chemical state is mostly used for characterizing measured binding energies, Auger electron kinetic energies, and **Auger parameters** with different oxidation states of a

given element in different chemical compounds, e.g. the Cr III oxidation state in Cr_2O_3 and $Cr(OH)_3$. In **AES**, the term chemical state is often used to characterize the shape of the **Auger electron spectrum** 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 may result in differences in the respective peak energies, satellite structures, lineshapes or **energy loss** features in the corresponding Auger or photoelectron spectra.

NOTE 5 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.

5.108
chemical-state plot
Wagner plot
〈XPS〉 plot of the measured **kinetic energy** of a sharp **Auger electron** peak versus the **binding energy** of a **photoelectron** peak for the same element

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

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

5.109
chopper, beam
〈SIMS〉 electrostatic or electromagnetic device used to generate pulses of ions from a continuous **ion beam**

cf. **beam blanking**, **beam bunching**

NOTE The beam chopper can be used to define the pulse length and hence the mass resolution in a **time-of-flight** mass spectrometer and it can also be used to select particular ions in a beam that contains more than one species.

5.110
chromatic aberration
non-ideal focus of an electron or ion optical system for electrons or ions of different energies

5.111
cluster ion
ion composed of many atoms of **chemical species**

NOTE 1 The cluster may have a positive or negative charge.

NOTE 2 Cluster ions are used for primary-ion sources with enhanced properties compared with those of monatomic ions. Examples of such sources are: Au_3^+, Au_5^+, Bi_3^+, Bi_5^+, C_{60}^+, $H_3O^+(H_2O)_n$, $[Os_3(CO)_{12}]^+$ and SF_5^+.

5.112
cluster SIMS
〈SIMS〉 **SIMS** but utilizing a **primary beam** composed of **cluster ions**

NOTE Cluster ion sources are often used in **static SIMS** to enhance molecular signals and in **dynamic SIMS** to enhance **depth resolution**.

5.113
collective motion
〈SIMS, sputtering〉 movement of a number of atoms or molecules at the same time and in the same region

5.114
collision cascade
sequential energy transfer between atoms in a solid as a result of bombardment by an energetic species

[ASTM E673-03[1]]

cf. **atomic mixing**, **cascade mixing**, **knock-on**, **recoil implantation**

5.115
compositional depth profile
CDP
chemical or atomic composition measured as a function of distance normal to the **surface**

5.116
constant ΔE mode
constant analyser energy mode
CAE mode
fixed analyser transmission mode
FAT mode
mode of **electron energy analyser** operation that varies the **electron retardation** but keeps the **pass energy** constant in the energy-dispersive portion of the analyser

NOTE This mode is often used in **XPS** to maintain a high and constant **energy resolution** throughout the spectrum. In this case, the analyser transmission usually falls with increasing **kinetic energy** of the analysed electrons.

5.117
constant $\Delta E/E$ mode
constant retardation ratio mode
CRR mode
fixed retardation ratio mode
FRR mode
mode of **electron energy analyser** operation that varies the retarding potential so that the **pass energy** in the energy-dispersive portion of the analyser is a constant fraction of the original **vacuum level** referenced **kinetic energy**

NOTE This mode is often used in **AES** to improve the **signal-to-noise ratio** 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.

5.118
cooperative uplifting
collective motion of atoms or molecules under an atom or molecule at a **surface**, causing its desorption

5.119
Coster-Kronig transition
Auger process involving an electron from the same principal shell as the initial vacancy

cf. **Auger transition**, **super Coster-Kronig transition**

EXAMPLES $L_1L_2M_5$; $M_1M_2N_5$.

5.120
counts
total number of pulses recorded by a detector system in a defined time interval

NOTE 1 The counts may be representative, one-for-one with the particles being detected (in the absence of **dead time** losses in the counting measurement) in which case they follow Poissonian statistics (unless other **noise** sources are present) or they may simply be proportional to the number of particles being detected. The type of measure needs to be clearly stated.

NOTE 2 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.

5.121
crater depth
average depth of the region of a crater from which the measured signal is derived

NOTE 1 The crater is generally formed by ion bombardment in **sputter depth profiling** and, in this case, can be different from the thickness of sample material removed by **sputtering** due to dilation of the **altered layer**.

NOTE 2 The crater depth can be modified by the formation of a reacted layer (e.g. an oxide) following any exposure to the atmosphere or other environments necessary when conducting the crater depth measurement.

5.122
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**

5.123
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]

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

NOTE 2 A cross section of σ per atom for the removal of particles from a given state in a beam will lead to a reduction $\mathrm{d}N$ in the number N of particles in that state in a distance $\mathrm{d}x$, given by the relationship:

$$\mathrm{d}N = N\sigma n\ \mathrm{d}x$$

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

Integration leads to the relationship:

$$N = N_{\mathrm{o}}\exp(-n\sigma x)$$

where N_{o} is the value of N at the origin of x.

5.124
cross section, damage
cross section 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

cf. **cross section, disappearance**

NOTE 1 The particular entities can, for example, be specific molecules on a **surface**, specific observed ion fragments, atoms in a given chemical state or polymer cross-linking as inferred from spectral data.

NOTE 2 Generally, the larger the entity, the larger the damage cross section.

NOTE 3 As a result of the break-up of larger entities, the observed entity may increase or decrease in intensity.

NOTE 4 Cross sections are often expressed as an area per target entity (atom, molecule, etc.) for the relevant process.

NOTE 5 Either as a result of the damage or as a result of electron or ion **sputtering**, the damaged material can be removed from the sample. For bulk samples, this can reduce any change in the relevant signal observed. For **monolayer** samples, such sputtering can increase any change in the relevant signal observed. **Preferential sputtering** can also change the relevant signal observed.

NOTE 6 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:

$$dN = NJ\sigma\, dt$$

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

Integration leads to the relation:

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

where N_o is the initial value of N.

The observed value of the number of a given entity can also depend on sources creating that entity as discussed in Note 3.

5.125
cross section, disappearance
⟨SIMS⟩ **cross section** for the loss of intensity of an ion signal observed as a result of the bombardment by **primary ions**

cf. **cross section, damage**

NOTE 1 The ion signal used is usually that for a large or characteristic fragment of the molecule, such as a **cationized**, **protonated** or **deprotonated ion** from the molecule, at a **surface**.

NOTE 2 Generally, the larger the molecule, the larger the disappearance cross section.

NOTE 3 It is often assumed that the material being studied is present as a **monolayer**; however, this is an experimentally measured parameter and a value can be obtained irrespective of the precise form of the material under study. The disappearance cross section has practical significance and might or might not be simply related to the **damage cross section**.

5.126
cross section, elastic scattering
cross section for **binary elastic scattering**

5.127
cross section, elastic scattering, differential
quotient of the **elastic scattering cross section** for scattering into a particular infinitesimal solid angle far from the **target** by that infinitesimal solid angle

NOTE The differential elastic scattering cross section is related to the elastic scattering cross section, σ_e, by

$$\sigma_e = \int_{4\pi} \frac{d\sigma_e(\Omega)}{d\Omega}\, d\Omega$$

where $d\sigma_e(\Omega)/d\Omega$ is the differential elastic scattering cross section for scattering into solid angle Ω.

5.128
cross section, enhanced elastic
⟨EIA, RBS⟩ **cross section** of an atom for **elastic scattering** that is greater than the **Rutherford cross section** due to partial penetration of a nucleus in the sample by the incident particle

5.129
cross section, inelastic scattering
⟨AES, EELS, EMPA, XPS⟩ cross section for **inelastic scattering** by an electron traversing a material

5.130
cross section, ionization
cross section for a process that will produce, in an atom, a vacancy in a previously occupied shell

NOTE 1 Total ionization cross section refers to removal of an electron from any atomic shell or sub-shell of the atom.

NOTE 2 Partial or sub-shell ionization cross section refers to removal of an electron from a specified shell or sub-shell of the atom.

NOTE 3 A partial ionization cross section can be expressed per electron in a shell or sub-shell or for the total number of these electrons in a shell or sub-shell of the particular atom.

NOTE 4 An atom can have multiple vacancies following an initial ionization or as the result of subsequent **Auger** or **Coster-Kronig processes**.

5.131
cross section, nuclear reaction
〈EIA〉 **cross section** at a given **beam energy** and emission direction of the detected product for a particular nuclear reaction per atom

NOTE This cross section is usually expressed per atom as an area in units of barns (one barn = 10^{-28} m^2).

5.132
cross section, photoionization
total **ionization cross section** for an incident photon of a given energy interacting with a material to produce one or more photoelectrons from all sub-shells that are energetically accessible

cf. **ionization cross section**, **sub-shell photoionization cross section**

5.133
cross section, Rutherford
〈RBS〉 **elastic scattering cross section** calculated using classical mechanics and a Coulomb potential

cf. **elastic scattering cross section**, **enhanced elastic cross section**

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

5.134
cross section, stopping
〈EIA, RBS, sputtering〉 quotient of the rate of **energy loss** of a particle with distance along its trajectory in a sample by the atomic density of sample atoms for an infinitesimal sample thickness

cf. **stopping force**, **stopping power**

NOTE 1 The stopping cross section is usually expressed in units of eV·m^2/atom and not as an area per atom as is customary for **cross sections**.

NOTE 2 The atomic density is usually taken as the number density, N, but sometimes as the mass density, ρ, so that the units will be eV·m^2/atom or eV·m^2/kg. The stopping cross section $S(E)$ is thus given either by

$$S(E) \equiv (1/N)\,(\mathrm{d}E/\mathrm{d}x)$$

or by

$$S(E) \equiv (1/\rho)\,(\mathrm{d}E/\mathrm{d}x)$$

where $\mathrm{d}E/\mathrm{d}x$ is the rate of loss of energy E with distance x along the particle trajectory. Note that $\mathrm{d}E/\mathrm{d}x$ is often called the stopping power although it is not in units of power.

NOTE 3 In some texts, the stopping cross section and stopping power are used interchangeably so that $S(E) \equiv (\mathrm{d}E/\mathrm{d}x)$. This inconsistency for the term stopping power leads to its deprecation.

NOTE 4 Older texts can be found with the stopping cross section given in keV·cm^2/gm (meaning “per gram”) and in many other forms.

5.135
cross section, sub-shell photoionization
cross section for an incident photon interacting with a material to produce one or more photoelectrons from a given sub-shell

cf. **photoionization cross section**

NOTE Photoionization from one sub-shell may lead to **shake-up** or **shake-off** of electrons from other shells.

5.136
cross section, transport
σ_{tr}
quotient of the fractional momentum loss of a particle incident on the sample arising from **elastic scattering** by the areic density of the sample atoms, for an infinitesimally thin sample

NOTE 1 This **cross section** is expressed as an area per atom.

NOTE 2 The cross section for the loss of any momentum, however small, is simply the **elastic scattering cross section**. By contrast, the transport cross section is a measure of the probability of the loss of a substantial fraction of the initial momentum, analogous to **stopping cross section** which is a measure of the probability of the loss of a substantial amount of energy.

NOTE 3 The transport cross section is related to the **differential elastic scattering cross section**, $\mathrm{d}\sigma_e(\Omega)/\mathrm{d}\Omega$, by

$$\sigma_{tr} = 2\pi \int_0^{\pi} \frac{\mathrm{d}\sigma_e(\Omega)}{\mathrm{d}\Omega} (1-\cos\theta) \sin\theta \, \mathrm{d}\theta$$

where θ is the **angle of scattering**.

5.137
cross-sectioning
sample preparation in which the sample is cleaved, cut or polished in a plane perpendicular to the **interface** under study, so that associated compositional differences or gradients can be observed in that plane

5.138
damage limit
particle **fluence** above which significant changes in the spectrum or in a stated peak, arising from damage processes, are observed

cf. **static limit**

5.139
dark space
⟨GDS⟩ region of a **glow discharge** that emits little light compared to the surrounding regions, thereby appearing dark to the human eye

5.140
dark space, anode
⟨GDS⟩ **dark space** between the **positive column** and the **anode glow** in a **glow discharge**

cf. **Aston dark space**, **cathode dark space**, **Faraday dark space**

5.141
dark space, Aston
⟨GDS⟩ very thin **dark space** immediately adjacent to the **cathode** in a **glow discharge**

cf. **cathode dark space**, **Faraday dark space**, **anode dark space**

NOTE In **glow discharge spectrometry** used for surface chemical analysis, the Aston dark space is often not noticeable.

5.142
dark space, cathode
Crookes' dark space (deprecated)
Hittorf dark space (deprecated)
⟨GDS⟩ **dark space** between the **cathode layer** and the **negative glow** in a **glow discharge**

cf. **Aston dark space**, **Faraday dark space**, **anode dark space**

NOTE 1 In **glow discharge spectrometry** used for surface chemical analysis, the cathode dark space usually appears to occupy all of the space between the **cathode** surface and the negative glow.

NOTE 2 In dc glow discharge spectrometry, the cathode dark space is characterized by a large positive space charge and a strong electric field. This situation also occurs in an rf glow discharge over a large majority of the rf cycle. As a result, efficient acceleration of charged particles occurs in the cathode dark space.

5.143
dark space, Faraday
⟨GDS⟩ **dark space** between the **negative glow** and the **positive column** in a **glow discharge**

cf. **Aston dark space**, **cathode dark space**, **anode dark space**

5.144
daughter ion
electrically charged product formed from a **parent ion** or from a neutral entity generally of a larger size

NOTE Formation of the product need not necessarily involve **fragmentation**. It could, for example, involve a change in the number of charges carried. Thus, all **fragment ions** are daughter ions, but not all daughter ions are necessarily fragment ions.

5.145
dc bias
dc offset
self bias
⟨GDS, rf operation⟩ time-averaged electric potential, relative to ground, developed on the **surface** of the electrode to which the rf power is applied

NOTE 1 The dc bias arises as a result of the very different mobilities of the **plasma** electrons and the positively charged plasma ions.

NOTE 2 The dc bias effectively limits **sputtering** to the sample surface, preventing sputtering of other surfaces in contact with the plasma.

NOTE 3 For a properly designed rf **glow discharge** device used for surface chemical analysis, the magnitude of the dc bias is slightly less than one-half of the applied rf peak-to-peak potential difference.

5.146
dead time
time per pulse for which a pulse-counting system is unavailable for further counting

5.147
dead time, extended
dead time for a system where the pulse lengths are extended by extra pulses arriving during the dead time associated with an earlier pulse

5.148
dead time, multidetector
effective **dead time** of the whole detector, treating it as a single detector

5.149
dead time, non-extended
dead time for a system where the pulse lengths are not extended by extra pulses arriving during the dead time associated with earlier pulses

5.150
decay length
value of l for an intensity exhibiting a response $e^{\pm x/l}$ with distance x

cf. **attenuation length**

5.151
decay length, average emission function
negative reciprocal slope of the logarithm of a specified exponential approximation to the **emission depth distribution function** over a specified range of depths, as determined by a straight-line fit to the emission depth distribution function plotted on a logarithmic scale versus depth on a linear scale

[ASTM E673-03[1]]

5.152
decay length, deep emission function
asymptotic value of the **emission function decay length** for increasing depths from the **surface**

5.153
decay length, emission function
negative reciprocal slope of the logarithm of the **emission depth distribution function** at a specified depth

[ASTM E673-03[1]]

5.154
decay length, leading edge
value of the **decay length** for an increasing **signal intensity** as a function of depth prior to a maximum

NOTE This term is mainly used in the **SIMS depth profiling** of **delta layers**. It is also used in **AES** and **XPS sputter depth profiles**.

5.155
decay length, trailing edge
value of the **decay length** for a decreasing **signal intensity** as a function of depth following a maximum

NOTE This term is mainly used in the **SIMS depth profiling** of **delta layers**. It is also used in **AES** and **XPS sputter depth profiles**.

5.156
degree of ionization
ionization coefficient (deprecated)
⟨SIMS, FABMS⟩ quotient of the number of ions of a species emitted by the number of sputtered particles of that species

5.157
delayed onset
X-ray energy, in an X-ray absorption spectrum, at which there is a significant increase of absorption and for which the increased absorption occurs at a higher energy than a core-level **binding energy**

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

5.158
delta layer
layer of discrete composition, one atom thick, formed during growth of material on a substrate

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

5.159
dendrimer
molecule comprising a multifunctional core molecule with a dendritic wedge of highly branched monomers regularly attached to each functional site, leading to a monodisperse, tree-like or generational, structure

NOTE Dendrimer synthesis occurs in polymer chemistry and involves stepwise reactions in which the dendrimer is built up one monomer layer, or generation, at a time. The core molecule is referred to as "generation 0". Each successive repeat unit along all branches forms the next generation, "generation 1", "generation 2", and so on until the terminating generation.

5.160
deprotonated ion
parent molecule or fragment from which a proton has been removed to form a negative ion

5.161
depth distribution function, emission
⟨for a measured signal of particles or radiation emitted from a surface⟩ probability that the particle or radiation leaving the **surface** in a specified state and in a given direction originated from a specified depth measured normally from the surface into the material

5.162
depth distribution function, excitation
probability that specified excitations are created at specified depths measured, normally from a **surface** into the material, by a beam of specified particles or radiation incident on the surface in a given direction

[ASTM E673-03[1]]

5.163
depth profiling
monitoring of **signal intensity** as a function of a variable that can be related to distance normal to the **surface**

cf. **compositional depth profile**

NOTE The signal intensity is usually measured as a function of **sputtering** time.

5.164
depth resolution
depth range over which a signal changes by a specified quantity when reconstructing the profile of an ideally sharp **interface** between two media or a **delta layer** in one medium

NOTE The precise quantity to be used depends on the signal function with depth. However, for routine analytical use, a convention often used in **AES** and **XPS** is the depth at an interface over which the signal from an overlayer or a substrate changes from 16 % to 84 % of the total variation between plateau values.

5.165
depth resolution, instrumental
⟨AES, SIMS, XPS⟩ **depth resolution** in the sample arising from parameters of the instrument

NOTE In **sputter depth profiling**, these parameters involve the system alignment and may include the **ion species**, energy and **angle of incidence** as well as the option to rotate the sample whilst **sputtering**.

5.166
depth resolution, instrumental
⟨MEIS, RBS⟩ **depth resolution** in the sample arising from the **energy resolution** of the spectrometer

5.167
depth resolution parameter
parameter which may be used as (i) a coefficient in an analytic fit to a measured **compositional depth profile** or (ii) a qualitative way of describing that profile

cf. **depth resolution**

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

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

NOTE 2 Parameter definitions should be used consistently.

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

5.168
detection limit
smallest amount of an element or compound that can be measured under specified analysis conditions

NOTE 1 By convention, the detection limit is often taken to correspond to the amount of material for which the total signal for that material minus the **background signal** is three times the standard deviation of the signal above the background signal. This convention might not be applicable to all measurements, however, and, for a fuller discussion of detection limits, Reference [5] should be consulted.

NOTE 2 The detection limit can be expressed in many ways, depending on the purpose. Examples of ways of expressing it are mass or weight fraction, atomic fraction, concentration, number of atoms and mass or weight.

NOTE 3 The detection limit will generally be different for different materials.

5.169
detector efficiency
fraction of particles or photons incident on the detector that result in the detected signal

5.170
differential electron elastic reflection coefficient
⟨EPES⟩ ratio, per solid angle, of the number of electrons backscattered quasi-elastically from a solid **surface** at a given **scattering angle** to the number of incident electrons

NOTE The differential elastic reflection coefficient for electrons depends on the atomic composition of the surface layer of the solid, on the **differential elastic scattering cross sections** of the different atoms for electrons, on the corresponding **inelastic mean free path**, on the energy of the incident electrons and on the scattering geometry.

5.171
differential spectrum
⟨AES (and, rarely, XPS)⟩ differential of the **direct spectrum** with respect to energy, E, by an analogue electrode **modulation** method or by numerical differentiation of that spectrum

NOTE The modulation amplitude in eV or the number of points and the type of differentiating function should be given.

5.172
dilute limit
⟨SIMS⟩ atomic fraction or concentration of impurity species in a homogeneous matrix below which the SIMS process can safely be assumed to be linear with composition

5.173
direct spectrum
⟨AES and XPS⟩ intensity of electrons transmitted and detected by a spectrometer with a dispersing energy analyser, as a function of energy, E

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

NOTE 2 By convention, direct spectra in **XPS** are often presented in the **constant ΔE mode**, in which the spectrum approximates the true spectrum, whereas, in **AES**, spectra are often presented in the **constant $\Delta E/E$ mode**, in which the spectrum approximates to E times the true spectrum.

5.174
dose
synonym of **areic dose**

5.175
dose, areic
dose density (deprecated)
D
quotient of $\mathrm{d}N$ by $\mathrm{d}A$, where $\mathrm{d}N$ is the number of energetic particles of a specified type introduced into a solid through a surface area $\mathrm{d}A$:

$$D = \mathrm{d}N/\mathrm{d}A$$

NOTE 1 The energetic particles are atoms or atom clusters, which can be electrically charged or neutral, and the surface area $\mathrm{d}A$ is the geometric surface area.

NOTE 2 For a stationary parallel beam, the areic dose equals the **fluence** times $\cos\theta$, where θ is the **angle of incidence** of the beam to the surface normal.

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

NOTE 4 For a discussion of areic dose in relation to ion-implanted **reference materials**, see Reference [6].

5.176
dose, implanted areic
D^{imp}
quotient of $\mathrm{d}N^{\mathrm{imp}}$ by $\mathrm{d}A$, where $\mathrm{d}N^{\mathrm{imp}}$ is the number of energetic particles of a specified type incident on a solid within a surface area $\mathrm{d}A$ and stopped within the solid:

$$D^{\mathrm{imp}} = \mathrm{d}N^{\mathrm{imp}}/\mathrm{d}A$$

NOTE Particles which are not stopped within the solid are either backscattered or transmitted.

5.177
dose, nominal areic
D^{nom}
areic dose, as measured by an approximating procedure

NOTE Typically, D^{nom} for a beam of charged particles is derived by forming the quotient of the particle equivalent of the current integral over time and the surface area over which the beam is scanned with lateral uniformity. Hence, D^{nom} is generally an approximate average measure of D.

5.178
dose, non-implanted areic
areic dose representing the fraction of the **received areic dose** not trapped in the sample

NOTE The sum of the **implanted areic dose** and the non-implanted areic dose equals the received areic dose.

5.179
dose rate, areic
G
quotient of dD by dt, where dD is the **areic dose** introduced into a solid in time interval dt:

$$G = \mathrm{d}D/\mathrm{d}t$$

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

5.180
dose, received areic
D^{rec}
quotient of dN^{rec} by dA, where dN^{rec} is the number of energetic particles of a specified type incident on a solid within a surface area dA:

$$D^{rec} = \mathrm{d}N^{rec}/\mathrm{d}A$$

5.181
dose, retained areic
D^{ret}
quotient of dN^{ret} by dA, where dN^{ret} is the number of energetic particles of a specified type incident on a solid within a surface area dA which are stopped within the solid and remain therein:

$$D^{ret} = \mathrm{d}N^{ret}/\mathrm{d}A$$

NOTE 1 Particles which are stopped within the solid but do not remain therein might be either thermally evaporated or re-emitted by sputter erosion of the solid.

NOTE 2 The retained areic dose is a fractional quantity of the **implanted areic dose**.

5.182
dose, sputtered areic
areic dose representing the fraction of the **implanted areic dose** lost from the sample by **sputtering**

NOTE The sputtered areic dose is a fractional quantity of the **implanted areic dose**.

5.183
dual-beam profiling
⟨SIMS⟩ **sputter depth profiling** involving two ion guns

NOTE 1 Two similar ion guns can be used in opposite azimuths of the sample to reduce the development of topography.

NOTE 2 In **time-of-flight** mass spectrometers, one beam is used with a short on-time for the **SIMS** analysis whilst a second is used during the period when the first is off and the mass analysis has been completed in each cycle. The second gun provides the ions for sputter removal of the sample to form the **depth profile**. This combination allows practical **sputtering rates** to be achieved and the profiling to be optimized separately from the optimization for the SIMS analysis.

5.184
dynamic emittance matching
electron or ion optical method of steering a spectrometer axis to align with the impact area of the **primary beam** at all points of a **raster** scan on the sample **surface**

5.185
efficiency
〈SIMS〉 quotient of the measured yield of an **ion species** per **primary ion** and the **disappearance cross section**

cf. **ionization efficiency**

5.186
elastic peak
quasi-elastic peak
peak in the electron spectrum, produced by quasi-elastically scattered electrons detected by an **electron spectrometer**

cf. **elastic peak electron spectroscopy**, **EPES**, **inelastic scattering**, **recoil effect**, **reflected electron energy loss spectroscopy**, **REELS**

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

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

5.187
electron energy analyser
device for measuring the number of electrons, or an intensity proportional to that number, as a function of the electron **kinetic energy**

cf. **electron spectrometer**

5.188
electron flooding
irradiation of a sample with low-energy electrons in order to change or stabilize the **charging potential**

5.189
electron retardation
〈AES, XPS〉 method of measuring the **kinetic energy** distribution by retarding the emitted electrons before or within the **electron energy analyser**

[ASTM E673-03[1]]

5.190
electron spectrometer
device, the essential part of which is an **electron energy analyser**

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

5.191
emission yield
⟨GDOES⟩ quotient of the time-integrated optical emission signal minus the signal background at a specified wavelength by the mass of the emitting element sputtered in the time interval of interest

5.192
energy acceptance window
range of energies accepted by a spectrometer, leading to a detected signal

5.193
energy edge
⟨EIA, RBS⟩ values of the **backscattering energy** for an element, or for an isotope, that is located at the **surface** of the sample

5.194
energy eigenvalue
energy value of a single bound electron level in an atom, molecule, ion or solid obtained by solving the single-electron Schrödinger or Dirac equation in the Dirac-Fock representation of the electronic structure of an atom in its ground state

NOTE 1 Eigenvalues are the solutions to certain integral equations, a special case of which is the Schrödinger equation for electrons in atoms, molecules, ions or solids.

NOTE 2 In the **frozen-orbital approximation**, the **binding energy** of a **hole state** is given by the negative of the corresponding single-electron energy eigenvalue.

5.195
energy, impact
kinetic energy of the **particles** on impact with the sample **surface**

cf. **beam energy**, **incident-particle energy**

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

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

5.196
energy loss
energy dissipated by particles as they interact with the sample

cf. **characteristic electron energy losses**, **plasmon**

5.197
energy loss spectrum, electron
energy spectrum of electrons from a nominally monoenergetic source emitted after inelastic interactions with the sample, often exhibiting peaks due to specific inelastic loss processes

cf. **characteristic electron energy losses**, **plasmon**

NOTE 1 The spectrum obtained using an incident-electron beam of about the same energy as an **AES** or **XPS** peak approximates to the energy loss spectrum associated with that peak.

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

5.198
energy of incident beam (deprecated)
See **impact energy**.

5.199
energy per channel
energy difference between successive spectral channels

5.200
energy, surface approximation
⟨EIA, RBS⟩ simplification of calculations involving the energy of an ion passing through a solid sample, where the energy of the ion at the **surface** is used in place of a properly averaged energy

[Adapted from ASTM E673-03[1]]

NOTE This approximation is used to determine the energy at which scattering or **stopping cross sections**, or both, are evaluated.

5.201
enhancement factor
$K_{n,1}$
⟨SIMS, sputtering⟩ ratio of the ion or neutral **sputtering yield** using a primary-ion cluster of n similar atoms to n times the ion or neutral sputtering yield using a **primary ion** of one of those atoms where the primary-ion energy per atom is the same in each case

NOTE An enhancement factor greater than unity in **SIMS** is usually used to show that the yield from a cluster source is greater than the yield that would be predicted for a **linear collision cascade**.

5.202
erosion rate
⟨surface⟩ quotient of the change in the position of the **surface** as a result of particle or photon irradiation by the time of irradiation

cf. **sputtering rate**

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

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

NOTE 3 The rate may be measured as a velocity.

5.203
escape depth, mean
average depth normal to the **surface** from which the specified particles or radiations escape as defined by:

$$\int_0^\infty z\phi(z,\theta)\,\mathrm{d}z \Big/ \int_0^\infty \phi(z,\theta)\,\mathrm{d}z$$

where $\phi(z,\theta)$ is the **emission depth distribution function** for depth z from the surface into the material and for **angle of emission** θ with respect to the surface normal

[ASTM E673-03[1]]

5.204
excitation, electron impact
⟨GDS⟩ electronic excitation of an atom, molecule or ion resulting from collision with an electron

NOTE 1 For example, $M + e^- \rightarrow M^* + e^-$, where M* is a transition metal in an electronically **excited state**.

NOTE 2 In a **glow discharge** used for surface chemical analysis, electron-impact excitation is believed to account for most of the electronic excitations. Therefore, it is a very important physical mechanism for **glow discharge optical emission spectrometry**.

5.205
excited state
state of a system with energy higher than that of the ground state

NOTE This term is generally used to characterize a molecule in one of its electronically excited states, but can also refer to vibrational and/or rotational excitation in the electronic ground state.

5.206
extraction bias
⟨SIMS⟩ voltage between the electrodes used to define the **extraction field** occurring in the period between ion pulses in the pulsed-extraction mode

NOTE 1 This term is used in **time-of-flight SIMS** instruments.

NOTE 2 The extraction bias can be set to zero or it can be set at a particular value to deflect low-energy electrons to the sample for **charge neutralization** or, in dual-ion-beam systems for **depth profiling**, to deflect **secondary ions** generated by the **sputter depth profiling** ion gun in order to prevent them from entering the mass spectrometer and generating background **counts**.

5.207
extraction field
⟨SIMS⟩ electric field above the sample, operational during ion emission from the sample

NOTE The extraction field may be pulsed or constant, depending on the type of instrument.

5.208
extractor voltage
⟨SIMS⟩ voltage, referenced to the sample, of the electrode defining the field above the sample and used to facilitate the introduction of emitted ions into the mass spectrometer

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

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

5.209
FAB-SIMS
⟨SIMS⟩ **SIMS** in which the primary-ion beam is replaced by a fast-atom beam

5.210
Faraday cup
detector with a cup-shaped electrode for collection of the electric charge carried by a beam of charged particles passing into the cup, designed such that emission of charged particles from the detector is minimized

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

5.211
Fermi energy
Fermi level
⟨conductors⟩ maximum energy of electrons in the valence band at zero kelvins

cf. **vacuum level**

NOTE For insulators and semiconductors, the Fermi level is usually between the valence and conduction bands.

5.212
Fermi level referencing
⟨XPS, UPS⟩ establishing the **binding energy** scale for a particular sample by assigning the **kinetic energy** corresponding to the **Fermi level**, as determined by analysis of the sample's **XPS** or **UPS** spectrum, as the point of zero binding energy

[ASTM E673-03[1]]

cf. **vacuum level referencing**

5.213
FIB
focussed ion beam system
ion beam system used for machining small regions with sub-micron precision

NOTE 1 In general, FIBs use an LMIS to generate a finely focussed ion beam with diameters typically in the range 7 nm to 300 nm and of sufficient **flux**, typically 4 pA to 20 nA, to machine small items for study by **AES**, **SIMS** or TEM in an economic time. They are also used to manufacture **SPM** tips, those for **AFM** having radii down to 2 nm.

NOTE 2 FIB-machined **surfaces** may have an ion-damaged surface that needs to be removed.

5.214
field-induced migration
effect occurring in insulators where internal electric fields created by ion or electron bombardment cause the migration of sample atoms

5.215
final state
⟨AES, EMPA, XPS⟩ state of an atom resulting after a particular **Auger**, X-ray or **photoemission process**

5.216
floating potential
⟨GDS⟩ electric potential that develops on an isolated substrate immersed in a **plasma**

NOTE An isolated substrate cannot conduct charge to other parts of the instrument. Therefore, averaged over time, the **fluxes** of electrons and positively charged ions to its **surface** must be equal. Given that electrons are much more mobile than positively charged ions, equal fluxes arise when the floating potential is typically a few volts more negative than the **plasma potential**.

5.217
fluence
F
⟨for a parallel beam of particles⟩ quotient of $\mathrm{d}N$ by $\mathrm{d}A$, where $\mathrm{d}N$ is the number of particles of a specified type incident on an area $\mathrm{d}A$ at right angles to the direction of the beam:

$$F = \mathrm{d}N/\mathrm{d}A$$

NOTE 1 For a scanned parallel beam, the fluence may be referred to the laboratory coordinate system or to the scanned beam's own moving coordinate system. The latter will generally give the higher value. The usage of fluence in these situations requires a clear statement of the coordinate system being used.

NOTE 2 In some texts, the term **fluence** is used for **areic dose**. This is incorrect and has led to confusion. See Note 2 in 5.175.

NOTE 3 For a parallel beam, **fluence** rate and **flux** density are equivalent measures.

5.218
fluence
F
⟨for particles moving in many directions⟩ quotient of dN by dA, where dN is the number of particles of a specified type incident on a sphere of cross-sectional area dA

5.219
fluorescence
⟨AES, TXRF, XPS⟩ X-rays generated by a transition of an electron from a filled shell to a core **hole**, created by incident radiation, at a higher **binding energy**

5.220
fluorescence yield
⟨AES, TXRF, XPS⟩ probability that an atom with a vacancy in a particular inner shell will relax by X-ray **fluorescence**

5.221
flux
Φ
⟨for a beam of particles⟩ quotient of dN by dt, where dN is the number of particles of a specified type passing in the time interval dt

$$\Phi = dN/dt$$

NOTE For a parallel beam, **fluence** rate and **flux** density are equivalent measures.

5.222
fragment ion
charged dissociation product arising from ionic **fragmentation**

[IUPAC[3]]

cf. **daughter ion**, **metastable ion**

NOTE Fragment ions may dissociate further to form other electrically charged molecular or atomic moieties of successively lower mass.

5.223
fragmentation
breakdown of a molecule or ion to form one or more ions or neutral species of lower mass whilst conserving the total charge

5.224
frozen-orbital approximation
assumption that the one-electron wavefunctions of the electrons remaining in an atom or molecule are unchanged after ionization

NOTE In the frozen-orbital approximation, the **binding energy** of an electron is given by the negative of the **energy eigenvalue**.

5.225
gate, digital
system allowing the data associated with any selected group of image pixels to be summed to produce cumulative data from any desired area

5.226
gate, electronic
system consisting of a counter or detector which is enabled or disabled by signals from the beam scanning system so that **counts** only accumulate when the **primary beam** is incident on a selected part of the imaged area

5.227
gated area
defined area within a larger area from which the signal may be obtained

NOTE The defined area is often in the central region of a crater and may be defined by an **optical aperture**, an **electronic gate** or a **digital gate**.

5.228
glow discharge
phenomenon that results from the passage of electrical current through a gas and that is characterized by emission of light, a low current density (about 0,01 A/m^2 to 1 000 A/m^2) and a potential that is above the ionization potential of the gas but below the sparking potential

NOTE 1 In glow discharge surface-analytical instruments, sample material is introduced into the gaseous discharge via bombardment of the **surface** by positive ions and energetic neutral species. Sputtered atoms are then excited and ionized by collisions in the discharge.

NOTE 2 Analytical glow discharge devices are usually operated in argon at a pressure in the range 10 Pa to 2 000 Pa.

5.229
glow discharge, abnormal
⟨GDS⟩ **glow discharge** operated in a current/voltage regime in which an increase in current is accompanied by an increase in voltage

cf. **glow discharge, normal**

NOTE Glow discharge devices used for surface chemical analysis are usually operated in the abnormal mode, rather than the normal mode. This is because abnormal operation provides **sputtering** of the entire exposed **surface** of the sample, as well as increased signal intensities.

5.230
glow discharge, boosted
⟨GDS⟩ **glow discharge** sustained by a secondary means of coupling energy into the **plasma** in addition to the primary means, sometimes providing enhanced analytical signals

NOTE Forms of boosting the glow discharge include the use of microwave and rf fields (not to be confused with unboosted rf glow discharge, in which rf excitation is the only power source), as well as the injection of extra plasma electrons by means of filaments or other electron sources.

5.231
glow discharge, normal
⟨GDS⟩ **glow discharge** operated in a current/voltage regime in which an increase in current is accompanied by little or no detectable change in voltage

cf. **glow discharge, abnormal**

NOTE Glow discharge devices used for surface chemical analysis are not usually operated in the normal mode. This is because a portion of the exposed sample **surface** remains unsputtered and signal intensities may be unacceptably weak. Such devices are usually operated in the abnormal mode.

5.232
glow discharge, pulsed
⟨GDS⟩ **glow discharge** in which one or more of the discharge operating parameters are intentionally varied in time in order to provide improved analytical performance

NOTE 1 The most common pulsed glow discharge involves **modulation**, in accordance with a square-wave or similar function, of the electrical power maintaining the **plasma**. However, other forms of pulsed glow discharge are possible.

NOTE 2 Both pulsed-dc and pulsed-rf glow discharges have been devised.

5.233
glow discharge source, jet-assisted
glow discharge source, jet-enhanced
⟨GDS⟩ **glow discharge** device incorporating a means of directing high-velocity jets of plasma-support gas directly towards the sample **surface**, intended to provide enhanced analytical signals

NOTE 1 This form of glow discharge device has been used predominantly for glow discharge atomic absorption spectrophotometry. The jets enhance atomic absorption by aiding the transport of sputtered material from the sample surface into the region of the **negative glow** in which light absorption is measured.

NOTE 2 Jet-enhanced glow discharge devices find little use for **depth profiling** because the craters formed on the sample surface are not usually flat.

5.234
gold decoration
⟨XPS⟩ a method whereby a very small quantity of gold, deposited as unconnected islands on an insulator, is used for **charge referencing**

cf. **adventitious carbon referencing**, **internal carbon referencing**

NOTE 1 The gold may be deposited by evaporation or by immersion of the **surface** in a solution that produces a colloidal gold deposit.

NOTE 2 The **binding energy** for the Au $4f_{7/2}$ peak is often taken as 84,0 eV, although measured values of this binding energy for gold deposited on a conducting substrate vary with the average gold island diameter.

5.235
grazing exit
glancing exit
geometrical arrangement in which the angle of the scattered (or emitted) particles is near 90° from the normal to the sample **surface**

NOTE This configuration generally results in improved surface sensitivity and can also improve **depth resolution**.

5.236
grazing incidence
glancing incidence
geometrical arrangement in which the angle of the incident particles is near 90° from the normal to the sample **surface**

NOTE This configuration can result in improved surface sensitivity (e.g. in **TXRF**).

5.237
hole
electronic vacancy in an atom, molecule or solid

5.238
hole state
electronic configuration of an atom, molecule or solid containing a **hole**

5.239
image depth profile
three-dimensional representation of the spatial distribution of a particular elemental or molecular species (as indicated by emitted **secondary ions** or electrons) as a function of depth or material removed by **sputtering**

[ASTM E673-03[1]]

5.240
impact energy per ion
kinetic energy of the **beam particles** on impact

cf. **impact energy**

5.241
incident-particle energy
kinetic energy of a particle incident on the sample **surface**

cf. **beam energy**, **impact energy**

NOTE The incident energy can also be expressed per atom for an incident atomic cluster; however, to avoid confusion, the phrase "per atom" should then be used.

5.242
inelastic electron scattering background subtraction
⟨AES, XPS⟩ process for subtracting a chosen **inelastic scattering** background from the measured spectrum

cf. **inelastic background**, **Shirley background**, **Tougaard background**

NOTE For **AES** and **XPS**, the inelastic background associated with a particular **Auger electron** or photoelectron peak has been approximated by a measured **electron energy loss spectrum** for which the incident-electron energy is close to the energy of the peak. 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.

5.243
inelastic mean free path, electron
average distance that an electron with a given energy travels between successive inelastic collisions

cf. **attenuation length**

5.244
inelastic scattering
interaction between a moving energetic particle and a second particle or assembly of particles in which the total **kinetic energy** is not conserved

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

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

5.245
information area
area of a region in the plane of the **surface** from which useful information is obtained

NOTE 1 The information area can be identified with the minimum surface area from which a specified percentage (e.g. 95 % or 99 %) of the detected signal originates.

NOTE 2 The information area can be determined from a measured, calculated or estimated measure of the **signal intensity** as a function of position on the sample surface.

5.246
information depth
maximum depth, normal to the **surface**, from which useful information is obtained

NOTE 1 The information depths for the different surface analysis methods differ significantly. The information depth for each technique depends on the material being analysed, the particular signals being recorded from that material, and the instrument configuration.

NOTE 2 The information depth can be identified with the sample thickness from which a specified percentage (e.g. 95 % or 99 %) of the detected signal originates.

NOTE 3 The information depth can be determined from a measured, calculated or estimated **emission depth distribution function** for the signal of interest.

5.247
information radius
maximum radius of a circular region, in the plane of the **surface**, from which useful information is obtained

NOTE 1 This definition is useful only for surface analyses of a homogeneous sample and for either normal incidence of the **primary beam** or normal detection of the signal particles, in which it is expected that the **signal intensity** as a function of position on the surface will depend only on the radial distance from the axis of symmetry. If these conditions are not met, it is more appropriate to make use of the **information area**.

NOTE 2 The information radius can be identified with the radius within which a specified percentage (e.g. 95 % or 99 %) of the detected signal originates.

NOTE 3 The information radius can be determined from a measured, calculated or estimated measure of the signal intensity as a function of radius.

5.248
initial state
⟨AES, EPMA⟩ core-hole **excited state** of an atom prior to an **Auger transition** or to X-ray emission

5.249
initial state
⟨XPS⟩ ground state of an atom prior to photoelectron emission

5.250
instrumental detection efficiency
ratio of the quantity of a detected event to the quantity of that event available for measurement

5.251
intensity, peak
measure of signal intensity for a constituent spectral peak

NOTE 1 Intensity is usually measured for quantitative purposes which, for direct electron spectra or for mass spectra, could be the height of the peak above a defined background or the **peak area**. The units could be **counts**, counts·eV, counts per second, counts·eV per second, counts per amu, counts per second per amu, etc. For **differential spectra**, the intensity could be the peak-to-peak height or the peak-to-background height. The measure of intensity should be defined and the units stated in each case.

NOTE 2 The meaning is very rarely the literal meaning of the intensity value at the top of the measured peak either before or after removal of any background.

5.252
intensity, signal
strength of a measured signal at a spectrometer detector or after some defined processing

NOTE 1 The signal intensity is subject to significant change between the points of generation and detection of the signal and, further, between the points of detection and display on the measuring instrument.

NOTE 2 The signal intensity can be expressed in **counts** (per channel) or counts per second (per channel) or counts·eV per second or other units. In **AES**, the differential of the signal intensity might be obtained by analogue **modulation** of an electrode in the spectrometer or by numerical differentiation of the spectrum. The type of signal thus needs to be defined.

NOTE 3 In an electron or **mass spectrum**, the measured spectrum integrated over energy or mass and solid angle is equal to a current. If the spectrometer has been calibrated, the units of intensity could be current·eV^{-1}·sr^{-1} or current·amu^{-1}·sr^{-1}. If the spectrum has been normalized to unit **primary-beam** current, the appropriate units would be eV^{-1}·sr^{-1} or amu^{-1}·sr^{-1}. If the spectrum has also been integrated over the emission solid angle, the appropriate units would be eV^{-1} or amu^{-1}.

5.253
interface
boundary between two bulk phases having different chemical, elemental or physical properties

5.254
interface width, observed
⟨AES, XPS, SIMS⟩ distance over which a 16 % to 84 %, or 84 % to 16 %, change in **signal intensity** is measured at the junction of two dissimilar matrices, the thicknesses of which are more than six times that distance

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

5.255
interfacial region
volume between two bulk phases having chemical, elemental or physical properties different from either bulk phase

5.256
interference signal
⟨mass spectrometry, optical spectroscopy, TXRF⟩ signal, measured at the mass, energy or wavelength position of interest, due to another, undesired, species

NOTE In general laboratory use, interference could be used more broadly to indicate electrical **noise**, line pick-up or other unwanted contributions to the detected signal.

5.257
internal carbon referencing
⟨XPS⟩ method by which the **charging potential** of a particular sample is determined from a comparison of the experimentally determined C 1s **binding energy** arising from a specific carbon group within the sample with a standard binding energy value for that carbon group

cf. **adventitious carbon referencing**, **Fermi level referencing**

NOTE A hydrocarbon group within the sample is often used for this purpose.

5.258
internal scattering
process in which some particles strike internal **surfaces** of the spectrometer in such a way that scattered or secondary particles are detected as unwanted intensity in the spectrum

5.259
ion beam
directed **flux** of charged atoms or molecules

[ASTM E673-03[1]]

5.260
ion beam induced mass transport
movement of atoms in a sample caused by ion bombardment

5.261
ion beam ratio
⟨GDMS⟩ intensity of the analyte ion divided by the intensity of the matrix ion, both corrected for isotopic abundance

5.262
ion image
⟨SIMS⟩ two-dimensional representation of the spatial distribution of the amount of a particular **secondary ion** emitted from within a specific area of the sample

cf. **map, elemental**

5.263
ion implantation
injection of ions into a sample

[ASTM E673-03[1]]

5.264
ion lifetime
average time that an ion exists in a particular electronic configuration, for example as a vacancy in a particular shell of an atom

5.265
ion neutralization
⟨ISS, SIMS⟩ **charge exchange** process in which an ion loses its charge through interactions with a material **surface** or with gas-phase atoms or molecules

5.266
ion-scattering spectrometer
⟨ISS⟩ instrument capable of generating a **primary beam** of principally monoenergetic, singly charged, low-energy ions and determining the energy distribution of the **primary ions** that have been scattered from a solid **surface** through a known angle

[ASTM E673-03[1]]

NOTE For applications in surface chemical analysis, the primary ions are commonly of rare-gas atoms with energies in the range 0,1 keV to 10 keV.

5.267
ion-scattering spectrum
⟨ISS⟩ plot of the intensity of ions, scattered from a sample, as a function of the ratio of the **scattered-ion energy** to the incident-ion energy

5.268
ion species
type and charge of ion

EXAMPLES Ar^+, O^- and H_2^+.

NOTE If an isotope is used, it should be specified.

5.269
ion yield, fractional
ratio of the number of ions of a particular species sputtered from a sample to the total number of particles of that species sputtered from that sample

cf. **fractional sputtering yield**, **partial sputtering yield**

5.270
ion yield, negative
ratio of the total number of negative **secondary ions** sputtered from a sample to the total number of incident primary particles

cf. **fractional ion yield**, **partial ion yield**, **total ion yield**

5.271
ion yield, positive
ratio of the total number of positive **secondary ions** sputtered from a sample to the total number of incident primary particles

cf. **fractional ion yield**, **partial ion yield**, **total ion yield**

5.272
ion yield, useful
〈SIMS〉 ratio of the number of ions of a particular isotope detected to the total number of atoms of the same element sputtered from the sample

5.273
ionization efficiency
ratio of the number of ions formed to the number of electrons, ions or photons used in an ionization process

[IUPAC[3]]

5.274
ionization, electron impact
〈GDS〉 ionization resulting from collision of an atom, molecule or ion with an electron

NOTE 1 For example, $M + e^- \rightarrow M^+ + e^-$, where M^+ is a transition metal ion.

NOTE 2 Electron impact ionization is possible only if the **kinetic energy** of the relative motion of the collision partners exceeds the difference between (1) the product of the magnitude of the electronic charge and the ionization potential of the particle to be ionized and (2) the potential energy of that particle prior to collision.

NOTE 3 In a **glow discharge** used for surface chemical analysis, electron impact ionization usually accounts for a large fraction of the total ionization occurring in the **plasma**. Therefore, it is a very important physical mechanism for **glow discharge mass spectrometry**.

5.275
ionization, Penning
〈GDS〉 ionization resulting from collision with an atom that is in an electronically **excited state**

NOTE 1 For example, $Ar^{ms} + M \rightarrow Ar + M^+$, where Ar^{ms} is a metastable Ar atom and M is a transition metal.

NOTE 2 Penning ionization is possible only if the sum of the excitation potential of the excited-state atom and the **kinetic energy** of the relative motion of the collision partners exceeds the difference between (1) the product of the magnitude of the electronic charge and the ionization potential of the particle that is to be ionized and (2) the potential energy of that particle prior to collision.

NOTE 3 The probability of Penning ionization is directly related to the excited-state lifetime of the excited-state collision partner. For this reason, Penning ionization usually occurs through collisions with metastable species.

NOTE 4 In a **glow discharge** used for surface chemical analysis, Penning ionization is usually an important ionization mechanism, owing to the fact that the metastable energy levels of Ar, the discharge gas most commonly employed, lie sufficiently above the ionization potentials of most atomic analytes.

5.276
jump ratio
⟨EPMA, TXRF⟩ ratio of the X-ray **absorption coefficient** at an energy just above an absorption edge to that at an energy just below the edge

NOTE X-ray absorption spectra can have complex shapes for X-ray energies in the vicinity of photoionization thresholds, and a well-defined edge is not always observed at the threshold.

5.277
kinematic factor
⟨EIA, RBS, ISS⟩ ratio of the projectile energy after an elastic collision to that before the collision in the laboratory frame of reference

NOTE The symbol K is often used for the kinematic factor and might have a subscript added in ISS or **RBS** measurements, denoting the target atom as either, say, K_{Si} or K_{28}. The subscript for atomic mass is preferred since the isotope is correctly identified.

5.278
kinetic energy
energy of motion

NOTE The energy of a charged particle due to motion is not necessarily constant and varies with the local electric potential. If all local electrodes are at ground potential, the kinetic energy of the particle varies with the local **vacuum level**. This vacuum level may vary over a range of 1 eV in different regions of **AES** and **XPS** instruments and measured electron energies may similarly vary. This variation is removed if the kinetic energies are referred to the **Fermi level**. In XPS, by convention, the Fermi level is always used but in AES both **vacuum** and **Fermi level referencing** are practised. Instruments capable of both AES and XPS are Fermi level referenced. Fermi level referencing is recommended for accurate measurements of energies in AES. In **electron spectrometers**, Fermi level referenced energies are typically 4,5 eV greater than those referenced to the vacuum level. It is convenient in AES to assume a **standard vacuum level** of 4,500 eV above the Fermi level so that the energies of **Auger electron** peaks, referenced to the Fermi level, can be converted in a consistent way to energies referenced to the vacuum level and *vice versa*.

5.279
knock-in
knock-on
recoil implantation
movement of constituent atoms of the sample deeper into the sample as a result of collisions with a primary particle

cf. **atomic mixing**, **cascade mixing**, **collision cascade**

NOTE The knock-in process refers only to the forward movement of the constituent atoms (in the direction of the primary bombardment) whereas cascade mixing refers, in addition, to the backward movement of these atoms.

5.280
Koopmans energy
calculated energy of an electron in an orbital, on the assumption that its removal to infinity is unaccompanied by electronic **relaxation**

[ASTM E673-03[1]]

5.281
Langmuir-Blodgett film
LB film
film comprising one or more **monolayers** of organic molecules

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

5.282
line scan
plot of the output **signal intensity** from the spectrometer, the signal intensity from another detector, or processed intensity information from the available software along a line corresponding to a line on the sample **surface**

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

5.283
linear cascade
linear collision cascade
dilute **collision cascade** in which the number of atoms set in motion by an energetic primary particle is proportional to the amount of recoil energy deposited in the material

cf. **spike**, **thermal spike**

NOTE The **sputtering** of solids by monatomic **primary ions** in the energy range below 20 keV, usually used for surface analysis, is often assumed to be described by a linear collision cascade.

5.284
lineshape
measured shape of a particular spectral feature

5.285
lineshape, intrinsic
lineshape, natural
⟨AES, UPS, XPS⟩ **lineshape** of a spectral feature after removal of all instrumental contributions

NOTE 1 A background might or might not be removed from the lineshape of interest, depending on the circumstances. The procedure for determination of the intrinsic lineshape might be complex and should therefore be clearly stated.

NOTE 2 In **AES**, a background due to **inelastic scattering**, **secondary electrons** or **backscattered electrons** might be removed. See **inelastic background**, **Sickafus background**.

NOTE 3 In **XPS**, a background due to other **photoemission** processes and to inelastic scattering processes in the sample might be removed. See inelastic background.

5.286
linewidth, intrinsic
linewidth, natural
⟨AES, UPS, XPS⟩ full width at half maximum intensity of a spectral feature for a particular transition after removal of the background and all instrumental terms including the contribution of the exciting source

NOTE The measured linewidth is determined from the measured **lineshape** which is a convolution of the **intrinsic lineshape** with broadening contributions of the sample and of the instrument (for example, the linewidth of the X-ray source in **XPS** and **spectrometer energy resolution** in both **AES** and XPS).

5.287
linewidth, intrinsic
⟨instrument⟩ See **resolution of a spectrometer**.

5.288
liquid-metal ion gun
LMIG
ion gun utilizing a liquid-metal Taylor cone as the source of the **primary ions**

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

5.289
map
image (deprecated)
two- or three-dimensional representation of the sample **surface** where the information at each point in the representation, given by a brightness or colour or as a length in a third dimension, is related to the output signal from a detector or processed intensity information from the available software

NOTE 1 By convention, the term image is usually applied to cases where the information is primarily optical.

NOTE 2 Maps are usually formed either by using a rectangular **raster** of the **primary beam** or by using an imaging detection system.

NOTE 3 Map intensities can be presented in a normalized fashion to have the maximum and minimum signal intensities set at, for example, full white and full black, respectively, or on a colour scale. The contrast scale should be defined.

5.290
map, chemical
map using signals proportional to the quantity of an element in a particular chemical state in the sample

5.291
map, elemental
map using signals proportional to the quantity of an element present in the sample

5.292
mass accuracy
systematic deviation of a measured mass from a reference value for that mass

NOTE In practice, this accuracy can be expressed as a fractional error (i.e. the ratio of the mass error to the mass at which that error is established) or as an absolute error (i.e. the mass error at a particular mass). Most commonly, the fractional error is used and is expressed in parts per million. This fractional error is the **relative mass accuracy**.

5.293
mass accuracy, relative
quotient of the **mass accuracy** and the mass relevant to that accuracy value

NOTE In practice, this accuracy can be expressed, as for mass accuracy (see the Note in 5.292), as a fractional error, often expressed in parts per million, or as an absolute error (the mass accuracy or the mass error at a particular mass). Most commonly, the relative mass accuracy is used.

5.294
mass analyser
device for dispersing and detecting particles as a function of their **mass-to-charge ratio**

5.295
mass spectrum
plot of the measured particle signal as a function of particle **mass-to-charge ratio**

5.296
mass-to-charge ratio
modulus of the quotient of the particle mass in **u** and the particle charge in units of electronic charge

5.297
matrix effects
change in the intensities or spectral information per atom of the analyte arising from change in the chemical or physical environment

NOTE Examples of these environments are: varying sample morphologies (e.g. **thin films**, clusters, fibres, nanostructures) of different dimensions, the amorphous or crystalline state, changes of matrix species, and the proximity of other physical phases or **chemical species**.

5.298
matrix factor
factor, arising from the composition of the matrix, for multiplying the quotient of the measured intensity and the appropriate sensitivity factor in equations to determine the composition using surface analytical techniques

cf. **average matrix sensitivity factor**, **pure-element sensitivity factor**

NOTE In methods such as **AES**, the matrix factor is determined in part by the composition of the sub-surface material and in part by the composition of the **analysis volume** in the sample.

5.299
mean free path, transport
λ_{tr}
average distance that an energetic particle must travel before its momentum in its initial direction of motion is reduced to 1/e of its initial value by **elastic scattering** alone

cf. **inelastic mean free path**

NOTE For a homogeneous and isotropic solid, in which only **binary elastic scattering** occurs, the transport mean free path is related to the **transport cross section**, σ_{tr}, by

$$\lambda_{tr} = \frac{1}{N\sigma_{tr}}$$

where N is the number of scattering centres per unit volume.

5.300
metastable ion
ion that spontaneously fragments between emission and detection

cf. **background, metastable**

NOTE 1 In general, metastable ions have a lifetime of less than 1 µs.

NOTE 2 In **reflectron time-of-flight** mass spectrometers, the decay of metastable ions leads to broad peaks at a mass dependent on the drift energy and **reflector voltage**. Good design minimizes these **background signals**.

5.301
modulation
⟨AES, differential spectrum⟩ periodic waveform added to the spectrometer **pass energy** or applied to the sample in order to generate a display of the **differential spectrum**

NOTE The amplitude of the modulation should be given as eV peak-to-peak, thereby including any relevant geometrical **factor** of the spectrometer, rather than volts peak-to-peak. The frequency and waveform shape should also be given.

5.302
molecular fragment
ion or neutral particle that was part of a larger molecular structure and contains information about that structure

5.303
molecular image
image of a **surface** formed from ions characteristic of a particular molecule

cf. **static limit**

5.304
molecular ion
ion formed by the removal from (positive ions) or addition to (negative ions) a molecule of one or more electrons without **fragmentation** of the molecular structure

[IUPAC[3]]

cf. **deprotonated molecular ion**, **protonated molecular ion**

NOTE Protonated and deprotonated molecular ions are often of greater intensity than the molecular ion.

5.305
molecular ion, deprotonated
molecular ion that has lost a proton to form a negative ion

5.306
molecular ion, protonated
molecular ion that has gained a proton to form a positive ion

5.307
monolayer
⟨chemisorption, physisorption, segregation⟩ complete coverage of a substrate by one atomic or molecular layer of a species

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

5.308
monolayer capacity
⟨chemisorption⟩ amount of adsorbate which is needed to occupy all adsorption sites as determined by the structure of the adsorbent and by the chemical nature of the adsorptive

[Appendix to Manual of symbols and terminology for physico-chemical quantities and units[7]]

5.309
monolayer capacity
⟨physisorption⟩ amount of adsorbate which is needed to cover the **surface** with a complete **monolayer** of atoms or molecules in a close-packed array

[Appendix to Manual of symbols and terminology for physico-chemical quantities and units[7]]

NOTE The type of close packing needs to be stated.

5.310
multilayer
structure composed of two or more chemically distinct layers

cf. **delta layer**

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

5.311
multilayer
⟨chemisorption, physisorption⟩ coverage of a substrate surface by more than one atomic or molecular layer of the adsorptive or segregated species

cf. **monolayer**

5.312
multiplet splitting
〈AES〉 splitting of an **Auger electron** line into two or more components, caused by the interactions of the atomic vacancies created by the **Auger process**

5.313
multiplet splitting
exchange splitting
〈XPS〉 splitting of a photoelectron line caused by the interaction of the unpaired electron, created by **photoemission**, with other unpaired electrons in the atom

[ASTM E673-03[1]]

5.314
negative glow
glow region (deprecated)
〈GDS〉 region of a **glow discharge** from which most light is emitted and from which analytical signals for surface chemical analysis are usually derived

cf. **cathode layer**, **positive column**, **anode glow**

5.315
noise
time-varying disturbances superimposed on the analytical signal with fluctuations, leading to uncertainty in the **signal intensity**

NOTE 1 An accurate measure of noise can be determined from the standard deviation of the fluctuations. Visual or other estimates, such as peak-to-peak noise in a spectrum, might be useful as semi-quantitative measures of noise.

NOTE 2 The fluctuations in the measured intensity can arise from a number of causes, such as **statistical noise** and electrical interference.

5.316
noise, statistical
noise in the spectrum due solely to the statistics of randomly detected single events

NOTE 1 For single-particle counting systems exhibiting Poisson statistics, the standard deviation of a large number of measures of an otherwise steady count rate, N, each in the same time interval, is equal to the square root of N.

NOTE 2 In multidetector systems, the data processing required to generate the output spectrum might lead to statistical correlation between adjacent channels and also an apparent noise in each channel that is less than Poissonian.

5.317
nominal mass
particle mass, in **unified atomic mass units**, **u**, rounded to the nearest integer

5.318
oligomer molecule
molecule of intermediate relative molecular mass, the structure of which essentially comprises a small plurality of units derived, actually or conceptually, from molecules of lower relative molecular mass

[IUPAC[3]]

NOTE 1 A molecule is regarded as having an intermediate relative molecular mass if it has properties which vary significantly with the removal of one or a few of the units.

NOTE 2 If a part or the whole of the molecule has an intermediate relative molecular mass and essentially comprises a small plurality of units derived, actually or conceptually, from molecules of lower relative molecular mass, it can be described as oligomeric or by the term oligomer used adjectivally.

5.319
optical aperture
optical gate (deprecated)
system consisting of a combination of a photon or particle lens and an aperture in an optical or particle spectrometer to limit the field of view for signal detection

5.320
orbital energy
⟨XPS⟩ **Koopmans energy** corrected for intra-atomic **relaxation**

[ASTM E673-03[1]]

5.321
overpotential
U
⟨AES⟩ ratio of the electron **beam energy** to the **binding energy** of a particular shell or sub-shell of an atom

NOTE Overpotential values are typically in the range 2 to 200.

5.322
parent ion
ion that subsequently fragments into smaller ions or neutral particles

5.323
partial intensity
⟨AES, EPES, REELS, XPS⟩ total number of electrons in an electron spectrum, originating from a given **Auger transition** or photoelectric transition, or associated with **primary electrons** backscattered from a **surface**, per unit of excitation or of backscattering, that reach the detector after participating in a given number of inelastic interactions of a given type

NOTE 1 The zero-order partial intensity is the number of electrons, originating from the peak of interest in the spectrum, that reach the detector without any inelastic interaction in the solid or the vacuum. This intensity is the area under the photoelectron or **Auger electron** peak of interest or under the peak corresponding to the elastically **backscattered electrons**.

NOTE 2 In a solid, an electron can experience different types of **inelastic scattering**, such as those associated with volume or surface effects. The inclusion or exclusion of specific types of inelastic scattering in calculations of partial intensities should be stated.

NOTE 3 The partial intensity is a dimensionless number.

5.324
partial intensity, reduced
⟨AES, EPES, REELS, XPS⟩ ratio of the **partial intensity** to the zero-order partial intensity

NOTE The reduced partial intensity is a dimensionless number.

5.325
pass energy
⟨AES, ISS, XPS⟩ mean **kinetic energy** of the detected particles in the energy-dispersive portion of the energy analyser

5.326
peak area
area under a peak in a spectrum after background removal

cf. **inelastic electron scattering background subtraction**, **signal intensity**

NOTE The peak area can be expressed in **counts**, counts per second, counts·eV, counts·eV per second, counts per amu or other units.

5.327
peak energy
〈AES, EELS, ISS, UPS, XPS〉 energy value corresponding to the intensity maximum in a **direct spectrum** or to the intensity minimum (i.e. the negative excursion) for a **differential spectrum**

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

NOTE 2 For the differential spectrum in **AES**, the **modulation** or differentiating amplitude should be given.

NOTE 3 The peak energies for the differential spectrum in AES are higher in **kinetic energy** than those for the direct spectrum.

5.328
peak fitting
a procedure whereby a spectrum, generated by **peak synthesis**, is adjusted to match a measured spectrum

NOTE 1 A least-squares optimization procedure is generally used in a computer programme for this purpose.

NOTE 2 The selected peak shape and the background shape should be defined. Any constraints imposed on the adjustment process should also be defined.

5.329
peak synthesis
curve resolving (deprecated)
a procedure whereby a synthetic spectrum is generated, using either model or experimental peak shapes, in which the number of peaks, the peak shapes, the **peak widths**, the peak positions, the peak intensities and the background shape and intensity are adjusted for **peak fitting**

cf. **peak fitting**

NOTE The selected peak shape and the background shape should be defined.

5.330
peak-to-background ratio
signal-to-background ratio
ratio of the maximum height of the peak above the background intensity to the magnitude of that background intensity

NOTE 1 Signal-to-background ratio is the more commonly used term for **GDS**, where it is abbreviated to SBR. Peak-to-background ratio is the more commonly used term for types of electron spectroscopies such as **AES** and **XPS**.

NOTE 2 The method of estimating the background intensity needs to be given. For AES, the background intensity is often determined at a **kinetic energy** just above the peak of interest.

5.331
peak width
line width (deprecated)
width of a peak at a defined fraction of the peak height

cf. **intrinsic linewidth**

NOTE 1 Any background subtraction method used should be specified.

NOTE 2 The most common measure of peak width is the full width of the peak at half maximum (FWHM) intensity.

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

5.332
photoelectric effect
interaction of a photon with bound electrons in atoms, molecules and solids, resulting in the production of one or more photoelectrons

5.333
photoelectron X-ray satellite peaks
photoelectron peaks in a spectrum resulting from **photoemission** induced by characteristic minor X-ray lines associated with the X-ray spectrum of the **anode** material

[ASTM E673-03[1]]

EXAMPLES Kα′, $K\alpha_{3,4}$, $L\alpha_{5,6}$ and Kβ are all minor X-ray lines.

5.334
photoelectron X-ray satellite subtraction
removal of **photoelectron X-ray satellite peaks** from a spectrum

[ASTM E673-03[1]]

NOTE For unmonochromated Al and Mg X-rays, the satellites usually removed are $K\alpha_{3,4}$ and $K\alpha_{5,6}$. More sophisticated subtraction methods also remove the $K\alpha_2$, Kα′ and Kβ satellites.

5.335
photoemission
emission of electrons from atoms or molecules caused by the **photoelectric effect**

[ASTM E673-03[1]]

5.336
pileup
⟨EIA, RBS⟩ **counts** in a **backscattering spectrum** arising from two or more separate events that occur so closely in time that the signals are not resolved by the detection system and cause counts to be recorded in erroneous channels

cf. **dead time**

5.337
plasma
⟨GDS⟩ gas consisting of ions, electrons and neutral particles

NOTE Gases are weakly ionized in **glow discharge**.

5.338
plasma potential
space potential (deprecated)
⟨GDS⟩ electric potential of **plasma** relative to an appropriate reference such as ground potential

NOTE The plasma potential of direct current **glow discharge** varies with location in the plasma. The plasma potential of an rf glow discharge varies with both location in the plasma and time, according to the phase of the rf excitation.

5.339
plasmon
bulk plasmon
volume plasmon
excitation of valence-band electrons in a solid in which collective oscillations are generated

cf. **characteristic electron energy losses**

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

NOTE 2 Plasmons are prominent in some materials and not others.

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

5.340
polyatomic fragment
ion or neutral particle composed of three or more atoms

5.341
polyatomic ion
charged multi-atom species

NOTE Dimer and trimer ions are specific examples of polyatomic ions containing two and three atoms, respectively.

5.342
positive column
⟨GDS⟩ diffuse, luminous region of **glow discharge** between the **Faraday** and **anode dark spaces**

cf. **cathode layer**, **negative glow**, **anode glow**

NOTE The positive column is usually absent in glow discharge devices operated for surface chemical analysis, owing to the gas pressure and the small separation between the electrodes.

5.343
post-acceleration detector voltage
post-acceleration voltage
voltage applied to the front of the detector to increase the **impact energy** of incident electrons or ions

NOTE Voltages are often referred to reference points in the instrumental electronics but here the reference zero is such that a post-acceleration detector voltage of 5 kV leads to an impact energy of 5 keV, etc. Post-acceleration detector voltages of 5 kV to 20 kV are generally used.

5.344
preburn
presputtering period
⟨GDS, bulk materials⟩ period during which **preburning** occurs

NOTE 1 Preburning is used for stabilizing the **glow discharge**. Typical preburn times for **GDOES** range from 30 s to 60 s, while those for **GDMS** can be much longer.

NOTE 2 Glow discharge conditions used for preburn are usually identical to those employed during signal registration. However, for some applications, they might be different.

5.345
preburning
presputtering
⟨GDS, bulk materials⟩ process of **sputtering**, prior to signal registration, employed to allow **steady-state sputtering** to be established and analytical signals to stabilize

NOTE Preburning is used for stabilizing the **glow discharge**.

5.346
primary electron
electron extracted from a source and directed at a sample

cf. **secondary electron**

5.347
primary electron
⟨GDS⟩ electron that enters the **negative glow** region from the **cathode dark space**, having been accelerated by the strong electric field within the cathode dark space, thereby having a **kinetic energy** that is among the highest of the kinetic energies of any electrons present within the **plasma**

cf. **secondary electron** ⟨GDS⟩

NOTE This term is defined differently for **AES**, EPMA and SEM.

5.348
primary ion
ion extracted from a source and directed at a sample

cf. **probe ion**, **secondary ion**

5.349
probe ion
ionic species intentionally produced by an ion source and directed onto the sample **surface** at a known **angle of incidence** and a known energy

5.350
profile, depth
profile, vertical
chemical or elemental composition, **signal intensity** or processed intensity information from the available software measured in a direction normal to the **surface**

cf. **compositional depth profile**

5.351
profile, lateral
chemical or elemental composition, **signal intensity** or processed intensity information from the available software measured in a specified direction parallel to the **surface**

cf. **line scan**

5.352
projected range
⟨EIA, RBS, SIMS⟩ distance from the **surface** at which an energetic ion or atom comes to rest in the sample, projected along the direction of the beam

cf. **range straggling**

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

5.353
protonated ion
parent molecule to which a proton has been added to form a positive ion

5.354
pulse rate
〈SIMS〉 number of ion pulse cycles per second

cf. **repetition rate**

5.355
pulse width
〈SIMS〉 full width at half maximum of the time distribution of the pulse of ions generated by the **beam chopper** and, optionally, the use of **beam bunching**

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

5.356
pulsed extraction field
〈SIMS〉 **extraction field** around the sample that is pulsed to the working value for extracting ions for the time necessary for operation of a **time-of-flight** mass spectrometer but is otherwise at a low value

NOTE This is the usual mode in time-of-flight **SIMS** systems either for studying insulators, where the **charge neutralization** is established whilst the **extraction field** is off, or for **depth profiling** using a second **ion beam** whilst the extraction field is off.

5.357
quantitative analysis
determination of the amounts of analytes detected in a sample

NOTE 1 The analytes can be elemental or compound in nature.

NOTE 2 The amounts can be expressed, for example, as atomic or mass percent, atomic or mass fraction, mole or mass per unit volume, as appropriate or as desired.

NOTE 3 The sample material might be inhomogeneous so that a particular model structure might need to be assumed in the interpretation. Details of that model need to be stated.

5.358
radial sectioning
sample preparation in which a sample is polished by a cylinder in order to expose compositional changes below the original sample **surface** with the intent that the depth of these layers can be related to the position on the surface created by the cylinder

cf. **angle lapping**, **ball cratering**

5.359
radiation-enhanced diffusion
radiation-induced diffusion
atom movement in the solid, well beyond the typical penetration depth of an incident particle, due to particle beam damage or bombardment-induced defects

[ASTM E673-03[1]]

5.360
radical
free radical (deprecated)
molecular entity possessing an unpaired electron

NOTE 1 Molecular entities such as $^{\bullet}CH_3$, $^{\bullet}SnH_3$ and $Cl^{\bullet}$ have formulae in which the dot symbolizing the unpaired electron is placed so as to indicate the atom of highest spin density, if this is possible. Paramagnetic metal ions are not normally regarded as radicals.

NOTE 2 Depending upon the core atom that possesses the unpaired electron, the radicals can be described as carbon-, oxygen-, nitrogen- or metal-centred radicals. If the unpaired electron occupies an orbital having considerable "s" or more or less pure "p" character, the respective radicals are termed σ- or π-radicals.

NOTE 3 The adjective "free" is no longer used. The term free radical might in future be restricted to those radicals that do not form parts of radical pairs.

5.361
radical ion
radical carrying an electric charge

NOTE A positively charged radical is called a "radical cation" (e.g. the benzene radical cation $C_6H_6^{\bullet+}$); a negatively charged radical is called a "radical anion" (e.g. the benzene radical anion $C_6H_6^{\bullet-}$ or the benzophenone radical anion $Ph_2C\text{-}O^{\bullet-}$). Commonly, but not necessarily, the odd electron and the charge are associated with the same atom. Unless the positions of unpaired spin and charge can be associated with specific atoms, superscript dot and charge designations should be placed in the order $\bullet+$ or $\bullet-$ as suggested by the name "radical ion" (e.g. $C_3H_6^{\bullet+}$).

5.362
random raster
digital **raster** array in which the coordinates of sequential ion pulses filling a frame are random

NOTE 1 The coordinates may be addressed in the same "random" sequence in each frame.

NOTE 2 A random raster, as opposed to a traditional or saw-tooth raster, can be used for analysing insulating samples to reduce the instantaneous accumulation of charge in any local region.

5.363
range straggling
⟨EIA, RBS, SIMS⟩ standard deviation of the **projected ranges** of energetic ions or atoms of a given energy

cf. **transverse straggling**

5.364
raster
two-dimensional pattern generated by the deflection of a **primary beam**

NOTE Commonly used rasters cover square or rectangular areas.

5.365
raw-data file
unprocessed-data file of information provided by an instrument

NOTE For **time-of-flight SIMS** instruments, this file usually contains the x- and y-coordinates of the **ion beam raster** address as well as the recorded flight times and signal intensities since these files are used retrospectively to generate **secondary-ion maps** or spectra from the whole or selected parts of the map, or to generate these from all or selected time regions.

5.366
recoil effect
⟨EPES⟩ effect resulting from the change in movement of a scatterer atom as a result of quasi-elastic electron scattering

NOTE The energy shift and energy broadening of the **quasi-elastic peak** for a scattered electron beam due to atomic recoil depend on the mass of the scatterer atom, the energy of the **primary electrons** and the **scattering angle**. In addition, the energy broadening due to atomic recoil depends on the sample temperature. The quasi-elastic peak in **EPES** for multicomponent materials contains contributions from each component. Recoil effects are most easily observable in electron spectra taken at high **energy resolution** with low atomic number scattering atoms. Hydrogen can be directly detected by its recoil shift.

5.367
recombination
ion-electron recombination
〈GDS〉 addition of an electron to an ion with a net positive charge, resulting in a net charge that is one elementary charge unit more negative

NOTE Energy and momentum cannot be simultaneously conserved in an ion-electron recombination process that involves the collision of only an ion and an electron and that releases no additional particles. For this reason, recombination proceeds only through the involvement of a third collision partner, such as another electron or a **surface**, or through the release of a photon.

5.368
recombination, radiative
〈GDS〉 **ion-electron recombination** involving the release of a photon

5.369
redeposition
deposition of sputtered sample material back onto the sample **surface**

5.370
reference material
RM
material or substance one or more of whose property values are sufficiently homogeneous and well established to be used for the calibration of an apparatus, for the assessment of a measurement method or for assigning values to materials

[ISO Guide 30:1992[8]]

NOTE Some RMs involving surface properties can be in the form of wafers or foils. For these, the material is often homogeneous for the property values across the **surface** but not in the direction perpendicular to the surface and into the bulk. Examples are a) implanted silicon wafers to calibrate dopant levels and b) thin oxide layers on substrates to calibrate depth or thickness in analytical **depth profiling** instruments.

5.371
reference material, certified
CRM
reference material, accompanied by a certificate, one or more of whose property values are certified by a procedure which establishes its traceability to an accurate realization of the unit in which the property values are expressed, and for which each certified value is accompanied by an uncertainty at a stated level of confidence

[ISO Guide 30:1992[8]]

NOTE 1 CRMs are usually prepared in batches for which the property values are determined within stated uncertainty limits by measurements on samples representative of the whole batch.

NOTE 2 All CRMs lie within the definition of “measurement standards” given in the international vocabulary of metrology, ISO/IEC Guide 99[9].

NOTE 3 Some **RMs** and CRMs have properties which, because they cannot be correlated with an established chemical structure or for other reasons, cannot be determined by exactly defined physical and chemical measurement methods. Such materials include certain biological materials such as vaccines to which an international unit has been assigned by the World Health Organization.

5.372
reference method
thoroughly investigated method, clearly and exactly describing the necessary conditions and procedures for the measurement of one or more property values, that has been shown to have accuracy and precision commensurate with its intended use and that can therefore be used to assess the accuracy of other methods for the same measurement, particularly in permitting the characterization of a **reference material**

[ISO Guide 30:1992[8]]

5.373
reflector voltage
⟨SIMS⟩ voltage set on the reflector electrode of a **reflectron** mass spectrometer with the zero referenced such that an ion emitted from the sample with an energy numerically equal to the reflector voltage would just be on the point of reflection or transmission by the reflector electrode

5.374
reflectron
⟨SIMS⟩ **time-of-flight** mass spectrometer in which ions are reflected through an angle approaching 180° in order to reduce the flight time dependence on the particular energy of the ions

5.375
relative instrument spectral response function
RISR
⟨AES, SIMS, XPS⟩ ratio of the **spectrometer response function** to the response function of a reference instrument, or the average for several such instruments, as a function of energy (**AES**, **XPS**, etc.) or mass (SIMS)

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

5.376
relative resolution of a spectrometer
⟨energy, mass or optical⟩ ratio of the **resolution of a spectrometer** at a given energy, mass or wavelength to that energy, mass or wavelength

cf. **resolving power of a spectrometer**

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

NOTE 2 It can be convenient to specify the relative **energy resolution** of an **electron spectrometer**, the relative mass resolution of a mass spectrometer or the relative wavelength resolution of an optical spectrometer.

NOTE 3 In practice, the relative resolution of a spectrometer can be deduced using a source with an emission line of known width, usually chosen to be as narrow as possible.

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

NOTE 5 The relative resolution is often expressed as a percentage.

5.377
relative sputtering rate
quotient of the **sputtering rate** of a sample and the sputtering rate of a reference sample sputtered under the same conditions

5.378
relaxation
process by which an atom, molecule or ion is transformed from a higher potential-energy state to a lower potential-energy state

cf. **relaxation, electronic**

5.379
relaxation, electronic
relaxation resulting from the transition of an electron between energy levels, resulting in the release of energy

NOTE The energy release can result in the ejection of a photon or other particle.

5.380
relaxation energy
〈XPS〉 energy associated with intra-atomic or extra-atomic electronic readjustment to the removal of an atomic electron, so as to minimize the energy of the **final state** of the system

[ASTM E673-03[1]]

5.381
relaxation energy, extra-atomic
screening energy
diminished energy of an ionized atom in a solid due to coulombic attraction of electrons in the immediate environment

5.382
repeat unit, polymer
smallest structure that, repeated many times, describes the molecular structure of the polymer

5.383
repetition rate
〈SIMS〉 rate at which the whole cycle of primary-ion pulse, ion extraction, mass analysis and removal of slow ions is repeated to build up a **mass spectrum** in a **time-of-flight** mass spectrometer

5.384
resolution, energy
full width at half maximum (FWHM) intensity of the measured energy distribution for monoenergetic particles

5.385
resolution, lateral
distance, measured either in the plane of the sample **surface** or in a plane at right angles to the axis of the image-forming optics, over which changes in composition can be separately established with confidence

NOTE 1 The choice of plane should be stated.

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

5.386
resolution of a spectrometer
spectrometer resolution
〈energy, mass or optical〉 contribution of the spectrometer to the measured full width at half maximum (FWHM) intensities of spectral peaks above their local backgrounds

cf. **relative resolution of a spectrometer**, **resolving power of a spectrometer**

NOTE 1 It can be convenient to specify the **energy resolution** of an **electron spectrometer**, the mass resolution of a mass spectrometer or the wavelength resolution of an optical spectrometer.

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

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

5.387
resolution, system
⟨EIA, RBS⟩ energy or depth resolution measured in the **backscattering spectrum** for a monoenergetic incident-ion beam

5.388
resolving power of a spectrometer
⟨energy, mass or optical⟩ ratio of the energy, mass or wavelength to the **resolution of the spectrometer** at that energy, mass or wavelength

cf. **relative resolution of a spectrometer**

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

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

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

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

5.389
resonance reaction
⟨EIA⟩ nuclear reaction that has a narrow peak in the **nuclear reaction cross section** as a function of energy, the nuclear reaction cross section at the peak being so much larger than the nuclear reaction cross sections at adjacent energies on either side of the peak that essentially all the particles detected from the reaction are due to the peak

[Adapted from ASTM E673-03[1]]

5.390
sample area viewed by the analyser
two-dimensional region of a sample **surface**, measured in the plane of that surface, from which the analyser can collect an analytical signal from the sample or a specified percentage of that signal

5.391
sample bias
potential applied to the whole or part of the sample, referenced to the potential of the sample holder

cf. **sample voltage**

5.392
sample charging
change in the electrical potential in the sample or on the sample **surface** caused by particle or photon bombardment

5.393
sample voltage
voltage of the sample referenced to ground

cf. **sample bias**

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

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

5.394
scattered-ion energy
⟨ISS⟩ **kinetic energy** of a **primary ion** after a collision

NOTE Following **binary elastic scattering**, the kinetic energy of the primary or **probe ion**, E_s, is given by:

$$E_s = E_0\left[M_0/(M_0+M_1)\right]^2\left\{\cos\theta+\left[(M_1/M_0)^2-\sin^2\theta\right]^{1/2}\right\}^2$$

where

E_s is the kinetic energy of the scattered probe ion;

E_0 is the kinetic energy of the incident probe ion prior to scattering;

M_0 is the mass of the probe ion;

M_1 is the mass of the target atom;

θ is the angle between the initial and final velocity vectors for the probe ion, as determined from a common origin in the laboratory coordinate system, expressed as a value between 0° and 180°.

5.395
scattered-ion energy ratio
⟨ISS⟩ ratio of the **scattered-ion energy** to the energy of the incident **probe ion** prior to a collision

5.396
scattered-ion intensity, experimental
⟨ISS⟩ measured response of the energy filtering and detection system as a consequence of bombarding the sample material with an **ion beam**, usually presented as the ordinate of an **ion-scattering spectrum**

5.397
scattered-ion intensity, theoretical
⟨ISS⟩ calculated intensity for the **probe ions** scattered into a specified solid angle at a given direction

NOTE For **binary elastic scattering**, the scattered-ion intensity is defined by:

$$I_i(\theta) = I_0 N_i P_i \alpha_i (\mathrm{d}\sigma_i/\mathrm{d}\Omega)\theta\,\Delta\Omega\,T$$

where

$I_i(\theta)$ is the scattered-ion intensity from atoms of species i at a given **angle of scattering**, θ, in ions·s^{-1};

I_0 is the intensity of incident probe ions, in ions·s^{-1};

N_i is the number of scattering centres of species i per unit area of **surface** accessible to the incident beam, in atoms·m^{-2};

P_i is the probability that the probe ion remains ionized after interacting with an atom of species i;

α_i is the geometric or shadowing **factor** for species i in the given environment and geometry;

$(\mathrm{d}\sigma_i/\mathrm{d}\Omega)\theta$ is the **differential elastic scattering cross section** for species i, taken at the angle for which scattering is measured, i.e. the angular distribution of the scattered-ion intensity per unit **flux** of incident ions per atom of species i, in $m^2 \cdot atom^{-1} \cdot sr^{-1}$;

$\Delta\Omega$ is the solid angle of acceptance, determined by the entrance of the filtering and detection system, in sr;

T is the fractional transmission of the analysing and detection system.

5.398
screening
response arising from the atom's electrons, causing an apparent reduction in the coulomb potential of the nucleus

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

5.399
screening function
⟨IBA⟩ **factor** by which the **Rutherford cross section** is reduced as a result of **screening** in a given situation

5.400
secondary cathode
⟨GDS⟩ electrically conductive mask, containing an aperture, used to allow **sputtering** of an electrically non-conductive sample **surface** in a direct-current **glow discharge** device

NOTE 1 The secondary cathode is placed in direct contact with the insulating-sample surface, and both the secondary cathode and the surface of the sample within the aperture are exposed to the glow discharge. The secondary cathode is held at **cathode** potential, resulting in sputtering of its surface. Some of the material sputtered from the secondary cathode is deposited on the insulating-sample surface within the aperture, causing that surface to become electrically conductive. This results in sputtering of the insulating sample.

NOTE 2 When electrically non-conductive samples must be analysed, the secondary-cathode technique provides a useful alternative to an rf glow discharge.

5.401
secondary electron
electron, generally of low energy, leaving a **surface** as a result of an excitation induced by an incident electron, photon, ion or neutral particle

NOTE By convention, electrons with energies $\leqslant$50 eV are considered as secondary electrons unless otherwise specified. Calculations of the energy distribution of the electrons emitted from a surface show that 50 eV is a useful cut-off energy to contain most of the electrons. The cut-off is artificial, and secondary electrons with energies greater than 50 eV usually exist. This convention is not usually observed for **GDS**.

5.402
secondary electron
⟨GDS⟩ electron with a **kinetic energy** intermediate between the kinetic energies of primary and **thermalized electrons**, produced through ionization or incomplete thermalization of **primary electrons**

NOTE This term is defined differently for general use in 5.401. Both definitions are used in **GDS**, depending on the context.

5.403
secondary-electron yield
secondary-electron emission coefficient
δ
⟨AES, EPMA⟩ ratio of the total number of electrons emitted from a sample with energies less than 50 eV to the total number of electrons incident at a given energy and **angle of incidence**

5.404
secondary-electron yield
secondary-electron emission coefficient
⟨GDS, SIMS⟩ ratio of the total number of electrons emitted from a sample to the total number of particles incident upon the sample **surface**

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

5.405
secondary-electron yield, total
σ
⟨AES, EPMA⟩ ratio of the total number of electrons emitted from a sample to the total number of electrons incident at a given energy and **angle of incidence**:

$$\sigma = \delta + \eta$$

where δ is the **secondary-electron yield** and η is the **backscattering coefficient**

cf. **backscattering yield**, **secondary-electron yield**

NOTE The total secondary-electron yield is often simply called the secondary-electron yield. This leads to confusion with the term of that name which is restricted to **secondary electrons** with energies $\leqslant$50 eV.

5.406
secondary ion
ion ejected from a sample **surface** as a result of energy and momentum transfer from a **primary ion**

5.407
secondary-ion angular distribution
number of **secondary ions** as a function of **angle of emission**

5.408
secondary-ion energy distribution
number of **secondary ions** as a function of their **kinetic energy** at a specified collection angle

5.409
secondary-ion yield
ratio of the total number of ions sputtered from a sample to the total number of ions incident with a given mass, energy, charge and **angle of incidence**

5.410
segregation
partitioning of a species from one region to another as a result of kinetic or thermodynamic effects

NOTE Segregation is often observed at **surfaces** and **interfaces**.

5.411
selected-area aperture
⟨XPS, SIMS⟩ aperture in the electron or ion optical system restricting the detected signal to a small area of the sample **surface**

cf. **optical aperture**

5.412
self-absorption
⟨GDOES⟩ absorption of emitted light by a species, identical to the emitting species, positioned between the emitting species and the optical detector

NOTE Self-absorption results in non-linear calibration curves. Further, it produces broadened spectral peaks because the probability of photon absorption is at a maximum near the peak maximum.

5.413
self-assembled monolayer
SAM
film, one molecule thick, covalently assembled on a **surface**

5.414
self-reversal
⟨GDOES⟩ severe **self-absorption** that produces a local minimum of intensity near the centre of a spectral peak

5.415
sensitivity factor, absolute elemental
coefficient for an element by which the measured intensity for that element is divided to yield the atomic concentration or atomic fraction of the element present in the sample

cf. **relative elemental sensitivity factor**

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

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

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

NOTE 4 Sensitivity factors depend on parameters of the excitation source, the spectrometer and the orientation of the sample to these parts of the instrument. Sensitivity factors also depend on the matrix being analysed, and in **SIMS** this has a dominating influence.

5.416
sensitivity factor, average matrix relative
AMRSF
⟨AES, XPS⟩ coefficient proportional to the intensity, calculated for an element in an average matrix, by which the measured intensity for that element is divided in calculations to yield the atomic concentration or atomic fraction of the element present in the sample

cf. **sensitivity factor**, **relative elemental sensitivity factor**, **pure-element relative sensitivity factor**

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

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

NOTE 3 The source of sensitivity factors should be given. **Matrix factors** are taken to be unity for average matrix relative sensitivity factors.

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

5.417
sensitivity factor, pure-element relative
PERSF
⟨AES, XPS⟩ coefficient, proportional to the intensity measured for a pure sample of an element, by which the measured intensity for that element is divided in calculations to yield the atomic concentration or atomic fraction of the element present in the sample

cf. **sensitivity factor**, **relative elemental sensitivity factor**, **average matrix relative sensitivity factor**

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

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

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

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

5.418
sensitivity factor, relative
RSF
⟨GDMS⟩ coefficient for an element by which the measured intensity of a mass peak for that element, divided by the measured intensity of a mass peak for a matrix element, is multiplied to yield the mass fraction of that element in the sample divided by the mass fraction of the matrix element

NOTE For a given **GDMS** instrument, the relative sensitivity factors for all elements in the periodic table usually fall within approximately one order of magnitude, making semi-quantitative GDMS analysis possible without the use of **reference materials** for calibration. However, quantitative GDMS analysis requires the use of reference materials with a matrix similar to that of the sample in order to measure the relative sensitivity factors for the elements of interest in that matrix using that particular GDMS instrument.

5.419
sensitivity factor, elemental relative
⟨AES, XPS, TXRF⟩ coefficient proportional to the **absolute elemental sensitivity factor**, where the constant of proportionality is chosen such that the value for a selected element and transition is unity

NOTE 1 Elements and transitions commonly used are C 1s or F 1s for **XPS** and Ag $M_{4,5}VV$ for **AES**.

NOTE 2 The type of sensitivity factor used should be appropriate for the type of sample analysed, for example homogeneous samples or segregated layers.

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

NOTE 4 Sensitivity factors depend on parameters of the excitation source, the spectrometer and the orientation of the sample to these parts of the instrument. Sensitivity factors also depend on the matrix being analysed, and in **SIMS** this has a dominating influence.

5.420
sensitivity factor, elemental relative
⟨dynamic SIMS⟩ coefficient for an element by which the measured intensity of a mass peak for that element, divided by the measured intensity of a mass peak for the matrix, is multiplied to yield the atomic concentration of the element present in the sample

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

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

5.421
sensitivity factor, relative isotopic
⟨dynamic SIMS⟩ coefficient for an element by which the measured intensity for an isotope of that element, divided by the measured intensity for a matrix ion, is multiplied to yield the atomic concentration of that isotope of the element present in the sample

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

5.422
shakeoff
⟨AES, XPS⟩ multi-electron process in which two or more electrons are emitted, partitioning between them the excess **kinetic energy**

cf. **shakeup**

NOTE Shakeup leads to peak structure at kinetic energies below that of a parent peak whereas shakeoff leads to a continuum background intensity, also at kinetic energies below that of the parent peak in the electron spectrum.

5.423
shakeup
⟨AES, XPS⟩ multi-electron process in which an atom is left in an **excited state** following a photoionization or **Auger electron** process, so that the outgoing electron has a characteristic **kinetic energy** slightly less than that of the parent photoelectron

cf. **shakeoff**

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

5.424
sheath
electrode sheath
⟨GDS⟩ region of **plasma** adjacent to an electrode **surface**, characterized by a **plasma potential** that changes with distance from the electrode, being equivalent to the electrode potential at the electrode surface and approaching the plasma potential of the surrounding plasma at sufficiently large distances

NOTE These terms are usually applied to an rf **glow discharge**, though they can also be applied to a dc glow discharge.

5.425
sheath potential
⟨GDS⟩ electric potential drop across a **sheath**

NOTE In surface chemical analysis, this term is usually applied to an rf **glow discharge**, rather than to a dc glow discharge, for which terms such as **cathode fall** are much more commonly employed. However, sheath potential can also be applied to a dc glow discharge.

5.426
shots per pixel
⟨SIMS⟩ number of ion pulses incident at each pixel in an image for one **raster** frame

5.427
signal-to-noise ratio
ratio of the **signal intensity** to a measure of the total **noise** in determining that signal

cf. **statistical noise**

NOTE The noise in **AES** is often measured at a convenient region of the spectral background close to the peak.

5.428
smoothing
mathematical treatment of data to reduce the apparent **noise**

5.429
spectator hole
hole state in the electronic structure of an atom that can be present during processes such as **Auger electron** and X-ray photoelectron emission but is not created or destroyed in the process

5.430
spectrometer dispersion
analyser dispersion
⟨energy or mass⟩ quotient of the change in position, Δx, of the dispersed particles at the exit of an analyser or a spectrometer by the fractional change in particle energy, $\Delta E/E$, or mass, $\Delta m/m$

5.431
spectrometer dispersion
analyser dispersion
⟨optical⟩ quotient of the change in position, Δx, of the radiation at the exit of the spectrometer by the change in wavelength, $\Delta\lambda$

5.432
spectrometer étendue
integral of the product of the **spectrometer transmission** and an element of area of a plane **surface**, normal to the analyser axis passing through the centre of the **analysis area**, over that surface

NOTE The units of étendue can be sr·m^2·eV, sr·m^2·amu or sr·m^3.

5.433
spectrometer response function
quotient of the number of particles detected with a spectrometer by the number of such particles per solid angle and per interval of the dispersing parameter available for measurement as a function of the dispersing parameter

cf. **spectrometer transmission function**, **spectrometer étendue**

NOTE 1 The dispersing parameter is commonly energy, mass or wavelength.

NOTE 2 The units of transmission can be sr·eV, sr·amu or sr·m.

NOTE 3 The spectrometer response function is similar to the spectrometer transmission function or étendue but includes the efficiencies of all other components of the measurement chain, such as detectors and the electronic processing and recording equipment.

NOTE 4 For some methods of **quantitative analysis**, the energy dependence of the response function is needed in order to use **relative sensitivity factors**. For these cases, a function is determined which is proportional to the absolute response function, where the proportionality constant is not necessarily important.

5.434
spectrometer transmission function
analyser transmission function
quotient of the number of particles transmitted by the analyser by the number of such particles per solid angle and per interval of the dispersing parameter (e.g. energy, mass or wavelength) available for measurement as a function of the dispersing parameter

cf. **spectrometer response function**

NOTE 1 The units of transmission can be sr·eV, sr·amu or sr·m.

NOTE 2 Often, an incomplete use of the term occurs where just the solid angle of acceptance of the spectrometer, in sr, or a fraction of the 2π solid angle of available space is given. This usage is deprecated, cf. **solid angle of analyser**.

NOTE 3 This term is often used incorrectly instead of spectrometer response function, which includes contributions from the detector and the signal-processing system.

5.435
spectrum, aligned incidence
⟨EIA, ISS⟩ **backscattering spectrum** recorded with the analysing beam aligned with crystallographic axes or planes of the sample that produce **channelling**

[ASTM E673-03[1]]

5.436
spectrum, random incidence
⟨EIA, ISS⟩ **backscattering spectrum** recorded with the analysing beam incident on the sample in a direction such as to produce no **channelling**

[ASTM E673-03[1]]

5.437
spike
⟨SIMS, sputtering⟩ limited region in space and time within which the majority of atoms in an irradiated material are in rapid motion

cf. **thermal spike**

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

5.438
spin coating
coating of a thin layer of an organic material deposited from solution, under the action of high-speed rotation, on a flat substrate wetted by that solution

NOTE 1 Rotation speeds of about 4 000 revolutions per minute are commonly used, producing films generally thinner than 100 nm.

NOTE 2 Some users place a drop of solution in the centre and some flood the whole sample, prior to the high-speed rotation that removes the solvent.

5.439
spin orbit splitting
splitting of p, d or f levels in an atom arising from coupling of the spin and orbital angular momentum

5.440
sputter depth profile
SDP
compositional depth profile obtained when the surface composition is measured as material is removed by **sputtering**

NOTE In some analytical methods such as **SIMS**, the sputtering is often accomplished by the **ion beam** used for analysis, but in other methods an ion beam might need to be added.

5.441
sputtering
process in which atoms and ions are ejected from the sample as a result of particle bombardment

5.442
sputtering, equilibrium surface composition
steady-state surface composition produced by **sputtering** a homogeneous sample under non-varying conditions

5.443
sputtering, preferential
change in the equilibrium surface composition of the sample which can occur when **sputtering** multicomponent samples

5.444
sputtering rate
quotient of the amount of sample material removed, as a result of particle bombardment, by time

cf. **erosion rate**

NOTE The rate can be measured as a velocity, a mass per unit area per unit time, or some other measure of quantity per unit time.

5.445
sputtering yield
ratio of the number of atoms and ions sputtered from a sample to the total number of incident primary particles

5.446
sputtering yield, fractional
ratio of the number of atoms and ions of a particular species sputtered from a sample to the total number of atoms and ions sputtered from the sample

cf. **fractional ion yield**, **negative-ion yield**, **partial ion yield**, **partial sputtering yield**, **positive-ion yield**, **total ion yield**

5.447
sputtering yield, partial
ratio of the number of atoms and ions of a particular species sputtered from a sample to the total number of incident particles

cf. **fractional ion yield**, **fractional sputtering yield**, **negative-ion yield**, **partial ion yield**, **positive-ion yield**, **total ion yield**

5.448
static limit
⟨SIMS⟩ ion **fluence** above which any significant changes in the spectrum, arising from beam damage, are observed

NOTE 1 Classically, a limit of 10^{12} ions/cm^2 or 10^{16} ions/m^2 is taken as the limit not to be exceeded in **static SIMS**. This limit is based on one incident ion for each 1 000 surface atoms.

NOTE 2 For imaging, the total molecular signal can be used, and here the limit can be higher and reach 100 times the limit given in Note 1.

NOTE 3 For large molecules, the **damage cross section** and **disappearance cross section** are both generally larger than for small molecules, leading to a static limit lower than 10^{12} ions/cm^2.

5.449
steady-state sputtering
⟨AES, GDS, SIMS⟩ state of the **sputtering** process in which important operational and analytical parameters are unchanging over a meaningful timescale

cf. **stoichiometric sputtering**

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

5.450
stoichiometric sputtering
⟨AES, GDS, SIMS⟩ state of the **sputtering** process in which the relative amounts of the elemental components sputtered from a sample are equal to their stoichiometry within the sample

cf. **steady-state sputtering**

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

5.451
stop event
⟨SIMS⟩ registration of a particle by a time-to-digital converter

NOTE The arrival time for each ion providing a pulse at the detector is registered by the time-to-digital converter (TDC). This is a stop event. TDCs might only record a fixed number of stop events during the time following each primary-ion pulse, for example 512 or 1 024, other events being lost.

5.452
stopping cross section, electronic
⟨EIA, RBS, sputtering⟩ **stopping cross section** arising from energy transfer to the electrons of the sample

NOTE 1 The total stopping cross section is the sum of the electronic and **nuclear stopping cross sections**.

NOTE 2 The maximum of the nuclear stopping cross section occurs at energies of the order of 1 keV per nucleon, whereas that of the electronic stopping cross section occurs at above 100 keV per nucleon. The absolute value of the electronic stopping cross section maximum is significantly greater than that for the nuclear stopping cross section.

5.453
stopping cross section factor
⟨EIA, RBS⟩ quotient of the total **energy loss** of a particle scattered at a given depth in the sample, and detected at a given angle, by the product of the atomic density of the sample atoms and the depth of scattering

5.454
stopping cross section, nuclear
⟨EIA, RBS, sputtering⟩ **stopping cross section** arising from energy transfer to atomic nuclei of the sample

NOTE 1 The total stopping cross section is the sum of the nuclear and **electronic stopping cross sections**.

NOTE 2 The maximum of the nuclear stopping cross section occurs at energies of the order of 1 keV per nucleon, whereas that of the electronic stopping cross section occurs at above 100 keV per nucleon. The absolute value of the electronic stopping cross section maximum is significantly greater than that for the nuclear stopping cross section.

5.455
stopping power
stopping force
⟨EIA, RBS, sputtering⟩ rate of **energy loss** of a particle with distance along its trajectory in a sample

cf. **stopping cross section**

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

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

NOTE 3 In older texts, this quantity might also be called, erroneously, the stopping cross section.

5.456
sum rule
⟨dielectric function⟩ equation that gives the value of an integral of a specified dielectric function

NOTE 1 Equations have been derived that give expected values of integrals of the imaginary part of the complex dielectric constant and of the imaginary part of the reciprocal of the complex dielectric constant for any material. The integrals involve the product of the specified dielectric function and either frequency or inverse frequency from zero frequency to an infinite frequency. The values of each integral can be used to assess the internal consistency of a set of dielectric data for a material by comparing values of the specified integrals to expected values. In practice, the integrations are made from low frequencies (corresponding to infrared or visible photon energies) to frequencies much higher than those corresponding to the largest K-shell **binding energy** of atoms in the material.

NOTE 2 The integral of the product of the specified dielectric function and frequency is proportional to the total number of electrons per atom or molecule in the material. This sum rule is often referred to as the f-sum rule, the oscillator-strength sum rule, or the Thomas-Reiche-Kuhn sum rule.

5.457
super Coster-Kronig transition
⟨AES, EPMA, XPS⟩ **Coster-Kronig transition** in which the ejected electron is from the same principal shell as the initial vacancy

cf. **Auger transition**

EXAMPLES $M_2M_4M_5$; $N_5N_7N_7$.

5.458
surface
interface between a condensed phase and a gas, vapour or free space

5.459
surface contamination
material, generally unwanted, on the sample **surface** which either is not characteristic of that sample and any process investigated or has arisen from exposure of the sample to particular environments other than those relevant for the original surface or the process to be studied

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

5.460
surface coverage
⟨chemisorption, physisorption⟩ quotient of the amount of a material at a **surface** by a measure of the surface area

NOTE The surface coverage can be expressed in atoms·m^{-2}, in mol·m^{-2}, in kg·m^{-2} or as a ratio of the amount to the **monolayer capacity**.

5.461
surface excitation parameter
SEP
⟨AES, EPES, REELS, XPS⟩ characteristic parameter in the exponential attenuation, describing the ratio of the intensity of a peak resulting from the presence of the **surface**, during a single crossing of a material surface, to that expected after traversing the same amount of material but in the absence of the surface

NOTE 1 If it is assumed that the SEP arises solely from surface excitations and that multiple surface excitations are governed by the Poisson stochastic process, the probability of experiencing n surface excitations is given by $(S^n/n!)[\exp(-S)]$, where S is the SEP. The SEP can then be interpreted as the average number of surface excitations during a single surface crossing, and the probability for not experiencing any surface excitation during that single surface crossing is given by $\exp(-S)$.

NOTE 2 The value of the SEP depends on the geometry of the experiment, and the contributions for incoming and for outgoing electrons in **EPES** and **REELS** can differ. The SEP decreases the intensities observed in REELS, EPES, **AES**, **XPS** and similar types of spectroscopy.

NOTE 3 Surface excitation decreases the intensity of the **quasi-elastic peak**. It is important in REELS and EPES.

5.462
surface plasmon
excitation of conduction- or valence-band electrons in a solid or liquid, associated with the termination of the material at the **surface**, in which collective oscillations are generated

cf. **characteristic electron energy losses**, **plasmon**

NOTE 1 **Plasmon** excitations are often observed as characteristic **energy loss** peaks associated with other peaks or structures in the spectrum, such as those of any elastically scattered **primary electrons**, photoelectron peaks, **Auger electron** peaks and ionization edges. Surface plasmons are important for many optical measurements.

NOTE 2 Plasmons are prominent in some materials and not in others.

NOTE 3 Two types of plasmon are commonly observed: **bulk plasmons** (often simply called plasmons) associated with material remote from a surface or **interface** and surface plasmons associated with a surface or interface. The bulk plasmon energy depends on the electronic structure of the material and is generally roughly proportional to the square root of the density of the valence-band electrons. The surface plasmon energy for a surface (i.e. a material-vacuum interface) is often approximately $(1/\sqrt{2})$ of the bulk plasmon energy for a planar surface; the actual ratio of the bulk and surface plasmon energies depends on the electronic structure of the material. For an interface between two materials, the surface plasmon energy depends on the electronic properties of each material. In the case of a thin oxide film on a free-electron-like metal, the surface plasmon energy of the metal will be reduced compared to the value for the clean metal surface due to the presence of the oxide.

5.463
surface segregation
partitioning of a species from the bulk of a material to the **surface** as a result of kinetic or thermodynamic effects

5.464
surfactant
substance that lowers the interfacial energy of a material in contact with a liquid or the surface energy of that liquid

NOTE 1 In practice, the liquid is usually water or a water-based medium. Emulsifiers, detergents and dispersing agents are examples of surfactants.

NOTE 2 In many cases, surfactant molecules have a hydrophilic or polar group at one end and a lipophilic or oleophilic group at the other.

5.465
synchrotron radiation
electromagnetic radiation (photons) with a continuous energy spectrum, created by the acceleration of electrons in a synchrotron or storage ring

NOTE Synchrotron radiation is a useful variable-energy source of photons for **Auger electron spectroscopy** and photoelectron spectroscopy. For photoelectron spectroscopy, the radiation is monochromated. Good intensities can be available for photons in the energy range 10 eV to 1 000 eV.

5.466
target
⟨EIA, RBS⟩ sample under investigation

5.467
target, thick
⟨EIA, RBS⟩ sample whose thickness produces backscattered particles whose energies, for each constitutive element, vary greatly with respect to the **system resolution**

[ASTM E673-03[1]]

5.468
target, thin
⟨EIA, RBS⟩ sample whose thickness is sufficiently small that the variation in energy of particles backscattered from atoms of each constitutive element is small with respect to the **system resolution**

[ASTM E673-03[1]]

5.469
thermal spike
⟨SIMS, sputtering⟩ **spike** in which energy deposition leading to local heating is the dominating process

NOTE Other processes proposed to generate spikes are pressure and shock waves.

5.470
thermalized electrons
ultimate electrons (deprecated)
⟨GDS⟩ electrons which, following collisions in the **plasma**, have an equilibrium energy distribution corresponding to the plasma temperature

5.471
thin film
layer of material, typically less than 100 nm in thickness, deposited or grown on a substrate

[ASTM E673-03[1]]

NOTE Films thinner than 10 nm are often called ultra-thin films.

5.472
time constant
⟨analogue electronic circuits⟩ time required for a signal to change by [1 – (1/e)], or 63,2 %, of its final value in response to a step function input

5.473
time of flight
TOF or **ToF**
⟨SIMS⟩ total time taken for ions of a particular mass to move from the sample to the detector

NOTE Usually, the clock timer is started with the **beam chopper** sequence selecting an ion pulse, and so the recorded flight time might include the additional time for the **primary ion** to travel to the sample **surface** from the pulse-forming region of the ion gun.

5.474
topographic contrast
contrast in a **map** or image arising from the topography of the sample **surface**

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

NOTE 2 Topographic contrast can change after ion **sputtering**.

5.475
total reflection
⟨TXRF⟩ condition where the **glancing angle** for the incident X-rays is at or less than the **critical angle** and the X-rays are either reflected or absorbed in a region very close to the **surface**

NOTE The reflected intensity is close to 100 % of the incident intensity and the transmitted intensity is zero.

5.476
transformation probability
⟨SIMS⟩ probability of a defined charged or neutral species being produced, by consumption of a defined parent atomic or molecular configuration at a **surface**, as a result of **sputtering**

5.477
transverse range
⟨EIA, RBS, SIMS⟩ distance, normal to the direction of an energetic ion or atom impacting a **surface**, at which the ion or atom comes to rest in the sample

cf. **projected range**

5.478
transverse straggling
⟨EIA, RBS, SIMS⟩ standard deviation of the **transverse ranges** of energetic ions or atoms of a given energy

cf. **range straggling**, **transverse range**

5.479
ultra-shallow depth profile
⟨SIMS⟩ **depth profile** for which the depth over which significant changes occur is less than 10 nm

5.480
unified atomic mass unit (CODATA)
u
unit equal to 1/12 of the mass of the nuclide ^{12}C at rest and in its ground state

NOTE 1 $1\ u \approx 1{,}660\ 538\ 86 \times 10^{-27}$ kg with a one-standard-deviation uncertainty of $\pm 0{,}000\ 000\ 28 \times 10^{-27}$ kg.[10] This is a non-SI unit, accepted for use with the International System, whose value in SI units is obtained experimentally.

NOTE 2 In the field of biochemistry, the unified atomic mass unit is also called the dalton, symbol Da.

NOTE 3 The above definition was agreed upon by the International Union of Pure and Applied Physics in 1960 and the International Union of Pure and Applied Chemistry in 1961, resolving a longstanding difference between chemists and physicists. The unified atomic mass unit replaced the atomic mass unit (chemical scale) and the atomic mass unit (physical scale), both having the symbol amu. The amu (physical scale) was one-sixteenth of the mass of an atom of oxygen-16. The amu (chemical scale) was one-sixteenth of the average mass of oxygen atoms as found in nature. In the 1998 CODATA, 1 u = 1,000 317 9 amu (physical scale) = 1,000 043 amu (chemical scale).

5.481
unimolecular dissociation
spontaneous dissociation of a molecule into two or more fragments

NOTE This term is often applied to the **fragmentation** of a **metastable ion**.

5.482
useful spatial resolution
⟨SIMS⟩ image resolution obtained in practice

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

5.483
vacuum level
electric potential of the vacuum at a point in space

[Adapted from ASTM E673-03[1]]

cf. **Fermi level**

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

5.484
vacuum level referencing
〈AES, XPS〉 method of establishing the **kinetic energy** scale in which the zero point corresponds to an electron at rest at the **vacuum level**

cf. **Fermi level referencing**

5.485
vacuum level, standard
electric potential 4,500 eV above the **Fermi level**

cf**. vacuum level**

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

5.486
valence-band spectrum
〈XPS〉 photoelectron energy distribution arising from excitation of electrons from the valence band of the sample material

5.487
work function
potential difference for electrons between the **Fermi level** and the maximum potential just outside a specified **surface**

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

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

5.488
X-ray ghost line
〈XPS〉 line in a spectrum due to **photoemission** induced by X-ray photons from an impurity in or on the X-ray **anode**, from the X-ray window, or from certain elements present in the sample

NOTE Ghost lines typically appear in dual-anode X-ray sources with Mg and Al coatings where a small fraction of Al X-rays appear when using the Mg source and *vice versa*. Other common ghost lines appear for oxygen X-rays as the coatings oxidize or copper X-rays from the coating substrate.

5.489
X-ray linewidth
energy width of the principal **characteristic X-ray** line

NOTE 1 In **XPS** the X-ray linewidth usually refers to that of the X-ray source.

NOTE 2 The X-ray linewidth contributes to the photoelectron **peak widths**.

5.490
X-ray monochromator
device used to eliminate photons of energies other than those in a narrow energy or wavelength band

NOTE For **XPS** using Al X-rays, the monochromator is usually aligned close to the Al $K\alpha_1$ energy.

5.491
yield, partial ion
sputtering yield, partial ion
ratio of the number of ions of a particular species sputtered from a sample to the total number of incident particles

cf. **fractional ion yield**, **fractional sputtering yield**, **negative-ion yield**, **partial sputtering yield**, **positive-ion yield**, **total ion yield**

5.492
yield, total ion
ratio of the total number of ions of both signs sputtered from a sample to the total number of incident particles

cf. **fractional ion yield**, **fractional sputtering yield**, **negative-ion yield**, **partial ion yield**, **partial sputtering yield**, **positive-ion yield**

NOTE The total ion yield is often used where, more correctly, the writer means the total negative-ion yield or the total positive-ion yield rather than their sum.

5.493
yield, volume
ratio of the total volume sputtered from a sample to the total number of incident particles

cf. **fractional ion yield**, **fractional sputtering yield**, **negative-ion yield**, **partial ion yield**, **partial sputtering yield**, **positive-ion yield**

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

5.494
zone of mixing
layer of the sample **surface** within which the **primary beam** causes **atomic mixing**

[ASTM E673-03[1]]

cf. **collision cascade**

6 Definitions of terms for multivariate analysis

6.1
centering
mean centering
centring (deprecated)
mean centring (deprecated)
⟨data preprocessing⟩ a **data-preprocessing** procedure in which each **variable** in the **data matrix** is centred by the subtraction of its mean value across all **samples**

cf. **scaling**, **transformation**

NOTE 1 Mean centering emphasizes the differences between samples rather than differences between the samples and the origin.

NOTE 2 Mean centering is generally recommended for **PCA**, **PLS** and **discriminant analysis** of **SIMS** and **XPS** data, where relative intensities of peaks across the samples are more important than their absolute deviation from zero intensities. Mean centering is not compatible with non-negativity constraints in **MCR** for the resolution of physically meaningful component spectra and contributions, which must have positive values.

NOTE 3 Mean centering is generally applied after other **data-preprocessing** methods, including data selection and **scaling**.

NOTE 4 All **data-preprocessing** methods imply some assumptions about the nature of the variance in the data set. It is important that these assumptions are understood and appropriate for the data set involved.

6.2
data matrix
table of numbers, with I rows and K columns, containing experimental data obtained for I **samples** over K values of one or more **variables**, where I and K are integers

NOTE 1 The term samples denotes any individual measurements made on a system and the term variables denotes the channels over which the measurements are made. For example, in **SIMS**, the variables refer to the mass or **time of flight** of **secondary ions** and, in **XPS**, the variables refer to the binding energies of photoelectrons detected.

NOTE 2 For a multivariate image with dimensions of I pixels $\times$ J pixels $\times$ K variables, the data is often "unfolded" prior to **multivariate analysis** to form a data matrix with dimensions $IJ \times K$. On completion of the analysis, the results can be "folded" to restore the original image dimensions.

6.3
data preprocessing
data pretreatment (deprecated)
manipulation of raw data prior to a specified data analysis treatment

NOTE 1 The terms preprocessing and pretreatment are often used interchangeably, but the latter is deprecated to reduce confusion with sample preparation/treatment prior to experimental analysis.

NOTE 2 Aside from the three main categories of data-preprocessing method (**centering**, **scaling** and **transformation**), data preprocessing can refer to any other procedures carried out on the raw data, including mass binning and peak selection. In the case of multivariate images, this can also include region-of-interest selection and image filtering or binning.

NOTE 3 All data-preprocessing methods imply some assumptions about the nature of the variance in the data set. It is important that these assumptions are understood and appropriate for the data set involved.

NOTE 4 More than one data-preprocessing method can be applied to the same data set. The order of data preprocessing is important and can affect assumptions made on the nature of variance in the data set.

6.4
discriminant analysis
DA
discriminant function analysis
DFA
a supervised multivariate technique for classifying **samples** into predefined groups using discriminant functions

NOTE 1 Discriminant functions are **factors** that maximize the variance between different groups while minimizing the variance within each group. **Loadings** on DFA factors can be used to provide information on the combination of **variables** which is best for predicting group membership.

NOTE 2 DFA is often applied after **PCA** to a multivariate data set. This removes colinearity from the multivariate data and ensures that the new predictor variables, which are PCA **scores**, are distributed normally. This method is referred to as principal-component discriminant function analysis (PC-DFA).