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Surface chemical analysis — Vocabulary

Analyse chimique des surfaces — Vocabulaire

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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 3.

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 International Standard may be the subject of patent rights. ISO shall not be held responsible for identifying any or all such patent rights.

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

Annex A of this International Standard is for information only.

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 may be materials scientists, chemists or physicists and may 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 techniques covered in this International Vocabulary extend from electron spectroscopy and mass spectrometry to optical spectrometry and X-ray analysis. 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 work for ISO 18115 started with a consideration, *inter alia*, of ASTM E 673-95a, *Standard terminology relating to surface analysis* [1], and a number of terms retain this reference. Such definitions have remained essentially unchanged. Some editorial changes have had to be made in all the cases where this reference appears since the ASTM definition structure differs from that adopted by ISO. Some other terms from the ASTM standard also appear, but with a revised text or significantly revised meaning. These terms are not referenced to the ASTM standard.

The terms of this International Vocabulary standard 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 two headings:

Clause 4: Definitions of the surface analysis methods.

Clause 5: Definitions of terms for surface analysis.

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

A single alphabetical index is given after the Bibliography. To assist retrieval, compound terms may be found in the index in both natural and reverse word order.

As standards are formulated by Technical Committee ISO/TC 201, *Surface chemical analysis*, new terms are defined. It is intended that these terms will be grouped conveniently into a supplement or supplements, to be used with this standard, until such time as this standard needs to be revised when they will be incorporated.

Surface chemical analysis — Vocabulary

1 Scope

This International Standard defines terms for surface chemical analysis.

2 Abbreviations

AES	Auger electron spectroscopy
CDP	compositional depth profile
CMA	cylindrical mirror analyser
eV	electron volt
EELS	electron energy loss spectroscopy
EIA	energetic-ion analysis
EPMA	electron probe microanalysis
ESCA	electron spectroscopy for chemical analysis
FABMS	fast atom bombardment mass spectrometry
FWHM	full width at half maximum
GDS	glow discharge spectrometry
GDOES	glow discharge optical emission spectrometry
GDMS	glow discharge mass spectrometry
HEISS	high-energy ion-scattering spectrometry
HSA	hemispherical sector analyser
IBA	ion beam analysis
LEISS	low-energy ion-scattering spectrometry
MEISS	medium-energy ion-scattering spectrometry
ptp	peak-to-peak
RBS	Rutherford backscattering spectrometry
RFA	retarding field analyser

SAM	scanning Auger microscope
SDP	sputter depth profile
SEM	scanning electron microscope
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 International Standard. 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 excitations. 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

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/m².

4.3

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.

4.4**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

4.5**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**

4.6**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**

4.7**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 which encompasses **GDOES** and **GDMS**.

4.8**ion beam analysis****IBA**

a method 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 LEISS, MEISS and RBS are all forms of IBA in which the probe ion energies are typically in the ranges 0,1 keV to 10 keV, 50 keV to 200 keV and 1 MeV to 2 MeV, respectively. These classifications represent three ranges in which fundamentally different physics is involved.

4.9**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**

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/m² in order to retain the surface in an essentially undamaged state.

4.10

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.

4.11

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/m² to an extent that depends on both the material of the sample and the size of the molecular fragments being analysed.

4.12

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**

4.13

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.

4.14

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 Al and Mg unmonochromated K α X-rays at 1 486,6 and 1 253,6 eV, respectively. Modern instruments also use monochromated Al K α X-rays. Some instruments make use of various X-ray sources with other anodes 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 and the mass density of the substance.

5.3

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. **internal carbon referencing**

NOTE 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.

5.4

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

EXAMPLE 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.

5.5

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

5.6

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

5.7

analysis volume

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

5.8

analysis volume

〈spectrometer〉 three-dimensional region within the spectrometer from which the entire analytical signal or a specified percentage of that signal may be detected

5.9

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

5.10

angle, glancing

〈TXRF〉 angle between the incident beam and the average surface plane

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

5.11

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.

5.12

angle, magic

⟨XPS⟩ angle at which the spectrometer entrance axis is aligned at $54,7^\circ$ 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 isolated 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.

5.13

angle of emission

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.

5.14

angle of incidence

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.

5.15

angle of scattering

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

5.16

angle-resolved AES

ARAES

angle-dependent AES

a procedure in which Auger electron intensities are measured as a function of the **angle of emission**

5.17

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.

5.18

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**

5.19

angle, solid, of detector

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

5.20**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.

5.21**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 according to

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

NOTE This formula relates to gases and is modified by the effects of elastic scattering when applied to solids.

5.22**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**

5.23**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.

5.24**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 an exponential decay due to the effects of elastic scattering. Where this approximation is valid, the term effective attenuation length is used.

5.25**attenuation length, effective**

average **emission function decay length** when the **emission depth distribution function** is sufficiently close to exponential for a given application

cf. **attenuation length**

NOTE Effective attenuation length is often used in **AES** and **XPS** to describe the transport of electrons that have not lost more than 1 eV as a result of inelastic scattering.

5.26

Auger de-excitation

⟨surface⟩

- a) process in which the energy of an excited atom or ion is given up by a non-radiative re-arrangement of electrons in that atom or ion
- b) process in which the energy in a metastable species near a solid surface is lost by interaction with the surface, and in the process enough energy is released to eject an electron from a surface atom

cf. **Auger neutralization**

NOTE For both processes, the electron may be ejected into the vacuum.

5.27

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.

5.28

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.

5.29

Auger electron yield

probability that an atom with a vacancy in a particular inner shell will relax by an **Auger process** ^[1]

5.30

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.

5.31

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.

5.32

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 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 which have similar binding energy shifts.

5.33

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.

5.34

Auger process

relaxation, by electron emission, of an atom with a vacancy in an inner electron shell [1]

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

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

5.35

Auger process, interatomic

(AES) **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

5.36

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, and LMM). When a valence electron is involved, the letter V is used (for example, LMV and KVV). When a particular sub-shell involved is known, this can also be indicated (for example, KL_1L_2). Coupling terms may also be added, where known, to indicate the final atomic state (for example, $L_3M_{4,5}M_{4,5}^1D$).

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 dash (for example, LL-VV and 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**.

5.37

Auger transition rate

quotient of the probability for an **Auger process** by time

5.38

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.

5.39

background, instrumental

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

5.40

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**

5.41

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 correct 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.

5.42

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**

5.43

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 may 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.

5.44

backscattered electron

(AES, EELS) 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.

5.45

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

5.46

backscattering energy

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

5.47

backscattering factor

(AES) factor defining the 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, as defined above, and sometimes unity plus that fractional increase. The latter usage is deprecated. For clarity, the particular usage needs to be defined.

5.48

backscattering spectrum

(EIA, RBS) plot of backscattering yield versus backscattering energy ^[1]

5.49

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**

5.50

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**

5.51

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.

5.52 beam current

I

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

$$I = dQ/dt$$

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 may or may not be equal to the d.c. or unpulsed beam current.

5.53 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.

5.54 beam current density

J

(for a parallel beam of charged particles) quotient of dI by dA where dI is the element of beam current incident on an area dA at right angles to the direction of the beam

$$J = dI/dA$$

cf. **fluence, flux, dose**

NOTE For a convergent or divergent beam, the area dA is replaced by a small sphere of cross-sectional area dA .

5.55 beam current, integrated

total electric charge transported in the beam over a specified time

5.56 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

5.57 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^[1]

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

5.58 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.

5.59**beam energy**

kinetic energy of the **beam particles**

cf. **beam 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.

5.60**beam impact energy**

kinetic energy of the **beam particles** on impact with the sample surface

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

NOTE 1 For primary ion beams in SIMS, the beam impact energy is given by the difference in electric potential between the ion source, strictly the plasma meniscus, 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.

5.61**beam particle**

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

5.62**beam, primary**

directed **flux** of particles or photons incident on a sample

5.63**beam profile**

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

5.64**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°.

5.65**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 ^[1]

5.66**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

5.67**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 ^[1]

5.68**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,

$$\varepsilon(A_x B_y) = x\varepsilon_A + y\varepsilon_B$$

where $\varepsilon(A_x B_y)$ is the stopping cross-section of the compound, $A_x B_y$, and ε_A and ε_B are the stopping cross-sections of elements A and B, respectively ^[1]

5.69**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 may also photoionize inner shells that would be energetically impossible by characteristic Al or Mg K α 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.

5.70**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, and are probably not significant as causes of sputter profile distortion.

5.71**channelling**

preferential motion of energetic particles along certain axial or planar directions of a crystalline solid as the particles move through the sample

NOTE The potentials of the individual atoms of the solid combine to reduce the scattering of the energetic particles from these directions.

5.72**characteristic electron energy losses**

⟨AES, EELS, XPS⟩ **inelastic scattering** of electrons in solids that produces a non-uniform energy loss spectrum determined by the characteristics of the material

cf. **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 may be due to a combination of plasmon excitation and single valence-electron excitations, and these excitations may 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).

5.73**characteristic X-rays**

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

5.74**charge modification**

alteration of the amount or the distribution of charge at a sample surface

5.75**charge neutralization**

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

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

5.76**charge referencing**

⟨AES, XPS⟩ 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 change

cf. **adventitious carbon referencing**

NOTE Charge referencing is often conducted using **adventitious carbon referencing** or by **gold decoration**.

5.77**charging potential**

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

NOTE Different charging potentials may 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

5.78**chemical effects**

⟨AES, EELS, EPMA, XPS⟩ change in the shape of a measured spectrum, or in the peak energy for an element, arising from chemical bonding

5.79

chemical shift

(AES, EELS, EMPA, XPS) change in **peak energy** arising from a change in the chemical environment of the atom

5.80

collision cascade

sequential energy transfer between atoms in a solid as a result of bombardment by an energetic species [1]

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

5.81

compositional depth profile

CDP

chemical or atomic composition measured as a function of distance normal to the surface

5.82

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.

5.83

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.

5.84

Coster-Kronig transition

(AES, EPMA, XPS) **Auger process** involving an electron from the same principal shell as the initial vacancy

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

EXAMPLES $L_1L_2M_5$; $M_1M_2N_5$.

5.85

counts

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

NOTE 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.

5.86

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, may be different from the thickness of sample material removed by sputtering due to dilation of the **altered layer**.

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

5.87

crater edge effect

signals from the crater edge which often originate from depths shallower than the central region of the crater formed in **depth profiling**

5.88

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 probability of reaction or process for the target entity by the incident-particle **fluence** ^[2]

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 dN in the number of N of particles in that state in a distance dx given by the relation:

$$dN = N\sigma n dx$$

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

Integration leads to the relation:

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

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

5.89

cross-section, elastic scattering

cross-section for binary elastic scattering

5.90

cross-section, elastic scattering, differential

quotient of the **cross-section for elastic 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 .

5.91

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

5.92

cross-section, inelastic scattering

(AES, EELS, EMPA, XPS) cross-section for **inelastic scattering** by an electron traversing a material

5.93

cross-section, ionization

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

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

NOTE 2 A 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 may 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 may have multiple vacancies following an initial ionization or as the result of subsequent Auger or **Coster-Kronig** processes.

5.94

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} m².

5.95

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**

5.96

cross-section, Rutherford

⟨RBS⟩ **elastic scattering cross-section** calculated using classical mechanics

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

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

5.97

cross-section, stopping

⟨EIA, RBS⟩ 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

NOTE 1 This stopping cross-section is usually expressed in units of eV·m²/atom and not an area per atom as is customary for **cross-sections**.

NOTE 2 The atomic density is sometimes taken as the number density, N , and sometimes as the mass density, ρ , so that the units will be eV·m²/atom or eV·m²/kg. The stopping cross-section ε is thus given either by

$$\varepsilon \equiv (1/N)(dE/dx)$$

or by

$$\varepsilon \equiv (1/\rho)(dE/dx)$$

where dE/dx is the rate of loss of energy E with distance x along the particle trajectory.

NOTE 3 Older texts may be found with the stopping cross-section given in keV·cm²/gm and in many other forms.

5.98

cross-section, sub-shell photoionization

cross-section for an incident photon interacting with a material to produce a 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.

5.99

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 energy.

NOTE 3 Transport cross-section is related to **differential elastic scattering cross-section**, $d\sigma_e(\Omega)/d\Omega$, by

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

where θ is the angle of scattering.

5.100

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 may be observed in that plane

5.101

dead time

time per pulse for which a pulse counting system is unavailable for further counting

5.102

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

5.103

dead time, multidetector

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

5.104

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

5.105

decay length

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

cf. **attenuation length**

5.106

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^[1]

5.107

decay length, deep emission function

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

5.108

decay length, emission function

negative reciprocal slope of the logarithm of the **emission depth distribution function** at a specified depth ^[1]

5.109

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**.

5.110

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**.

5.111

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

5.112

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.

5.113

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

5.114

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 ^[1]

5.115

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.

5.116

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 of the depth at an interface over which the signal from an overlayer or a substrate changes from 16 % to 84 % of their total variation between plateau values, is often used in AES and XPS.

5.117

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.

5.118 depth resolution, instrumental

(MEIS, RBS) depth resolution in the sample arising from the energy resolution of the spectrometer

5.119 depth resolution parameter

parameter which may be used as (i) a coefficient in an analytic fit to a measured compositional depth profile or (ii) as 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.

5.120 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 may not be applicable to all measurements and, for a fuller discussion of detection limits, [3] should be consulted.

NOTE 2 The detection limit may be expressed in many ways depending on the purpose. Examples of expressions 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.

5.121 detector efficiency

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

5.122 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.

5.123 dilute limit

(SIMS) atomic fraction or concentration of impurity species in an homogeneous matrix below which the SIMS process may safely be assumed to be linear with composition

5.124 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 may 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 E times the true spectrum.

5.125

dose

synonym of **areic dose**

5.126

dose, areic

dose density (deprecated)

D

quotient of dN by dA , where dN is the number of energetic particles of a specified type introduced into a solid through a surface area dA

$$D = dN/dA$$

NOTE 1 The energetic particles are atoms or atom clusters which may be electrically charged or neutral, the surface area dA is the geometric surface area.

NOTE 2 For a stationary parallel beam, areic dose equals **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 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 [4].

5.127

dose, implanted areic

D^{imp}

quotient of dN^{imp} by dA , where dN^{imp} is the number of energetic particles of a specified type incident on a solid within a surface area dA and stopped within the solid

$$D^{\text{imp}} = dN^{\text{imp}}/dA$$

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

5.128

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 to 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 .

5.129

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.

5.130**dose rate, areic** G

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

$$G = dD/dt$$

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

5.131**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

$$D^{\text{rec}} = dN^{\text{rec}}/dA$$

5.132**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 , stopped within the solid and remaining therein

$$D^{\text{ret}} = dN^{\text{ret}}/dA$$

NOTE 1 Particles which are stopped within the solid but do not remain therein may 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**.

5.133**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**.

5.134**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

5.135**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**

5.136**electron flooding**

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

5.137**electron retardation**

(AES, XPS) method of measuring the **kinetic energy** distribution by retarding the emitted electrons before or within the **electron energy analyser** ^[1]

5.138

electron spectrometer

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

NOTE 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 may be used to describe a complete working system with an energy analyser, possible electron-optical components, electron detector, excitation sources, vacuum pumps, control electronics and a data processing system. The meaning should be made clear by the context.

5.139

emission yield

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

5.140

energy edge

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

5.141

energy loss

energy dissipated by particles as they interact with the sample

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

5.142

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 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.

5.143

energy of incident beam (deprecated)

see **beam impact energy**

5.144

energy per channel

energy difference between successive spectral channels

5.145

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^[1]

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

5.146

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.

5.147

escape depth, mean

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

$$\frac{\int_0^{\infty} z\phi(z,\theta)dz}{\int_0^{\infty} \phi(z,\theta)dz}$$

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 ^[1]

5.148

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).

5.149

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.

5.150

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 ^[1]

cf. **vacuum level referencing**

5.151

field induced migration

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

5.152

final state

<AES, EMPA, XPS> state of an atom resulting after a particular **Auger**, X-ray or **photoemission process**

5.153
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

5.154
fluence

F

(for a parallel beam of particles) quotient of dN by dA , where dN is the number of particles of a specified type incident on an area dA at right angles to the direction of the beam

$$F = dN/dA$$

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 to the definition of areic dose.

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

5.155
fluorescence

(AES, TXRF, XPS) X-rays generated by a transition of an electron from a filled shell to a core hole at a higher binding energy created by incident radiation

5.156
fluorescence yield

(AES, TXRF, XPS) probability that an atom with a vacancy in a particular inner shell will relax by X-ray fluorescence

5.157
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.

5.158
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**.

5.159
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

5.160
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

5.161**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 (ca. 0,01 A/m² to 1 000 A/m²), 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.

5.162**gold decoration**

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

NOTE 1 The gold may be deposited by evaporation or by immersion of the surface in a solution which 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.

5.163**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 may also improve **depth resolution**.

5.164**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).

5.165**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** ^[1]

5.166**incident-particle energy**

kinetic energy of a particle incident on the sample surface

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

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

5.167**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.

5.168

inelastic mean free path, electron

average distance that an electron with a given energy travels between successive inelastic collisions

cf. **attenuation length**

5.169

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 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.

5.170

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 may be determined from a measured, calculated, or estimated **emission depth distribution function** for the signal of interest.

5.171

initial state

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

5.172

initial state

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

5.173

instrumental detection efficiency

ratio of the quantity of a detected event to the quantity of that event available for measurement

5.174

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, may be the height of the peak above a defined background or the **peak area**. The units may be counts, counts-eV, counts per second, counts-eV per second, counts per amu, counts per second per amu, etc. For **differential electron spectra**, the intensity may 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.

5.175**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 the detection of the signal and further between the points of detection and display on the measuring instrument.

NOTE 2 The signal intensity may 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 may 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 may 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.

5.176**interface**

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

5.177**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

5.178**interfacial region**

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

5.179**interference signal**

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

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

5.180**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**

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

5.181**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

5.182**ion beam**

directed **flux** of charged atoms or molecules ^[1]

5.183**ion beam induced mass transport**

movement of atoms in a sample caused by ion bombardment

5.184

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**

5.185

ion implantation

injection of ions into a sample ^[1]

5.186

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

5.187

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

5.188

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 the solid surface through a known angle ^[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.

5.189

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

5.190

ion species

type and charge of ion

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

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

5.191

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**

5.192

ion yield, negative

ratio of the total number of negative secondary ions sputtered from a sample to the total number of incident primary particles

5.193

ion yield, positive

ratio of the total number of positive secondary ions sputtered from a sample to the total number of incident primary particles

5.194**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

5.195**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.

5.196**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 may have a subscript added in **ISS** or **RBS** measurements denoting the target atom either as, say, K_{Si} or K_{28} . The subscript for atomic mass is preferred since the isotope is correctly identified.

5.197**kinetic energy**

energy of motion

NOTE The energy of a charged particle due to motion is not necessarily constant but 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*.

5.198**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.

5.199**Koopmans energy**

calculated energy of an electron in an orbital, on the assumption that its removal to infinity is unaccompanied by electronic relaxation ^[1]

5.200**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, may be in any arbitrary direction.

5.201

lineshape

measured shape of a particular spectral feature

5.202

lineshape, intrinsic

lineshape, natural

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

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

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

5.203

linewidth, intrinsic

⟨instrument⟩ see **resolution**

5.204

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 and 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).

5.205

map

image

two-dimensional representation of the sample surface where the information at each point in the representation is related to the output signal from the spectrometer, the signal from another detector, or processed intensity information from the available software

NOTE 1 By convention, map is usually applied to cases where the information is primarily composition-specific and image to those where it is primarily topographic.

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

NOTE 3 Map intensities may 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.

5.206

map, elemental

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

5.207

map, chemical

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

5.208

mass analyser

device for dispersing and detecting particles as a function of their mass-to-charge quotient

5.209**mass spectrum**

plot of the measured particle signal as a function of mass-to-charge quotient

5.210**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 proximity of other physical phases or chemical species.

5.211**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

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.

5.212**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

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 volumic number of scattering centres

5.213**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.

5.214**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 as opposed to those in **multilayers**.

5.215**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^[5]

5.216**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^[5]

NOTE The type of close packing needs to be stated.

5.217

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.

5.218

multilayer

〈chemisorption, physisorption〉 coverage of a substrate surface by more than one atomic or molecular layer of the adsorptive or segregated species

cf. **monolayer**

5.219

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

5.220

**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 ^[1]

5.221

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, may 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.

5.222

noise, statistical

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

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

5.223

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

5.224

orbital energy

〈XPS〉 **Koopmans energy** corrected for intra-atomic relaxation ^[1]

5.225 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.

5.226 pass energy

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

5.227 peak area

area under a peak in a spectrum after background removal

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

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

5.228 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**.

5.229 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.

5.230 peak synthesis

curve resolving (deprecated)

procedure whereby a synthetic spectrum is generated using either model or experimental peak shapes in which the number of peaks, the peak shapes, peak widths, peak positions, 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.

5.231 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 SBR. Peak-to-background ratio is the more commonly used term for types of electron spectroscopy 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.

5.232

peak width

line width

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.

5.233

photoelectric effect

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

5.234

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 ^[1]

EXAMPLES Minor X-ray lines are $K\alpha'$, $K\alpha_{3,4}$, $K\alpha_{5,6}$ and $K\beta$.

5.235

photoelectron X-ray satellite subtraction

removal of photoelectron X-ray satellite peaks from a spectrum ^[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 $K\alpha_2$, $K\alpha'$ and $K\beta$ satellites.

5.236

photoemission

emission of electrons from atoms or molecules caused by the **photoelectric effect** ^[1]

5.237

pileup

$\langle$ EIA, RBS $\rangle$ 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**

5.238

plasmon

$\langle$ AES, EELS, XPS $\rangle$ 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. Occasionally interface plasmons may 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.

5.239

polyatomic ion

charged multi-atom species

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

5.240

primary electron

electron extracted from a source and directed to a sample

cf. **secondary electron**

5.241

primary ion

ion extracted from a source and directed to a sample

cf. **probe ion, secondary ion**

5.242

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

5.243

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**

5.244

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**

5.245

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 same energy.

5.246

quantitative analysis

determination of the amounts of detected analytes in a sample

NOTE 1 The analyte may be elemental or compound in nature.

NOTE 2 The amount may be expressed, for example, as atomic or mass percent, atomic or mass fraction, mole or mass per unit volume, number (of atoms) per unit area, number (of atoms) per unit volume, as appropriate or as desired.

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

5.247

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**

5.248

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 ^[1]

5.249

range straggling

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

cf. **transverse straggling**

5.250

raster

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

NOTE Commonly used rasters cover square or rectangular areas.

5.251

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 may be convenient to specify the energy-relative resolution of an electron spectrometer, the mass-relative resolution of a mass spectrometer, or the wavelength-relative resolution of an optical spectrometer.

NOTE 3 In practice, the spectrometer-relative resolution 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.

5.252

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 ^[1]

5.253**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

5.254**resolution, energy**

full width at half maximum (FWHM) intensity of the measured energy distribution for monoenergetic particles

5.255**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 may 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 may be more appropriately chosen. 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 are used. The latter pair give the two sigma width for a Gaussian resolution function.

5.256**resolution of a spectrometer**

(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 may 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.

5.257**resolution, system**

(EIA, RBS) energy or depth resolution measured in the **backscattering spectrum** for a monoenergetic incident-ion beam

5.258**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 may 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.

5.259

resonance reaction

⟨EIA⟩ nuclear reaction that has a narrow peak in the **nuclear reaction cross-section** as a function of energy, which is so much larger than the nuclear reaction cross-sections at adjacent energies both above and below the peak that essentially all the particles detected from the reaction are due to the peak ^[1]

5.260

sample charging

change in the electrical potential in the sample or on the sample surface caused by particle or photon bombardment

5.261

scattered-ion energy

⟨ISS⟩ **kinetic energy** of the 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 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°.

5.262

scattered-ion energy ratio

⟨ISS⟩ ratio of the scattered-ion energy to the energy of the incident **probe ion** prior to a collision

5.263

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**

5.264

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

$$I_i(\theta) = I_0 N_i P_i \alpha_i (d\sigma_i/d\Omega) \theta \Delta\Omega T$$

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 $\text{atoms}\cdot\text{m}^{-2}$;
- 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;
- $(d\sigma_i/d\Omega)\theta$ is the **differential elastic scattering cross-section**, for species i , taken at the angle for which scattering is measured; that is, the angular distribution of scattered-ion intensity per unit flux of incident ions, per atom of species i , $\text{metre}^2\cdot\text{atom}^{-1}\cdot\text{steradian}^{-1}$;
- $\Delta\Omega$ is the solid angle of acceptance determined by the entrance of the filtering and detection system, steradians;
- T is the fractional transmission of the analysing and detection system.

5.265**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 ≤ 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**.

5.266**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**

5.267**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^+ .

5.268**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**

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

$$\sigma = \delta + \eta$$

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 ≤ 50 eV.

5.269**secondary ion**

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

5.270**secondary-ion angular distribution**

number of **secondary ions** as a function of **angle of emission**

5.271

secondary-ion energy distribution

number of secondary ions as a function of their **kinetic energy** at a specified collection angle

5.272

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**

5.273

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**.

5.274

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**

5.275

sensitivity factor, absolute elemental

coefficient for an element with 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. **sensitivity factor, relative elemental**

NOTE 1 The choice of use 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, of homogeneous samples or segregated layers.

NOTE 3 The source of the sensitivity factors should be given in order that the correct **matrix factors** or other parameters have been 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.

5.276

sensitivity factor, relative elemental

(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 analysis, for example, of homogeneous samples or segregated layers.

NOTE 3 The source of the sensitivity factors should be given in order that the correct **matrix factors** or other parameters have been 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.

5.277**sensitivity factor, relative elemental**

(dynamic SIMS) coefficient for an element with which the measured intensity for a mass peak of that element, divided by the measured intensity for a mass peak of the matrix is multiplied to yield the atomic concentration of the element present in the sample

NOTE 1 The elemental relative sensitivity factor may be obtained by dividing the **isotopic relative 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 the relative elemental sensitivity factors significantly.

5.278**sensitivity factor, relative isotopic**

(dynamic SIMS) coefficient for an element with 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 the relative elemental sensitivity factors significantly.

5.279**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.

5.280**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 in the range up to 100 eV less than the parent peak.

5.281**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.

5.282**smoothing**

mathematical treatment of data to reduce the apparent **noise**

5.283**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 ($\Delta m/m$)

5.284

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, $\Delta \lambda$

5.285

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 may be $\text{sr} \cdot \text{m}^2 \cdot \text{eV}$, $\text{sr} \cdot \text{m}^2 \cdot \text{amu}$ or $\text{sr} \cdot \text{m}^3$.

5.286

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 may be $\text{sr} \cdot \text{eV}$, $\text{sr} \cdot \text{amu}$ or $\text{sr} \cdot \text{m}$.

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.

5.287

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 may be $\text{sr} \cdot \text{eV}$, $\text{sr} \cdot \text{amu}$ or $\text{sr} \cdot \text{m}$.

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. **angle**, **solid of analyser**.

NOTE 3 This term is often used incorrectly instead of spectrometer response function which includes contributions from the detector and signal processing system.

5.288

spectrum, aligned incidence

⟨EIA, ISS⟩ **backscattering spectrum** recorded with the analysing beam aligned with crystallographic axes or planes of the sample that produce **channelling** ^[1]

5.289

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** ^[1]

5.290**spin orbit splitting**

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

5.291**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 may need to be added.

5.292**sputtering**

process in which atoms and ions are ejected from the sample as a result of particle bombardment

5.293**sputtering, equilibrium surface composition**

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

5.294**sputtering, preferential**

change in the **equilibrium surface composition** of the sample which may occur when sputtering multicomponent samples

5.295**sputtering rate**

quotient of the amount of sample material removed, as a result of particle bombardment, by time

cf. **erosion rate**

NOTE The rate may be measured as a velocity, a mass per unit area per unit time, or some other measure of quantity per unit time.

5.296**sputtering yield**

ratio of the number of atoms and ions sputtered from a sample to the total number of incident primary particles

5.297**sputtering yield, fractional****sputtering yield, partial**

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**

5.298**stopping cross-section, electronic**

(EIA, RBS) **stopping cross-section** arising from energy transfer to the electrons of the sample

NOTE The total stopping cross-section is the sum of the **electronic** and **nuclear stopping cross-sections**.

5.299**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