BS ISO 18115-1:2023

BSI Standards Publication

Surface chemical analysis — Vocabulary

Part 1: General terms and terms used in spectroscopy

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National foreword

This British Standard is the UK implementation of ISO 18115-1:2023. It supersedes BS ISO 18115-1:2013, which is withdrawn.

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

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

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INTERNATIONAL STANDARD

ISO 18115-1

Third edition
2023-06-19

Surface chemical analysis — Vocabulary —

Part 1: General terms and terms used in spectroscopy

Analyse chimique des surfaces — Vocabulaire —

Partie 1: Termes généraux et termes utilisés en spectroscopie

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Foreword

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

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

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

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For an explanation of the voluntary nature of standards, the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the World Trade Organization (WTO) principles in the Technical Barriers to Trade (TBT), see www.iso.org/iso/foreword.html.

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

This third edition cancels and replaces the second edition (ISO 18115-1:2013), which has been technically revised.

The main changes are as follows:

— revision of definitions related to resolution;

— introduction of definitions related to atom probe tomography;

— introduction of emerging methods such as HAXPES, NAPXPS, GEXRF;

— removal of repeated or redundant definitions and references;

— reorganisation of the terminology into subject-specific sections;

— removal of Annexes according to ISO requirements.

A list of all parts in the ISO 18115 series can be found on the ISO website.

Any feedback or questions on this document should be directed to the user's national standards body. A complete listing of these bodies can be found at www.iso.org/members.html.

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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 can be materials scientists, chemists, or physicists and can have a background that is primarily experimental or primarily theoretical. Those making use of the surface chemical data extend beyond this group into other disciplines.

With the present techniques of surface chemical analysis, compositional information is obtained for regions close to a surface (generally within 20 nm) and composition-versus-depth information is obtained with surface analytical techniques as surface layers are removed. The surface analytical terms covered in this document extend from the techniques of electron spectroscopy and mass spectrometry to optical spectrometry and X-ray analysis. The terms covered in ISO 18115-2 relate to scanning-probe microscopy. The terms covered in ISO 18115-3 relate to optical interface 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 terms are classified under Clauses 3 to 22:

— Clause 3: Terms related to general concepts in surface chemical analysis;

— Clause 4: Terms related to particle transport in materials;

— Clause 5: Terms related to the description of samples;

— Clause 6: Terms related to sample preparation;

— Clause 7: Terms related to instrumentation;

— Clause 8: Terms related to experimental conditions;

— Clause 9: Terms related to sputter depth profiling;

— Clause 10: Terms related to resolution;

— Clause 11: Terms related to electron spectroscopy methods;

— Clause 12: Terms related to electron spectroscopy analysis;

— Clause 13: Terms related to X-ray fluorescence, reflection and scattering methods;

— Clause 14: Terms related to X-ray fluorescence, reflection and scattering analysis;

— Clause 15: Terms related to glow discharge methods;

— Clause 16: Terms related to glow discharge analysis;

— Clause 17: Terms related to ion scattering methods;

— Clause 18: Terms related to ion scattering analysis;

— Clause 19: Terms related to surface mass spectrometry methods;

— Clause 20: Terms related to surface mass spectrometry analysis;

— Clause 21: Terms related to atom probe tomography;

— Clause 22: Terms related to multivariate analysis.

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INTERNATIONAL STANDARD **ISO 18115-1:2023**

Surface chemical analysis — Vocabulary —

Part 1: General terms and terms used in spectroscopy

1 Scope

This part of the ISO 18115 series defines terms for surface chemical analysis. It covers general terms and those used in spectroscopy, while ISO 18115-2 covers terms used in scanning-probe microscopy and ISO 18115-3 covers terms used in optical interface analysis.

2 Normative references

There are no normative references in this document.

3 Terms related to general concepts in surface chemical analysis

ISO and IEC maintain terminology databases for use in standardization at the following addresses:

— ISO Online browsing platform: available at https://www.iso.org/obp

— IEC Electropedia: available at https://www.electropedia.org/

3.1
interface
boundary between two phases having different chemical, elemental, or physical properties

3.2
surface
interface (3.1) between a condensed phase and a gas, vapour, or free space

3.3
measurand
quantity intended to be measured

[SOURCE: ISO/IEC Guide 99:2007,[1] 2.3, modified — The notes to entry have been deleted.]

3.4
analyte
substance or chemical constituent that is subjected to measurement

3.5
chemical species
atom, molecule, ion, or functional group

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3.6
unified atomic mass unit
u
dalton
Da
unit equal to 1/12 of the mass of the nuclide ^{12}C at rest and in its ground state

Note 1 to entry: 1 u ≈ 1,660 538 86 × 10^{-27} kg with a one-standard-deviation uncertainty of ±0,000 000 28 × 10^{-27} kg.[2] This is a non-SI unit, accepted for use with the International System, whose value in SI units is obtained experimentally.

Note 2 to entry: The term dalton, symbol Da, is preferred over unified atomic mass unit as it is both shorter and works better with prefixes.

Note 3 to entry: The above definition was agreed upon by the International Union of Pure and Applied Physics in 1960 and the International Union of Pure and Applied Chemistry in 1961, resolving a longstanding difference between chemists and physicists. The unified atomic mass unit replaced the atomic mass unit (chemical scale) and the atomic mass unit (physical scale), both having the symbol amu. The amu (physical scale) was one-sixteenth of the mass of an atom of oxygen-16. The amu (chemical scale) was one-sixteenth of the average mass of oxygen atoms as found in nature. In the 1998 CODATA, 1 u = 1,000 317 9 amu (physical scale) = 1,000 043 amu (chemical scale).

3.7
reference method
thoroughly investigated method, clearly and exactly describing the necessary conditions and procedures for the measurement of one or more property values, that has been shown to have accuracy and precision commensurate with its intended use and that can therefore be used to assess the accuracy of other methods for the same measurement, particularly in permitting the characterization of a *reference material* (5.1)

[SOURCE: ISO Guide 30:1992+A1:2008[3]]

3.8
quantitative analysis
determination of the amount of *analyte* (3.4) detected in, or on, a sample

Note 1 to entry: The analytes can be elemental or compound in nature.

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

Note 3 to entry: The sample material can be inhomogeneous so that a particular model structure may be assumed in the interpretation. Details of that model should be stated.

3.9
detection limit
smallest amount of an element or compound that can be measured under specified analysis conditions

Note 1 to entry: 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* (3.21) is three times the standard deviation of the signal above the background signal. This approach is simplistic and, for more accurate and rigorous definitions of detection limits, the References [4] and [5] should be consulted.

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

Note 3 to entry: The detection limit is generally different for different materials.

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3.10
matrix effects
change in the intensities or spectral information per atom of the *analyte* (3.4) arising from change in the chemical or physical environment

Note 1 to entry: Examples of these environments are varying sample morphologies [e.g. *thin films* (5.13), clusters, fibres, nanostructures] of different dimensions, the amorphous or crystalline state, changes of matrix species, and the proximity of other physical phases or *chemical species* (3.5).

3.11
matrix factor
factors, arising from the composition of the matrix, for multiplying the quotient of the measured intensity and the appropriate sensitivity factor in formulae to determine the composition using surface analytical techniques

Note 1 to entry: See average matrix sensitivity factor and pure-element sensitivity factor.

Note 2 to entry: In methods such as *AES* (11.1), 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* (8.48) in the sample.

3.12
absolute elemental sensitivity factor
coefficient for an element by which the measured intensity for that element is divided to yield the atomic concentration or atomic fraction of the element present in the sample

Note 1 to entry: See *elemental relative sensitivity factor* (12.92) (20.61).

Note 2 to entry: The choice of atomic concentration or atomic fraction should be made clear.

Note 3 to entry: The type of sensitivity factor utilized should be appropriate for the formulae used in the quantification process and for the type of sample analysed, for example homogeneous samples or segregated layers.

Note 4 to entry: The source of sensitivity factors should be given to ensure that the correct *matrix factors* (3.11) or other parameters are used.

Note 5 to entry: 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* (19.1) this has a dominating influence.

3.13
step size
distance between values in *measurand* (3.3) space from which individual data points are acquired

3.14
sweep
single, complete acquisition of one set of data

3.15
peak intensity
measure of *signal intensity* (3.17) for a constituent spectral peak

Note 1 to entry: Intensity is usually measured for quantitative purposes which can be the height of the peak above a defined background or the *peak area* (3.16). The units can be *counts* (3.18), counts·electron volts, counts per second, counts·electron volts per second, counts per amu, counts per second per amu, etc. For differential spectra, the intensity can 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 to entry: 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.

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3.16
peak area
area under a peak in a spectrum after background removal

Note 1 to entry: See *inelastic electron scattering background subtraction* (12.85) and *signal intensity* (3.17).

Note 2 to entry: The peak area can be expressed in *counts* (3.18), counts per second, counts·electron volts, counts·electron volts per second, counts per amu, or other units.

3.17
signal intensity
strength of a measured signal at a spectrometer detector or after some defined processing

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

Note 2 to entry: The signal intensity can be expressed in *counts* (3.18) (per channel) or counts per second (per channel) or counts·electron volts per second or other units. In *AES* (11.1), the differential of the signal intensity may be obtained by analogue *modulation* (12.61) of an electrode in the spectrometer or by numerical differentiation of the spectrum. The type of signal shall be defined.

Note 3 to entry: In an electron or *mass spectrum* (20.58), 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 can be current·eV^{-1}·sr^{-1} or current·amu^{-1}·sr^{-1}. If the spectrum has been normalized to unit *primary-beam* (8.10) 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}.

3.18
counts
total number of pulses recorded by a detector system in a defined time interval

Note 1 to entry: The counts can be representative, one-for-one with the particles being detected [in the absence of *dead time* (7.17) losses in the counting measurement] in which case they follow Poissonian statistics [unless other *noise* (3.19) sources are present] or they can simply be proportional to the number of particles being detected. The type of measure shall be clearly stated.

Note 2 to entry: In multidetector systems, the apportion of counts into relevant channels of the spectrum can lead to changes from the expected Poissonian statistics in each channel since the counts in neighbouring channels can be partly correlated.

3.19
noise
time-varying disturbances superimposed on the analytical signal with fluctuations, leading to uncertainty in the *signal intensity* (3.17)

Note 1 to entry: 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, can be useful as semiquantitative measures of noise.

Note 2 to entry: The fluctuations in the measured intensity can arise from a number of causes, such as *statistical noise* (3.20) and electrical interference.

3.20
statistical noise
noise (3.19) in the spectrum due solely to the statistics of randomly detected single events

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

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

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3.21
background signal
signal present at a particular position, energy, mass or wavelength due to processes or sources other than those of primary interest

Note 1 to entry: See *metastable background* (20.36), *Shirley background* (12.86), *Sickafus background* (12.87), and *Tougaard background* (12.88).

3.22
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 to entry: Signal-to-background ratio is the more commonly used term in *GDS* (15.1), where it is abbreviated to SBR. Peak-to-background ratio is the more commonly used term for types of electron spectroscopies such as *AES* (11.1) and *XPS* (11.6).

Note 2 to entry: The method of estimating the background intensity shall be given. For AES, the background intensity is often determined at a *kinetic energy* (3.35) just above the peak of interest.

3.23
signal-to-noise ratio
ratio of the *signal intensity* (3.17) to a measure of the total *noise* (3.19) in determining that signal

Note 1 to entry: See *statistical noise* (3.20).

Note 2 to entry: The noise in *AES* (11.1) is often measured at a convenient region of the spectral background close to the peak.

3.24
smoothing
mathematical treatment of data to reduce the apparent *noise* (3.19)

3.25
interference signal
<mass spectrometry, spectroscopy> signal, measured at the mass, energy, or wavelength position of interest, due to another, undesired, species

Note 1 to entry: In general laboratory use, interference can be used more broadly to indicate electrical *noise* (3.19), line pick-up, or other unwanted contributions to the detected signal.

3.26
relative standard deviation of the background
quotient of the standard deviation characterizing the *noise* (3.19) in the *background signal* (3.21) by the intensity of the background signal

3.27
lineshape
measured shape of a particular spectral feature

3.28
peak width
width of a peak at a defined fraction of the peak height

Note 1 to entry: See *intrinsic linewidth* (12.22).

Note 2 to entry: Any background subtraction method used should be specified.

Note 3 to entry: The most common measure of peak width is the full width of the peak at half maximum (FWHM) intensity.

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Note 4 to entry: For asymmetrical peaks, convenient measures of peak width are the half-widths of each side of the peak at half maximum intensity.

3.29
peak fitting
procedure whereby a spectrum, generated by *peak synthesis* (3.30), is adjusted to match a measured spectrum

Note 1 to entry: A least-squares optimization procedure is generally used in a computer programme for this purpose.

Note 2 to entry: The selected peak shape and the background shape should be defined. Any constraints imposed on the adjustment process should also be defined.

3.30
peak synthesis
procedure whereby a synthetic spectrum is generated, using either model or experimental peak shapes, in which the number of peaks, the peak shapes, the *peak widths* (3.28), the peak positions, the peak intensities, and the background shape and intensity are adjusted for *peak fitting* (3.29)

Note 1 to entry: The selected peak shape and the background shape should be defined.

3.31
lateral profile
chemical or elemental composition, *signal intensity* (3.17) or processed intensity information from the available software measured in a specified direction parallel to the *surface* (3.2)

Note 1 to entry: See *line scan* (8.56).

3.32
depth profile
vertical profile
chemical or elemental composition, *signal intensity* (3.17) or processed intensity information from the available software measured in a direction normal to the *surface* (3.2)

Note 1 to entry: See *compositional depth profile* (3.33).

3.33
compositional depth profile
CDP
atomic or molecular composition measured as a function of distance normal to the *surface* (3.2)

3.34
depth profiling
monitoring of *signal intensity* (3.17) as a function of a variable that can be related to distance normal to the *surface* (3.2)

Note 1 to entry: See *compositional depth profile* (3.33).

Note 2 to entry: In a *sputter depth profile* (9.1) the signal intensity is usually measured as a function of the *sputtering* (9.3) time.

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3.35
kinetic energy
energy of motion

Note 1 to entry: The energy of a charged particle due to motion is not necessarily constant and varies with the local electric potential. If all local electrodes are at ground potential, the kinetic energy of the particle varies with the local *vacuum level* (12.10). This vacuum level can vary over a range of 1 eV in different regions of *AES* (11.1) and *XPS* (11.6) instruments and measured electron energies can similarly vary. This variation is removed if the kinetic energies are referred to the *Fermi level* (12.9). In XPS, by convention, the Fermi level is always used but in AES both *vacuum* (12.76) and *Fermi level referencing* (12.75) 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* (12.58), 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* (12.11) of 4,500 eV above the Fermi level so that the energies of *Auger electron* (12.32) peaks, referenced to the Fermi level, can be converted in a consistent way to energies referenced to the vacuum level and vice versa.

3.36
ion species
type and charge of an ion

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

Note 1 to entry: If an isotope is used, it should be specified.

3.37
radical
atoms or molecular entity possessing an unpaired electron

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

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

Note 3 to entry: The adjective "free" is no longer used.

3.38
radical ion
radical (3.37) carrying an electric charge

Note 1 to entry: A positively charged radical is called a "radical cation" (e.g. the benzene radical cation $C_6H_6^{\bullet+}$); a negatively charged radical is called a "radical anion" (e.g. the benzene radical anion $C_6H_6^{\bullet-}$ or the benzophenone radical anion $Ph_2C{-}O^{\bullet-}$). Commonly, but not necessarily, the odd electron and the charge are associated with the same atom. Unless the positions of unpaired spin and charge can be associated with specific atoms, superscript dot and charge designations should be placed in the order $\bullet+$ or $\bullet-$ as suggested by the name "radical ion" (e.g. $C_3H_6^{\bullet+}$).

3.39
light ion
ion lighter than lithium

Note 1 to entry: See *intermediate-mass ion* (3.40) and *heavy ion* (3.41).

3.40
intermediate-mass ion
ion with mass between, and including, lithium and argon

Note 1 to entry: See *heavy ion* (3.41) and *light ion* (3.39).

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3.41
heavy ion
ion heavier than argon

Note 1 to entry: See *intermediate-mass ion* (3.40) and *light ion* (3.39).

3.42
anion
negatively charged ion

Note 1 to entry: See *cation* (3.43).

3.43
cation
positively charged ion

Note 1 to entry: See *anion* (3.42) and *cationized molecule* (20.22).

3.44
cluster ion
ion composed of many atoms or *chemical species* (3.5)

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

Note 2 to entry: Cluster ions are used to desorb molecular species from surfaces with enhanced efficiencies. Examples include ions produced in liquid metal sources (Au_n^+, Bi_n^+) as well as ions produced by electron impact [C_{60}^+, Ar_n^+ $(H_2O)_n^+$].

3.45
ionization efficiency
ratio of the number of ions formed to the number of electrons, ions, or photons used in an ionization process

[SOURCE: IUPAC]

3.46
ion neutralization
<ISS, SIMS> *charge exchange* (16.35) process in which an ion loses its charge through interactions with a material *surface* (3.2) or with gas-phase atoms or molecules

3.47
de Broglie wavelength
wavelength of a particle deduced from de Broglie's concept of wave-particle duality

Note 1 to entry: The wavelength is calculated as the quotient of Planck's constant and the particle momentum.

3.48
energy eigenvalue
energy value of a single bound electron level in an atom, molecule, ion, or solid obtained by solving the single-electron Schrödinger or Dirac formula in the Dirac-Fock representation of the electronic structure of an atom in its ground state

Note 1 to entry: Eigenvalues are the solutions to certain integral formulae, a special case of which is the Schrödinger formula for electrons in atoms, molecules, ions, or solids.

Note 2 to entry: In the *frozen-orbital approximation* (3.49), the *binding energy* (12.16) of a *hole state* (3.62) is given by the negative of the corresponding single-electron energy eigenvalue.

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3.49
frozen-orbital approximation
assumption that the one-electron wavefunctions of the electrons remaining in an atom or molecule are unchanged after ionization

Note 1 to entry: In the frozen-orbital approximation, the *binding energy* (12.16) of an electron is given by the negative of the *energy eigenvalue* (3.48).

3.50
Koopmans energy
calculated energy of an electron in an orbital, on the assumption that its removal to infinity is unaccompanied by *electronic relaxation* (3.58)

3.51
orbital energy
<XPS> *Koopmans energy* (3.50) corrected for intra-atomic *relaxation* (3.57)

3.52
spin orbit splitting
splitting of p, d, or f levels in an atom arising from coupling of the spin and orbital angular momentum

3.53
excited state
state of a system with energy higher than that of the ground state

Note 1 to entry: This term is generally used to characterize a molecule in one of its electronically excited states, but can also refer to vibrational and/or rotational excitation in the electronic ground state.

3.54
initial state
<AES> core-hole *excited state* (3.53) of an atom prior to an *Auger transition* (12.33) or to X-ray emission

3.55
initial state
<XPS> ground state of an atom prior to photoelectron emission

3.56
final state
<AES, XPS> state of an atom resulting after a particular Auger, X-ray, or *photoemission* (12.8) process

3.57
relaxation
process by which an atom, molecule, or ion is transformed from a higher potential-energy state to a lower potential-energy state

Note 1 to entry: See *electronic relaxation* (3.58).

3.58
electronic relaxation
relaxation (3.57) resulting from the transition of an electron between energy levels, resulting in the release of energy

Note 1 to entry: The energy release can result in the ejection of a photon or other particle.

3.59
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* (3.56) of the system

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3.60
extra-atomic relaxation energy
screening energy
diminished energy of an ionized atom in a solid due to coulombic attraction of electrons in the immediate environment

3.61
hole
electronic vacancy in an atom, molecule, or solid

3.62
hole state
electronic configuration of an atom, molecule, or solid containing a *hole* (3.61)

3.63
spectator hole
hole state (3.62) in the electronic structure of an atom that can be present during processes such as *Auger electron* (12.32) and X-ray photoelectron emission but is not created or destroyed in the process

3.64
X-ray fluorescence
<AES, TXRF, XPS> X-rays generated by a transition of an electron from a filled shell to a core *hole* (3.61), created by incident radiation, at a higher *binding energy* (12.16)

3.65
fluorescence yield
<AES, TXRF, XPS> probability that an atom with a vacancy in a particular inner shell relaxes by X-ray *fluorescence* (3.64)

3.66
characteristic X-rays
photons emitted by ionized atoms and having a particular distribution in energy and intensity which is characteristic of the atomic number and chemical environment of the atom

Note 1 to entry: In *XPS* (11.6), the term is applied to the X-ray source used to excite photoelectrons in the sample.

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

3.67
X-ray linewidth
energy width of the principal *characteristic X-ray* (3.66) line

Note 1 to entry: In *XPS* (11.6) the X-ray linewidth usually refers to that of the X-ray source.

Note 2 to entry: The X-ray linewidth contributes to the photoelectron *peak widths* (3.28).

3.68
X-ray monochromator
device used to eliminate photons of energies other than those in a narrow energy or wavelength band

3.69
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

3.70
Auger de-excitation
process in which the excess energy of an excited atom or ion is given up by the *Auger process* (12.30)

Note 1 to entry: See *Auger neutralization* (3.71).

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

3.71
Auger neutralization
<ion at a surface> process in which an electron, tunnelling from the conduction band of a solid, neutralizes an incoming ion and an electron is ejected from a surface atom

Note 1 to entry: The ejected electron can be emitted into the vacuum.

3.72
time constant
<analogue electronic circuits> time required for a signal to change by [1 − (1/e)], or 63,2 %, of its final value in response to a step function input

3.73
sum rule
<dielectric function> formula that gives the value of an integral of a specified dielectric function

Note 1 to entry: Formulae have been derived that give expected values of integrals of the imaginary part of the complex dielectric constant and of the imaginary part of the reciprocal of the complex dielectric constant for any material. The integrals involve the product of the specified dielectric function and either frequency or inverse frequency from zero frequency to an infinite frequency. The values of each integral can be used to assess the internal consistency of a set of dielectric data for a material by comparing values of the specified integrals to expected values. In practice, the integrations are made from low frequencies (corresponding to infrared or visible photon energies) to frequencies much higher than those corresponding to the largest K-shell *binding energy* (12.16) of atoms in the material.

Note 2 to entry: The integral of the product of the specified dielectric function and frequency is proportional to the total number of electrons per atom or molecule in the material. This sum rule is often referred to as the f-sum rule, the oscillator-strength sum rule, or the Thomas-Reiche-Kuhn sum rule.

4 Terms related to particle transport in materials

4.1
binary elastic scattering
elastic scattering
collision between a moving particle and a second particle in which the total *kinetic energy* (3.35) and the total momentum are conserved

Note 1 to entry: See *inelastic scattering* (4.2).

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

4.2
inelastic scattering
interaction between a moving energetic particle and a second particle or assembly of particles in which the total *kinetic energy* (3.35) is not conserved

Note 1 to entry: Kinetic energy is absorbed in solids by various mechanisms, for example inner-shell ionization, *plasmon* (12.47) and phonon excitation, and *bremsstrahlung* (12.57) generation. These excitations usually lead to a small change in direction of the moving particle.

Note 2 to entry: In particle collisions, the collision can be elastic in that the kinetic energy of the particles is conserved, but energy can still be lost by the incident particle. In the scattering of electrons by atoms, the energy lost is usually very small and is often ignored. Where it is not ignored, the scattering is often termed quasi-elastic [see *elastic peak* (12.42)].

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4.3
energy loss
energy dissipated by particles as they interact with the sample

Note 1 to entry: See *characteristic electron energy losses* (12.40) and *plasmon* (12.47).

4.4
backscattering energy
energy of a particle from the *primary beam* (8.10) after it has undergone a backscattering collision and escaped from the sample

4.5
Bohr's critical angle
angle of ion scattering from a nucleus given by the ratio of the *de Broglie wavelength* (3.47) and the distance of closest approach of the ion with the nucleus

Note 1 to entry: Quantum effects are usually ignored for *scattering angles* (8.4) larger than Bohr's critical angle. For surface analysis conditions, this angle is very small.

4.6
Compton scattering
scattering of X-rays and other photons by electrons

Note 1 to entry: The photon loses energy by recoil of the electron to an extent governed by the *scattering angle* (8.4).

4.7
cross section
<for a specified target entity and for a specified reaction or process produced by incident charged or uncharged particles of specified type and energy> quotient of the probability of reaction or process for the target entity by the incident-particle *fluence* (8.16)

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

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

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

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

Integration leads to the relationship

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

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

4.8
elastic scattering cross section
cross section (4.7) for *binary elastic scattering* (4.1)

4.9
differential elastic scattering cross section
quotient of the *elastic scatteringcross section* (4.8) for scattering into a particular infinitesimal solid angle far from the *target* (18.2) by that infinitesimal solid angle

Note 1 to entry: The differential elastic scattering cross section is related to the elastic scattering cross section, σ_e, by

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

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

4.10
transport cross section
σ_{tr}
quotient of the fractional momentum loss of a particle incident on the sample arising from *elastic scattering* (4.1) by the areic density of the sample atoms, for an infinitesimally thin sample

Note 1 to entry: This *cross section* (4.7) is expressed as an area per atom.

Note 2 to entry: The cross section for the loss of any momentum, however small, is simply the *elastic scattering cross section* (4.8). 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* (4.11) which is a measure of the probability of the loss of a substantial amount of energy.

Note 3 to entry: The transport cross section is related to the *differential elastic scattering cross section* (4.9), $d\sigma_e(\Omega)/d\Omega$, 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* (8.4).

4.11
stopping cross section
<ISS, RBS, sputtering> quotient of the rate of *energy loss* (4.3) 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 to entry: See *stopping power* (4.17).

Note 2 to entry: The stopping cross section is usually expressed in units of eV·m^2 per atom and not as an area per atom as is customary for *cross sections* (4.7).

Note 3 to entry: The atomic density is usually taken as the number density, N, but sometimes as the mass density, ρ, so that the units are eV·m^2/atom or eV·m^2/kg. The stopping cross section $S(E)$ is thus given either by

$$S(E) \equiv -(1/N)(dE/d\lambda)$$

or by

$$S(E) \equiv -(1/\rho)(dE/d\lambda)$$

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

Note 4 to entry: In some texts, the stopping cross section and stopping power are used interchangeably so that $S(E) \equiv -(dE/d\lambda)$. This inconsistency for the term stopping power leads to its deprecation.

Note 5 to entry: Older texts can be found with the stopping cross section given in keV·cm^2/gm (meaning "per gram") and in many other forms.

4.12
electronic stopping cross section
<EIA, RBS, sputtering> *stopping cross section* (4.11) arising from energy transfer to the electrons of the sample

Note 1 to entry: The total stopping cross section is the sum of the electronic and *nuclear stopping cross sections* (4.13).

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Note 2 to entry: The maximum of the nuclear stopping cross section occurs at energies of the order of 1 keV per nucleon, whereas that of the electronic stopping cross section occurs at above 100 keV per nucleon. The absolute value of the electronic stopping cross section maximum is significantly greater than that for the nuclear stopping cross section.

4.13
nuclear stopping cross section
<EIA, RBS, sputtering> *stopping cross section* (4.11) arising from energy transfer to atomic nuclei of the sample

Note 1 to entry: The total stopping cross section is the sum of the nuclear and *electronic stopping cross sections* (4.12).

Note 2 to entry: The maximum of the nuclear stopping cross section occurs at energies of the order of 1 keV per nucleon, whereas that of the electronic stopping cross section occurs at above 100 keV per nucleon. The absolute value of the electronic stopping cross section maximum is significantly greater than that for the nuclear stopping cross section.

4.14
Rutherford cross section
<RBS> *elastic scattering cross section* (4.8) calculated using classical mechanics and a Coulomb potential

Note 1 to entry: See *elastic scattering cross section* (4.8) and *enhanced elastic cross section* (4.21).

Note 2 to entry: The resulting cross section formula was first derived by Rutherford.

4.15
screening
response arising from the atom's electrons, causing an apparent reduction in the coulomb potential of the nucleus

Note 1 to entry: In *IBA* (17.1), when the incident ion is far from the target nucleus, the atom in which the nucleus sits looks neutral to the ion as a result of screening. The screening reduces the scattering *cross section* (4.7) slightly from the *Rutherford cross section* (4.14) (about 1 % per 50 increase in the target atomic number for 2 MeV He). The effect becomes more pronounced and increasingly uncertain as the energy decreases and, for *LEIS* (17.2), the cross section is no longer really well-known.

4.16
screening function
<IBA> factor by which the *Rutherford cross section* (4.14) is reduced as a result of *screening* (4.15) in a given situation

4.17
stopping power
stopping force
<EIA, RBS, sputtering> rate of *energy loss* (4.3) of a particle with distance along its trajectory in a sample

Note 1 to entry: See *stopping cross section* (4.11), *electronic stopping power* (4.18), and *nuclear stopping power* (4.19).

Note 2 to entry: Stopping power and stopping force are synonymous terms and are usually represented by $-\mathrm{d}E/\mathrm{d}\lambda$ for a particle of energy E moving along a path within a material.

Note 3 to entry: Stopping power is the official nomenclature of the International Commission on Radiation Units and Measurements (ICRU) but it is recognized that the term does not define a power but a force and so stopping force has been included here as a more precise synonymous term.

Note 4 to entry: In older texts, this quantity can also be called, erroneously, the stopping cross section.

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4.18
electronic stopping power
contribution to the *stopping power* (4.17) due to interactions between the particle and electrons in the material

Note 1 to entry: see also *electronic stopping cross section* (4.12).

4.19
nuclear stopping power
contribution to the *stopping power* (4.17) due to interactions between the particle and atomic nuclei in the material

Note 1 to entry: see also *nuclear stopping cross section* (4.13).

4.20
Bragg's rule
empirical rule formulated by W.H. Bragg and R. Kleeman that states that the *stopping cross section* (4.11) of a compound sample is equal to the sum of the products of the elemental stopping cross sections for each constituent and its atomic fraction, that is,

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

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

4.21
enhanced elastic cross section
<ISS, RBS> *cross section* (4.7) of an atom for *elastic scattering* (4.1) that is greater than the *Rutherford cross section* (4.14) due to partial penetration of a nucleus in the sample by the incident particle

4.22
nuclear reaction cross section
<EIA> *cross section* (4.7) at a given *beam energy* (8.33) and emission direction of the detected product for a particular nuclear reaction per atom

Note 1 to entry: This cross section is usually expressed per atom as an area in units of barns (1 barn = 10^{-28} m^2).

4.23
resonance reaction
<EIA> nuclear reaction that has a narrow peak in the *nuclear reaction cross section* (4.22) as a function of energy, the nuclear reaction cross section at the peak being so much larger than the nuclear reaction cross sections at adjacent energies on either side of the peak that essentially all the particles detected from the reaction are due to the peak

4.24
Fano plot
plot of data for the non-relativistic *kinetic energy* (3.35), E, times a specified factor versus the logarithm of E to evaluate the consistency with, or divergence from, the rate of energy loss for a fast charged particle with distance described by Bethe's theory

Note 1 to entry: The plot is named after U Fano[6] who, based on the theory of Bethe,[7] proposed a plot for testing the number of ionizations per unit path, S, for a fast charged particle in a gas. In his relativistic approach, $2\beta^2 S$ is plotted versus $\ln[\beta^2/(1-\beta^2)] - \beta^2$, where $\beta = v/c$, v being the particle velocity and c, the velocity of light. Fano plots have been utilized in analyses of sets of data for the electron *inelastic mean free path* (12.41), λ, in solid materials as a function of electron energy that were intended for use in *AES* (11.1) and XPS. In such applications, E/λ is plotted versus $\ln E$. In other applications, the product σE, where σ is the *cross section* (4.7) for a specified excitation or ionization, is plotted versus $\ln E$.

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4.25
Barkas effect
Barkas-Andersen effect
deviation, for *heavy particles* (18.7), of the *electronic stopping cross section* (4.12) from that of the Bethe theory

Note 1 to entry: The Bethe theory is derived in Reference [7].

Note 2 to entry: Published effects occur in the energy range above 0,5 MeV.

4.26
ionization cross section
cross section (4.7) for a process that produces, in an atom, a vacancy in a previously occupied shell

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

Note 2 to entry: 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 to entry: A partial ionization cross section can be expressed per electron in a shell or sub-shell or for the total number of these electrons in a shell or sub-shell of the particular atom.

Note 4 to entry: An atom can have multiple vacancies following an initial ionization or as the result of subsequent *Auger* (12.30) or *Coster-Kronig* (12.36) processes.

4.27
damage cross section
cross section (4.7) for the change in the number of particular entities considered to be a result of damage caused by bombardment by defined ions, electrons, or photons

Note 1 to entry: See *disappearancecross section* (20.16).

Note 2 to entry: The particular entities can, for example, be specific molecules on a *surface* (3.2), specific observed ion fragments, atoms in a given *chemical state* (12.23), or polymer cross-linking as inferred from spectral data.

Note 3 to entry: As a result of the break-up of larger entities, the observed entity can increase or decrease in intensity.

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

Note 5 to entry: Either as a result of the damage or as a result of electron or ion *sputtering* (9.3), the damaged material can be removed from the sample. For bulk samples, this can reduce any change in the relevant signal observed. For *monolayer* (5.6) samples, such sputtering can increase any change in the relevant signal observed. *Preferential sputtering* (9.26) can also change the relevant signal observed.

Note 6 to entry: A cross section of σ per atom for the removal of entities from a given state on a surface leads to a reduction $\mathrm{d}N$ in the number N of entities in that state in a time $\mathrm{d}t$ given by the relation:

$$\mathrm{d}N = -NJ\sigma\,\mathrm{d}t$$

where J is the primary-ion or electron *dose* (8.20) rate density.

Integration leads to the relation

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

where N_0 is the initial value of N.

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

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4.28
attenuation coefficient
quantity μ in the expression $\mu\Delta x$ for the fraction of a parallel beam of specified particles or radiation removed in passing through a thin layer Δx of a substance in the limit as Δx approaches zero, where Δx is measured in the direction of the beam

Note 1 to entry: See *attenuation length* (4.30) and *mass absorption coefficient* (4.39).

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

Note 3 to entry: The attenuation coefficient is the reciprocal of the attenuation length .

4.29
transport mean free path
λ_{tr}
average distance that an energetic particle travels before its momentum in its initial direction of motion is reduced to 1/e of its initial value by *elastic scattering* (4.1) alone

Note 1 to entry: See *inelastic mean free path* (12.41).

Note 2 to entry: 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* (4.10), σ_{tr}, by

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

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

4.30
attenuation length
quantity l in the expression $\Delta x/l$ for the fraction of a parallel beam of specified particles or radiation removed in passing through a thin layer Δx of a substance in the limit as Δx approaches zero, where Δx is measured in the direction of the beam

Note 1 to entry: See *attenuation coefficient* (4.28), *decay length* (4.31), *effective attenuation length* (12.45), *electroninelastic mean free path* (12.41), and *mass absorption coefficient* (4.39).

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

Note 3 to entry: For electrons in solids, the behaviour only approximates to an exponential decay due to the effects of *elastic scattering* (4.1). Nevertheless, for some measurement conditions in *AES* (11.1) and *XPS* (11.6), the *signal intensity* (3.17) can depend approximately exponentially on path length, but the exponential constant (the parameter l) is normally different from the corresponding inelastic mean free path. Where that approximation is valid, the term effective attenuation length is used.

4.31
decay length
value of l for an intensity exhibiting a response $e^{\pm x/l}$ with distance x

Note 1 to entry: See *attenuation length* (4.30).

4.32
emission function decay length
negative reciprocal slope of the logarithm of the *emission depth distribution function* (4.35) at a specified depth

4.33
average emission function decay length
negative reciprocal slope of the logarithm of a specified exponential approximation to the *emission depth distribution function* (4.35) 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

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4.34
deep emission function decay length
asymptotic value of the *emission function decay length* (4.32) for increasing depths from the *surface* (3.2)

4.35
emission depth distribution function
<for a measured signal of particles or radiation emitted from a surface> probability that the particle or radiation leaving the *surface* (3.2) in a specified state and in a given direction originated from a specified depth measured normally from the surface into the material

4.36
excitation depth distribution function
probability that specified excitations are created at specified depths measured, normally from a *surface* (3.2) into the material, by a beam of specified particles or radiation incident on the surface in a given direction

4.37
information depth
maximum depth, normal to the *surface* (3.2), from which useful information is obtained

Note 1 to entry: 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 to entry: 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 to entry: The information depth can be determined from a measured, calculated, or estimated *emission depth distribution function* (4.35) for the signal of interest.

4.38
mean escape depth
average depth normal to the *surface* (3.2) from which the specified particles or radiations escape as defined by

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

where $\phi(z,\theta)$ is the *emission depth distribution function* (4.35) for depth z from the surface into the material and for *angle of emission* (8.5)θ with respect to the surface normal

4.39
mass absorption coefficient
mass attenuation coefficient
quantity μ/ρ in the expression, $(\mu/\rho)\Delta(\rho x)$, for the fraction of a parallel beam of specified particles or radiation removed in passing through a thin layer of mass thickness $\Delta(\rho x)$ of a substance in the limit as $\Delta(\rho x)$ approaches zero, where $\Delta(\rho x)$ is measured in the direction of the beam

Note 1 to entry: See *attenuation length* (4.30).

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

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

Note 4 to entry: The mass attenuation (absorption) coefficient is the quotient of the *attenuation coefficient* (4.28) by the mass density of the substance.

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4.40
Beer's law
Beer-Lambert law
law in which the signal of interest decays exponentially with distance travelled

Note 1 to entry: In electron spectroscopies, in the approximation in which the electrons are assumed to travel in straight lines, the electron intensity of interest decays with distance with a decay constant given by the *attenuation length* (4.30). In a more complete approach in which the *elastic scattering* (4.1) of the electrons is considered, the electron intensity of interest decays with distance along the no-longer straight trajectory with a decay constant given by the *inelastic mean free path* (12.41).

4.41
projected range
<EIA, RBS, SIMS> distance from the *surface* (3.2) at which an energetic ion or atom comes to rest in the sample, projected along the direction of the beam

Note 1 to entry: See *range straggling* (4.43).

Note 2 to entry: Calculations usually deal with the mean or average projected range for a large number of ions or atoms of the same species and the same energy.

4.42
transverse range
<EIA, RBS, SIMS> distance, normal to the direction of an energetic ion or atom impacting a *surface* (3.2), at which the ion or atom comes to rest in the sample

Note 1 to entry: See *projected range* (4.41).

4.43
range straggling
<EIA, RBS, SIMS> standard deviation of the *projected ranges* (4.41) of energetic ions or atoms of a given energy

Note 1 to entry: See *transverse straggling* (4.44).

4.44
transverse straggling
<EIA, RBS, SIMS> standard deviation of the *transverse ranges* (4.42) of energetic ions or atoms of a given energy

Note 1 to entry: See *range straggling* (4.43).

4.45
infratrack
region of a *primary ion* (20.26) track in an organic material up to 1 nm from the track centre

Note 1 to entry: See *ultratrack* (4.46).

Note 2 to entry: The energy deposited electronically is deposited mainly as primary excitations and ionizations in this region.

4.46
ultratrack
region of a *primary ion* (20.26) track in an organic material from 1 to 100 nm from the track centre

Note 1 to entry: See *infratrack* (4.45).

Note 2 to entry: The energy deposited electronically in this region is deposited mainly through *secondary electrons* (12.2) produced as a result of primary processes in the infratrack. For fast ions, this fraction of the energy deposition can exceed that in the infratrack.

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4.47
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

5 Terms related to the description of samples

5.1
reference material
RM
material, sufficiently homogeneous and stable with respect to one or more specified properties, which has been established to be fit for its intended use in a measurement process

[SOURCE: ISO Guide 30:1992+A1:2008[3]]

EXAMPLE Implanted silicon wafers to calibrate dopant levels; thin oxide layers on substrates to calibrate depth or thickness in analytical *depth profiling* (3.34) instruments.

Note 1 to entry: Some RMs involving surface properties can be in the form of wafers or foils. For these, the material is often homogeneous for the property values across the *surface* (3.2) but not in the direction perpendicular to the surface and into the bulk.

5.2
certified reference material
CRM
reference material (5.1) characterized by a metrologically valid procedure for one or more specified properties, accompanied by a certificate that provides the value of the specified property, its associated uncertainty, and a statement of metrological traceability

[SOURCE: ISO Guide 30:1992+A1:2008[3]]

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

Note 2 to entry: All CRMs lie within the definition of "measurement standards" given in the international vocabulary of metrology, ISO/IEC Guide 99[6].

Note 3 to entry: Some *RMs* (5.1) and CRMs have properties which, because they cannot be correlated with an established chemical structure or for other reasons, cannot be determined by exactly defined physical and chemical measurement methods. Such materials include certain biological materials such as vaccines to which an international unit has been assigned by the World Health Organization.

5.3
interfacial region
volume between two bulk phases having chemical, elemental, or physical properties different from either bulk phase

5.4
segregation
partitioning of a species from one region to another as a result of kinetic or thermodynamic effects

Note 1 to entry: Segregation is often observed at *surfaces* (3.2) and *interfaces* (3.1).

5.5
surface segregation
partitioning of a species from the bulk of a material to the *surface* (3.2) as a result of kinetic or thermodynamic effects

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5.6
monolayer
<chemisorption, physisorption, segregation> complete coverage of a substrate by one atomic or molecular layer of a species

5.7
monolayer capacity
<chemisorption> amount of adsorbate which is required to occupy all adsorption sites as determined by the structure of the adsorbent and by the chemical nature of the adsorptive

5.8
monolayer capacity
<physisorption> amount of adsorbate which is required to cover the *surface* (3.2) with a complete *monolayer* (5.6) of atoms or molecules in a close-packed array

Note 1 to entry: The type of close packing shall be stated.

5.9
surface coverage
<chemisorption, physisorption> quotient of the amount of a material at a *surface* (3.2) by a measure of the surface area

Note 1 to entry: The surface coverage can be expressed in atoms·m^{-2}, in mol·m^{-2}, in kg·m^{-2}, or as a ratio of the amount to the *monolayer capacity* (5.7) (5.8).

5.10
multilayer
structure composed of two or more chemically distinct layers

Note 1 to entry: See *delta layer* (5.12).

Note 2 to entry: 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.

5.11
multilayer
<chemisorption, physisorption> coverage of a substrate surface by more than one atomic or molecular layer of the adsorptive or segregated species

Note 1 to entry: See *monolayer* (5.6).

5.12
delta layer
layer of discrete composition, one atom thick, formed during growth of material on a substrate

Note 1 to entry: These films are often formed during epitaxial growth on single-crystal substrates.

5.13
thin film
layer of material, typically less than 100 nm in thickness, deposited or grown on a substrate

Note 1 to entry: Films thinner than 10 nm are often called ultrathin films.

5.14
self-assembled monolayer
SAM
film, one molecule thick, covalently assembled on a *surface* (3.2)

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5.15
Langmuir-Blodgett film
LB film
film comprising one or more *monolayers* (5.6) of organic molecules

Note 1 to entry: The films are transferred from the *surface* (3.2) of a liquid bath onto solid substrates and by repeated immersions many layers can be deposited. Control of the liquid surface tension during this process allows the molecular density of the monolayers to be controlled.

5.16
surface contamination
material, generally unwanted, on the sample *surface* (3.2) which either is not characteristic of that sample and any process investigated or has arisen from exposure of the sample to particular environments other than those relevant for the original surface or the process to be studied

Note 1 to entry: Common surface contaminants are hydrocarbons and water. Local reactions with these and the environment can lead to a wide range of oxidation and other products.

5.17
charge modification
alteration of the amount or the distribution of charge at a sample *surface* (3.2)

5.18
field-induced migration
effect occurring in insulators where internal electric fields created by ion or electron bombardment cause the migration of sample atoms

5.19
bond cleavage
bond scission
breakage of a molecular bond

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

Note 2 to entry: For α- and β-cleavage, see Reference [8] or [9].

5.20
surfactant
substance that lowers the interfacial energy of a material in contact with a liquid or the surface energy of that liquid

Note 1 to entry: In practice, the liquid is usually water or a water-based medium. Emulsifiers, detergents, and dispersing agents are examples of surfactants.

Note 2 to entry: In many cases, surfactant molecules have a hydrophilic or polar group at one end and a lipophilic or oleophilic group at the other.

5.21
tethering
process of attaching a molecule to a surface

Note 1 to entry: Molecules can be attached to surfaces by functionalizing the surface, or first adsorbing other *cross-linker* (5.22) molecules.

5.22
cross-linker
<adsorption> molecule with appropriate end groups to bond to both molecules adsorbed on a surface and further molecules which do not adsorb on those adsorbed molecules

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5.23
polymer repeat unit
smallest structure that, repeated many times, describes the molecular structure of the polymer

5.24
dendrimer
molecule comprising a multifunctional core molecule with a dendritic wedge of highly branched monomers regularly attached to each functional site, leading to a monodisperse, tree-like, or generational structure

Note 1 to entry: Dendrimer synthesis occurs in polymer chemistry and involves stepwise reactions in which the dendrimer is built up one monomer layer, or generation, at a time. The core molecule is referred to as "generation 0". Each successive *repeat unit* (5.23) along all branches forms the next generation, "generation 1", "generation 2", and so on until the terminating generation.

6 Terms related to sample preparation

6.1
cross-sectioning
sample preparation in which the sample is cleaved, cut, or polished in a plane perpendicular to the *interface* (3.1) under stuy, so that associated compositional differences or gradients can be observed in that plane

6.2
angle lapping
sample preparation in which a sample is mechanically polished at an angle to the original *surface* (3.2)

Note 1 to entry: See *ball catering* (6.3) and *radial sectioning* (6.4).

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

6.3
ball cratering
procedure in which the sample is abraded by a sphere in order to expose compositional changes in layers below the original *surface* (3.2) with the intent that the depth of those layers can be related to the lateral position in the crater created by the abrasion

Note 1 to entry: See *angle lapping* (6.2) and *radial sectioning* (6.4).

6.4
radial sectioning
sample preparation in which a sample is polished by a cylinder in order to expose compositional changes below the original sample *surface* (3.2) with the intent that the depth of these layers can be related to the position on the surface created by the cylinder

Note 1 to entry: See *angle lapping* (6.2) and *ball catering* (6.3).

6.5
spin coating
coating of a thin layer of an organic material deposited from solution, under the action of high-speed rotation, on a flat substrate wetted by that solution

Note 1 to entry: Rotation speeds of about 4 000 r/min are commonly used, producing films generally thinner than 100 nm.

Note 2 to entry: Some users place a drop of solution in the centre and some flood the whole sample, prior to the high-speed rotation that removes the solvent.

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7 Terms related to instrumentation

7.1
synchrotron radiation
electromagnetic radiation (photons) with a continuous energy spectrum, created by the acceleration of electrons in a synchrotron or storage ring

7.2
instrumental background
intensity contribution, generally unwanted, arising from non-ideal behaviour of one or more parts of the instrument

7.3
internal scattering
process in which some particles strike internal *surfaces* (3.2) of the spectrometer in such a way that scattered or secondary particles are detected as unwanted intensity in the spectrum

7.4
solid angle of analyser
solid angle from a point on the sample that transmits particles or photons to the detector

Note 1 to entry: See *analyser transmission function* (7.15).

7.5
optical aperture
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

7.6
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* (3.2)

Note 1 to entry: See *optical aperture* (7.5).

7.7
contrast aperture
aperture, in an ion or electron optical system, designed to reduce unwanted *background signal* (3.21)

Note 1 to entry: This aperture can also govern the *spatial resolution* (10.14) and other properties of the system.

7.8
detector efficiency
fraction of particles or photons incident on the detector that result in the detected signal

7.9
instrumental detection efficiency
ratio of the quantity of a detected event to the quantity of that event available for measurement

7.10
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, $\Delta m/m$

7.11
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, $\Delta\lambda$

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7.12
spectrometer étendue
integral of the product of the spectrometer transmission and an element of area of a plane *surface* (3.2), normal to the analyser axis passing through the centre of the *analysis area* (8.49), over that surface

Note 1 to entry: The units of étendue can be sr·m^2·eV, sr·m^2·amu, or sr·m^3.

7.13
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

Note 1 to entry: See *spectrometer étendue* (7.12).

Note 2 to entry: The dispersing parameter is commonly energy, mass, or wavelength.

Note 3 to entry: The units of the spectrometer response function can be sr·eV, sr·amu, or sr·m.

Note 4 to entry: The spectrometer response function is similar to the *spectrometer transmission function* (7.15) 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 5 to entry: For some methods of *quantitative analysis* (3.8), the energy dependence of the response function is required in order to use *relative sensitivity factors* (12.91). For these cases, a function is determined which is proportional to the absolute response function, where the proportionality constant is not necessarily important.

7.14
relative instrument spectral response function
RISR
<AES, SIMS, XPS> ratio of the *spectrometer response function* (7.13) to the response function of a reference instrument, or the average for several such instruments, as a function of energy [*AES* (11.1), *XPS* (11.6), etc.] or mass (*SIMS* (19.1))

Note 1 to entry: The RISR can be used to relate spectra from one instrument to spectra from another when using similar excitation sources and geometries.

7.15
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

Note 1 to entry: See *spectrometer response function* (7.13).

Note 2 to entry: The units of transmission can be sr·eV, sr·amu, or sr·m.

Note 3 to entry: Often, an incomplete use of the term occurs where just the solid angle of acceptance of the spectrometer, in sr, or a fraction of the 2π solid angle of available space is given. This usage is deprecated, cf. *solid angle of analyser* (7.4).

Note 4 to entry: This term is often used incorrectly instead of spectrometer response function, which includes contributions from the detector and the signal-processing system.

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7.16
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 1 to entry: 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* (20.28) (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).

7.17
dead time
time per pulse for which a pulse-counting system is unavailable for further counting

7.18
non-extended dead time
dead time (7.17) for a system where the pulse lengths are not extended by extra pulses arriving during the dead time associated with earlier pulses

7.19
extended dead time
dead time (7.17) for a system where the pulse lengths are extended by extra pulses arriving during the dead time associated with an earlier pulse

7.20
multidetector dead time
effective *dead time* (7.17) of the whole detector, treating it as a single detector

7.21
post-acceleration detector voltage
post-acceleration voltage
voltage applied to the front of the detector to increase the *impact energy* (8.35) of incident electrons or ions

Note 1 to entry: Voltages are often referred to reference points in the instrumental electronics, but here the reference zero is such that a post-acceleration detector voltage of 5 kV leads to an impact energy of 5 keV, etc. Post-acceleration detector voltages of 5 kV to 20 kV are generally used.

7.22
beam blanking
electrostatic or electromagnetic process designed to prevent *beam particles* (8.9) from impacting the sample when activated

Note 1 to entry: See *beam bunching* (20.44) and *beam chopper* (20.48).

Note 2 to entry: For pulsed *ion beams* (8.8), the beam is usually deflected into a beam collector from which no particles can reach the sample and where the process of *sputtering* (9.3) causes minimal effect on nearby components of the ion optical system.

7.23
chromatic aberration
non-ideal focus of an particle optical system for particles of different energies

7.24
energy acceptance window
range of energies accepted by a spectrometer, leading to a detected signal

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7.25
dynamic emittance matching
electron or ion optical method of steering a spectrometer axis to align with the impact area of the *primary beam* (8.10) at all points of a *raster* (8.38) scan on the sample *surface* (3.2)

7.26
FIB
focussed ion beam system
ion beam (8.8) system used for machining small regions with sub-micron precision

Note 1 to entry: FIB-machined *surfaces* (3.2) can have an ion-damaged surface that requires removal.

7.27
gas cluster ion beam
GCIB
ion beam (8.8) formed of *cluster ions* (3.44) by ionising condensed clusters of atoms or molecules that are gaseous at ambient temperature and pressure

7.28
liquid-metal ion gun
LMIG
ion gun utilizing a liquid-metal Taylor cone as the source of the *primary ions* (20.26)

Note 1 to entry: The Taylor cone generates ion sources of very high brightness. This design enables the gun to provide *beam diameters* (8.30) in the range 50 nm to 1 µm for ion *beam energies* (8.33) in the range 5 keV to 30 keV, the lowest diameters generally being at the higher energies.

7.29
intrinsic linewidth
<instrument> see *resolution of a spectrometer* (10.6)

7.30
raw-data file
unprocessed-data file of information provided by an instrument

Note 1 to entry: For *time of flight* (20.49) SIMS instruments, this file usually contains the *x*- and *y*-coordinates of the *ion beam* (8.8)*raster* (8.38) address as well as the recorded flight times and signal intensities since these files are used retrospectively to generate secondary-ion *maps* (8.57) or spectra from the whole or selected parts of the map, or to generate these from all or selected time regions.

8 Terms related to experimental conditions

8.1
angle of incidence
incidence angle
angle between the incident beam and the local or average surface normal

Note 1 to entry: The particular surface normal, such as the surface normal to an elementary portion of a rough *surface* (3.2) or the normal to the average surface plane, shall be specified.

8.2
glancing angle
grazing angle
angle between the incident beam and the average surface plane

Note 1 to entry: The *angle of incidence* (8.1) and the glancing angle are complementary.

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