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Surface chemical analysis — Vocabulary —

Part 1: General terms and terms used in spectroscopy

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Analyse chimique des surfaces — Vocabulaire —

Partie 1: Termes généraux et termes utilisés en spectroscopie

ISO/FDIS 18115-1

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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).

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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.

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.

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

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: $1 \text{ u} \approx 1,660\,538\,86 \times 10^{-27} \text{ kg}$ with a one-standard-deviation uncertainty of $\pm 0,000\,000\,28 \times 10^{-27} \text{ kg}$.^[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, $1 \text{ u} = 1,000\,317\,9 \text{ amu}$ (physical scale) = $1,000\,043 \text{ amu}$ (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.

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.

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.

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.

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.

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 H₂⁺.

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 •CH₃, •SnH₃, and Cl• 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 C₆H₆^{•+}); a negatively charged radical is called a “radical anion” (e.g. the benzene radical anion C₆H₆^{•-} or the benzophenone radical anion Ph₂C–O^{•-}). 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 •+ or •- as suggested by the name “radical ion” (e.g. C₃H₆^{•+}).

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).

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^+ ($\text{H}_2\text{O})_n^+$].

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] standards.iteh.ai/catalog/standards/sist/f40bf6be-11e0-48f4-91d6-8e1adc5aad03/iso-fdis-18115-1

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.

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