

# INTERNATIONAL STANDARD

**ISO**  
**18115**

First edition  
2001-07-15

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## Surface chemical analysis — Vocabulary

*Analyse chimique des surfaces — Vocabulaire*

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Reference number  
ISO 18115:2001(E)

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Printed in Switzerland

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## Foreword

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

International Standards are drafted in accordance with the rules given in the ISO/IEC Directives, Part 3.

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

Attention is drawn to the possibility that some of the elements of this International Standard may be the subject of patent rights. ISO shall not be held responsible for identifying any or all such patent rights.

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

Annex A of this International Standard is for information only.

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

With the present techniques of surface chemical analysis, compositional information is obtained for regions close to a surface (generally within 20 nm) and composition-versus-depth information is obtained with surface analytical techniques as surface layers are removed. The surface analytical techniques covered in this International Vocabulary extend from electron spectroscopy and mass spectrometry to optical spectrometry and X-ray analysis. Concepts for these techniques derive from disciplines as widely ranging as nuclear physics and radiation science to physical chemistry and optics.

The wide range of disciplines and the individualities of national usages have led to different meanings being attributed to particular terms and, again, different terms being used to describe the same concept. To avoid the consequent misunderstandings and to facilitate the exchange of information, it is essential to clarify the concepts, to establish the correct terms for use and to establish their definitions.

The work for ISO 18115 started with a consideration, *inter alia*, of ASTM E 673-95a, *Standard terminology relating to surface analysis*<sup>[1]</sup>, and a number of terms retain this reference. Such definitions have remained essentially unchanged. Some editorial changes have had to be made in all the cases where this reference appears since the ASTM definition structure differs from that adopted by ISO. Some other terms from the ASTM standard also appear, but with a revised text or significantly revised meaning. These terms are not referenced to the ASTM standard.

### ISO 18115:2001

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

Clause 4: Definitions of the surface analysis methods.

Clause 5: Definitions of terms for surface analysis.

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

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

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

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# Surface chemical analysis — Vocabulary

## 1 Scope

This International Standard defines terms for surface chemical analysis.

## 2 Abbreviations

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

SAM	scanning Auger microscope
SDP	sputter depth profile
SEM	scanning electron microscope
SIMS	secondary-ion mass spectrometry
SNMS	sputtered neutral mass spectrometry
SSA	spherical sector analyser
TOF or ToF	time of flight
TXRF	total-reflection X-ray fluorescence spectroscopy
UPS	ultra-violet photoelectron spectroscopy
XPS	X-ray photoelectron spectroscopy

### 3 Format

#### 3.1 Use of terms printed boldface in definitions

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

#### 3.2 Non-preferred and deprecated terms

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

#### 3.3 Subject fields

Where a term designates several concepts, it is necessary to indicate the subject field to which each concept belongs. The field is shown lightface, between angle brackets, preceding the definition, on the same line.

### 4 Definitions of the surface analysis methods

#### 4.1

##### Auger electron spectroscopy

##### AES

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

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

#### 4.2

##### dynamic SIMS

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

**NOTE 1** Dynamic SIMS is often simply termed SIMS.

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



**4.3**

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

NOTE The term ESCA has fallen out of use as, in practice, it was only used to describe situations more clearly defined by the term X-ray photoelectron spectroscopy (XPS). Since 1980, the latter term has been preferred.

**4.4**

**fast atom bombardment mass spectrometry**  
**FABMS**

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

**4.5**

**glow discharge mass spectrometry**  
**GDMS**

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

**4.6**

**glow discharge optical emission spectrometry**  
**GDOES**

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

**4.7**

**glow discharge spectrometry**  
**GDS**

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

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

**4.8**

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

a method to elucidate composition and structure of the outermost atomic layers of a solid material, in which principally monoenergetic, singly charged **probe ions**, scattered from the **surface** are detected and recorded as a function of their energy or **angle of scattering**, or both

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

**4.9**

**secondary-ion mass spectrometry**  
**SIMS**

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

cf. **dynamic SIMS**, **static SIMS**

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

#### 4.10

##### **sputtered neutral mass spectrometry SNMS**

a method in which a mass spectrometer is used to measure the mass-to-charge quotient and abundance of secondary ionized neutral species emitted from a sample as a result of particle bombardment

NOTE The neutral species may be detected by using plasma, electron, or photon ionization methods.

#### 4.11

##### **static SIMS**

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

cf. **dynamic SIMS**

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

#### 4.12

##### **total reflection X-ray fluorescence spectroscopy TXRF**

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

#### 4.13

##### **ultra-violet photoelectron spectroscopy UPS**

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

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

#### 4.14

##### **X-ray photoelectron spectroscopy XPS**

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

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

## 5 Definitions of terms for surface analysis

### 5.1

#### **absorption coefficient, linear** linear **attenuation coefficient**

### 5.2

#### **absorption coefficient, mass** **attenuation coefficient, mass**

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

cf. **attenuation length**

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

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

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

### 5.3 adventitious carbon referencing

<XPS> determining the **charging potential** of a particular sample from a comparison of the experimentally determined C 1s binding energy, arising from adsorbed hydrocarbons on the sample, with a standard binding energy value

cf. **internal carbon referencing**

NOTE A nominal value of 285,0 eV is often used for the binding energy of the relevant C 1s peak, although some analysts prefer specific values in the range 284,6 eV to 285,2 eV depending on the nature of the substrate.

### 5.4 altered layer

<particle bombardment> surface region of a material under particle bombardment where the chemical state or physical structure is modified by the effects of the bombardment

EXAMPLE For silicon bombarded by 4 keV  $O_2^+$  at near normal incidence, after sputtering for a sufficient time to reach a steady state, the surface is converted to stoichiometric  $SiO_2$  to a depth of around 15 nm with lower oxygen concentrations at greater depths.

### 5.5 analysis area

<sample> two-dimensional region of a sample **surface** measured in the plane of that surface from which the entire analytical signal or a specified percentage of that signal is detected

### 5.6 analysis area

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

### 5.7 analysis volume

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

### 5.8 analysis volume

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

### 5.9 angle, critical

<TXRF> **glancing angle** at which the sample matrix X-ray fluorescence, when plotted against the glancing angle, is at the first point of inflection

### 5.10 angle, glancing

<TXRF> angle between the incident beam and the average surface plane

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

### 5.11

#### **angle lapping**

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

cf. **ball cratering, radial sectioning**

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

### 5.12

#### **angle, magic**

〈XPS〉 angle at which the spectrometer entrance axis is aligned at 54,7° to the direction of the X-rays at the sample surface

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

### 5.13

#### **angle of emission**

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

NOTE The particular surface normal needs to be specified.

### 5.14

#### **angle of incidence**

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

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

### 5.15

#### **angle of scattering**

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

### 5.16

#### **angle-resolved AES**

##### **ARAES**

#### **angle-dependent AES**

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

### 5.17

#### **angle-resolved XPS**

##### **ARXPS**

#### **angle-dependent XPS**

a procedure in which X-ray photoelectron intensities are measured as a function of the **angle of emission**

NOTE This procedure is often used to obtain information on the distribution with depth of different elements or compounds in a layer approximately 5 nm thick at the surface.

### 5.18

#### **angle, solid, of analyser**

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

cf. **analyser transmission function**

### 5.19

#### **angle, solid, of detector**

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

**5.20****angle, take-off**

angle between the trajectory of a particle as it leaves a surface and the local or average surface plane

NOTE 1 The particular surface plane needs to be specified.

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

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

**5.21****asymmetry parameter**

$\beta$

〈XPS〉 factor which characterizes the intensity distribution,  $L(\gamma)$ , of photoelectrons ejected by unpolarized X-rays from isolated atoms in a direction  $\gamma$  from the incident X-ray direction according to

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

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

**5.22****atomic mixing**

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

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

**5.23****attenuation coefficient**

quantity  $\mu$  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  $\Delta x$  of a substance in the limit as  $\Delta x$  approaches zero, where  $\Delta x$  is measured in the direction of the beam

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

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

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

**5.24****attenuation length**

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

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

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

NOTE 2 For electrons in solids, the behaviour only approximates an exponential decay due to the effects of elastic scattering. Where this approximation is valid, the term effective attenuation length is used.

**5.25****attenuation length, effective**

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

cf. **attenuation length**

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

## 5.26

### **Auger de-excitation**

<surface>

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

cf. **Auger neutralization**

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

## 5.27

### **Auger electron**

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

cf. **Auger transition**

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

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

## 5.28

### **Auger electron spectrum**

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

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

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

## 5.29

### **Auger electron yield**

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

## 5.30

### **Auger neutralization**

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

NOTE The ejected electron may be emitted into the vacuum.

## 5.31

### **Auger parameter**

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

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

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

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

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

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

### 5.32

#### Auger parameter, initial state

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

cf. Auger parameter, modified Auger parameter

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

### 5.33

#### Auger parameter, modified

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

cf. Auger parameter, initial state Auger parameter

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

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### 5.34

#### Auger process

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

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

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

### 5.35

#### Auger process, interatomic

(AES) **Auger transition** in which at least one of the final electron vacancies is localized in valence levels or molecular orbitals of atoms adjacent to the atom in which the initial vacancy occurred

### 5.36

#### Auger transition

**Auger process** involving designated electron shells or sub-shells

NOTE 1 The three shells involved in the Auger process are designated by three letters. The first letter designates the shell containing the initial vacancy and the last two letters designate the shells containing electron vacancies left by the Auger process (for example, KLL, and LMM). When a valence electron is involved, the letter V is used (for example, LMV and KVV). When a particular sub-shell involved is known, this can also be indicated (for example,  $KL_1L_2$ ). Coupling terms may also be added, where known, to indicate the final atomic state (for example,  $L_3M_{4,5}M_{4,5};^1D$ ).

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

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