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Surface chemical analysis — Vocabulary
AMENDMENT 1

Analyse chimique des surfaces — Vocabulaire
Amendement 1

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Foreword

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Amendment 1 to ISO 18115:2001 was prepared by Technical Committee ISO/TC 201, *Surface chemical analysis*, Subcommittee SC 1, *Terminology*.

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Introduction

In ISO 18115:2001, 350 terms for surface chemical analysis are provided. However, from time to time new terms need to be defined and these will appear in Amendments to ISO 18115. In this Amendment, five abbreviations and 71 terms are added. None of the previous terms are changed.

This Amendment has been prepared in conformance with the principles and style defined in ISO 1087-1, *Terminology work — Vocabulary — Part 1: Theory and application*, and ISO 10241, *International terminology standards — Preparation and layout*. It should be noted that, as in ISO 18115, a term printed boldface in a definition or a note is defined in another entry in the Amendment. However, the term is printed boldface only the first time it occurs in each entry. A term listed lightface is non-preferred or deprecated. The preferred term is listed boldface. 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.

The abbreviations given here add to those given in Clause 2 of ISO 18115. The terms given here in alphabetical order form a new Clause 6. An alphabetical index for this Amendment is given after the terms and definitions. The index for ISO 18115:2001 is given immediately after this for convenience. To assist retrieval, compound terms may be found in these indexes in both natural and reverse word order. It is recommended that users searching for a term start with these indexes.

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Surface chemical analysis — Vocabulary

AMENDMENT 1

Pages 1 and 2

Add the following abbreviations:

CRM	certified reference material
dc	direct current
rf	radio-frequency
RM	reference material
RSF	relative sensitivity factor

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Add the following clause:

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6 Definitions of supplementary terms for surface analysis

6.1

abundance sensitivity

⟨GDMS⟩ ratio of the maximum ion current recorded at a mass m to the ion current arising from the same species recorded at an adjacent mass ($m \pm 1$)

[IUPAC, 1997]

6.2

afterglow

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

6.3

anode

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

cf **cathode** ⟨GDS, dc operation⟩

6.4

anode

⟨GDS, rf operation⟩ electrode that is more positively charged over a large fraction of the rf cycle in a radio frequency powered **glow discharge** device

cf **cathode** ⟨GDS, rf operation⟩

NOTE 1 The rf power applied to a typical rf glow discharge device that is used for surface chemical analysis is sinusoidal and bipolar, with a time-averaged electric potential of zero relative to ground potential. The reason that the anode is not more positively charged over the entire rf cycle is that the magnitude of the **dc bias** is usually slightly less than one-half of the applied rf peak-to-peak potential.

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

6.5
anode glow

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

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

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

6.6
Auger vacancy satellite

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

6.7
background equivalent concentration

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

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

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6.8
background, relative standard deviation of the

quotient of the standard deviation characterizing the noise in the background signal and the background signal

6.9
cathode

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

cf. **anode** ⟨GDS, dc operation⟩

6.10
cathode

⟨GDS, rf operation⟩ electrode that is more negatively charged over a large fraction of the rf cycle in a radio frequency powered **glow discharge** device

cf. **anode** ⟨GDS, rf operation⟩

NOTE 1 The rf power applied to a typical rf glow discharge device that is used for surface chemical analysis is sinusoidal and bipolar, with a time-averaged electric potential of zero relative to ground potential. The reason that the cathode is not more negatively charged over the entire rf cycle is that the magnitude of the **dc bias** is usually slightly less than one-half of the applied rf peak-to-peak potential.

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

6.11 cathode fall fall potential

cathode drop

⟨GDS⟩ electric potential difference between the **cathode** surface and the **negative glow**

NOTE In direct-current **glow discharge spectrometry** typically used for surface chemical analysis, the cathode fall is usually in the range 200 V to 2 000 V, with the cathode surface being more negative. In an rf glow discharge, the cathode fall is time-varying, with a peak-to-peak value normally in the range 500 V to 2 000 V.

6.12 cathode layer

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

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

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

6.13 charge transfer charge exchange

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

6.14 charge transfer, asymmetric charge exchange, asymmetric

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

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

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

6.15 charge transfer, symmetric charge exchange, symmetric

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

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

6.16 chemical species

atom, molecule, ion or functional group

6.17 chemical state of an atom

⟨AES, EELS, UPS, XPS⟩ state of an atom arising from its chemical interaction with neighbouring atoms in a molecule, compound, solid, liquid or gas that leads to a characteristic energy or feature observable in electron spectroscopies

NOTE 1 Examples of features observed are satellite peaks, shifts in the peak energy positions, changes in the **lineshape** and changes in the **characteristic electron energy loss** spectra at lower **kinetic energies** than the photoelectron or **Auger electron** peaks.

NOTE 2 A full description of chemical state is denoted by the complete set of electronic states and the electron configuration in the core of the atom providing the signal, as well as the electronic and physical structure (including charge distribution, density of electronic states and electronic configuration) local to this atom.

NOTE 3 The chemical state of a selected atom is determined by its interaction (e.g. chemical bonding ionicity or covalency) with nearby atoms, most importantly its nearest neighbours. It is determined by the oxidation number of an atom in a compound, by the coordination (mostly by its stereo structure and number) and by the differences in the kinds of element in the position of the first nearest neighbour, second nearest neighbour, and so on. These all affect the effective charge and spin state of the selected atom.

NOTE 4 Different or distinguishable sets of chemical properties (different chemical states) of a chemical species may occur as a consequence of differing valence-band electronic structures, including charge distributions and electronic configurations, localized on the given chemical species. In XPS, the term “chemical state” is mostly used for characterizing measured binding energies, Auger-electron kinetic energies, and Auger parameters with different oxidation states of a given element in different chemical compounds, e.g. the Cr(III) oxidation state in Cr_2O_3 or $\text{Cr}(\text{OH})_3$. In AES, the term “chemical state” is often used to characterize the shape of the Auger electron spectrum for the atoms of an element in different chemical environments, e.g. the shape of the carbon Auger electron spectrum for graphite and for various carbides. Differences in the chemical properties of a chemical species in various environments may result in differences in the respective peak energies, satellite structures, lineshapes or energy loss features in the corresponding Auger or photoelectron spectra.

NOTE 5 The quantum theory of atoms in molecules defines an atom in a molecule or crystal as a bounded region of real space — an open quantum system. However, there is no wave function for the atom — only for the total system. Hence, there is no state designation for the atom — only for the total system. What physics provides are expectation values of all the observables, measurable or otherwise, for the bound atom. In this sense, its state is defined within the total system by the net charge and energy of the atom and how changes of charge and energy are reflected in the observed (e.g. Auger or photoelectron) spectra.

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6.18 chemical state plot Wagner plot

<XPS> plot of the measured **kinetic energy** of a sharp **Auger electron** peak versus the **binding energy** of a **photoelectron** peak for the same element

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

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

6.19 dark space

<GDS> region of a **glow discharge** that emits little light compared to the surrounding regions, thereby appearing dark to the human eye

6.20 dark space, anode

<GDS> dark space between the **positive column** and the **anode glow** in a **glow discharge**

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

6.21 dark space, Aston

<GDS> very thin dark space immediately adjacent to the cathode in a glow discharge

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

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

6.22**dark space, cathode**

Crookes' dark space

Hittorf dark space

〈GDS〉 dark space between the **cathode layer** and the **negative glow** in a **glow discharge**cf. **Aston dark space, Faraday dark space** and **anode dark space**

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

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

6.23**dark space, Faraday**〈GDS〉 dark space between the **negative glow** and the **positive column** in a **glow discharge**cf. **Aston dark space, cathode dark space** and **anode dark space****6.24****dc bias****dc offset****self bias**

〈GDS, rf operation〉 time-averaged electric potential, relative to ground, developed on the surface of the electrode to which the rf power is applied

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

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

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

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

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

6.26**energy eigenvalue**

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

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

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

6.27

excitation, electron impact

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

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

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

6.28

floating potential

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

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

6.29

frozen-orbital approximation

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

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

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6.30

glow discharge, abnormal

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

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cf. **glow discharge, normal** ⟨GDS⟩

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

6.31

glow discharge, boosted

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

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

6.32

glow discharge, normal

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

cf. **glow discharge, abnormal** ⟨GDS⟩

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

6.33**glow discharge, pulsed**

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

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

NOTE 2 Both pulsed direct-current and pulsed radio-frequency glow discharges have been devised.

6.34**glow discharge source, jet-assisted
glow discharge source, jet-enhanced**

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

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

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

6.35**hole**

electronic vacancy in an atom, molecule or solid

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6.36**hole state**

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

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6.37**ion beam ratio**

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

6.38**ionization, electron impact**

⟨GDS⟩ ionization resulting from collision of an atom, molecule or ion with an electron

NOTE 1 For example, $M + e^- \rightarrow M^+ + 2e^-$, where M^+ is a transition metal ion.

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

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

6.39**ionization, Penning**

⟨GDS⟩ ionization resulting from collision with an atom that is in an electronically excited state

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