International Standard

ISO 18118

Surface chemical analysis — Auger electron spectroscopy and X-ray photoelectron spectroscopy — Guide to the use of experimentally determined relative sensitivity factors for the quantitative analysis of homogeneous materials

**Third edition
2024-02**

Analyse chimique des surfaces — Spectroscopie des électrons Auger et spectroscopie de photoélectrons — Lignes directrices pour l'utilisation de facteurs expérimentaux de sensibilité relative pour l'analyse quantitative de matériaux homogènes

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Foreword

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This document was prepared by Technical Committee ISO/TC 201, *Surface chemical analysis*, Subcommittee SC 7, *Electron spectroscopies*.

This third edition cancels and replaces the second edition (ISO 18118:2015), which has been technically revised.

The main changes are as follows:

— The main equation for the use of sensitivity factors for analysis has been moved from Annex A to the main text

— Defined symbols and abbreviated terms from the Annexes have been consolidated to Clause 4.

— Several terms have been modified for formatting purposes, and some have been removed due to no longer being required.

— Several formulae have been removed from Annex A and replaced by references to formulae and databases of parameters that are more accurate. Such databases are now the recommended source for the parameters calculated using the removed formulae.

— Annex A has been redefined as an informative Annex.

— Multiple small additions have been made to provide new and updated sources for information.

— Editorial changes have been made throughout.

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

Auger electron spectroscopy (AES) and X-ray photoelectron spectroscopy (XPS) are surface-analytical techniques that are sensitive to the composition in the surface region of a material to depths of, typically, a few nanometres (nm). Both techniques yield a surface-weighted signal, averaged over the analysis volume. Most samples have compositional variations, both laterally and with depth, and quantification is often performed with approximate methods since it can be difficult to determine the magnitude of any compositional variations and the distance scale over which they can occur. The simplest sample for analysis is one that is homogeneous. Although this situation occurs infrequently, it is often assumed, for simplicity in the analysis, that the sample material of interest is homogeneous. This document provides guidance on the measurement and use of experimentally determined relative sensitivity factors for the quantitative analysis of homogeneous materials by AES and XPS.

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Surface chemical analysis — Auger electron spectroscopy and X-ray photoelectron spectroscopy — Guide to the use of experimentally determined relative sensitivity factors for the quantitative analysis of homogeneous materials

1 Scope

This document gives guidance on the measurement and use of experimentally-determined relative sensitivity factors for the quantitative analysis of homogeneous materials by Auger electron spectroscopy and X-ray photoelectron spectroscopy. The methods described only apply to polycrystalline and amorphous materials, as effects inherent to single-crystal samples are not addressed.

2 Normative references

The following documents are referred to in the text in such a way that some or all of their content constitutes requirements of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 18115-1, *Surface chemical analysis — Vocabulary — Part 1: General terms and terms used in spectroscopy*

ISO 21270, *Surface chemical analysis — X-ray photoelectron and Auger electron spectrometers — Linearity of intensity scale*

3 Terms and definitions

For the purposes of this document, the terms and definitions given in ISO 18115-1 and the following apply.

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
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 *relative elemental sensitivity factor*.

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* 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* this has a dominating influence.

[SOURCE: ISO 18115-1]

3.2
elemental relative sensitivity factor
<AES, XPS> coefficient proportional to the *absolute elemental sensitivity factor* (3.1)*,* where the constant of proportionality is chosen such that the value for a selected element and transition is unity

Note 1 to entry: Elements and transitions commonly used are C 1s or F 1s for *XPS* and Ag $M_{4,5}$VV for *AES*.

Note 2 to entry: The type of sensitivity factor used should be appropriate for the type of sample analysed, for example homogeneous samples or segregated layers.

Note 3 to entry: The source of sensitivity factors should be given to ensure that the correct *matrix factors* or other parameters are used.

Note 4 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* this has a dominating influence.

[SOURCE: ISO 18115-1]

3.3
average matrix relative sensitivity factor
AMRSF
<AES, XPS> coefficient, proportional to the intensity, calculated for an element in an average matrix, by which the measured intensity for that element is divided in calculations to yield the atomic concentration or atomic fraction of the element present in the sample

Note 1 to entry: See sensitivity factor, *elemental relative sensitivity factor* (3.2) and *pure element relative sensitivity factor* (3.4).

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. *Matrix factors* are taken to be unity for average matrix relative sensitivity factors.

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. The numerical values of the sensitivity factors can also depend on the method used to measure the peak intensities.

[SOURCE: ISO 18115-1]

3.4
pure-element relative sensitivity factor
PERSF
<AES, XPS> coefficient, proportional to the intensity measured for a pure sample of an element, by which the measured intensity for that element is divided in calculations to yield the atomic concentration or atomic fraction of the element present in the sample

Note 1 to entry: See sensitivity factor, *elemental relative sensitivity factor* (3.2), and *average matrix relative sensitivity factor* (3.3).

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 used 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* or other parameters are used. Matrix factors are significant and should be used with pure-element relative sensitivity factors.

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. The numerical values of the sensitivity factors can also depend on the method used to measure the peak intensities.

[SOURCE: ISO 18115-1]

3.5
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*.

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* (3.6) 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*, the energy dependence of the response function is needed in order to use *relative sensitivity factors*. For these cases, a function is determined which is proportional to the absolute response function, where the proportionality constant is not necessarily important.

[SOURCE: ISO 18115-1]

3.6
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* (3.5).

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*.

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.

[SOURCE: ISO 18115-1]

3.7
atomic relative sensitivity factor
ARSF
coefficient, proportional to the intensity measured for a single atom of an element, by which the measured intensity for that element is divided in calculations to yield the atomic concentration or atomic fraction of the element present in the sample.

Note 1 to entry: See *elemental relative sensitivity factor* (3.2).

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* 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* this has a dominating influence.

4 Symbols and abbreviated terms

AES	Auger electron spectroscopy
A_i	atomic mass of element i
$E_{b,i}$	binding energy of core level for element i
E_g	band-gap energy
E_i	kinetic energy of an auger electron or photoelectron from element i
E_p	free-electron plasmon energy
E_{pr}	primary electron energy
F_i	matrix correction factor for element i
F_j	matrix correction factor for element j
$H(\cos\alpha, \omega_i)$	Chandrasekhar function for parameters $\cos\alpha$ and ω_i
I_{key}	measured intensity of the chosen peak in the key material
C_i	number of atoms of element i in the molecular formula of the compound
$I_{i,ref}$	measured intensity of element i in the reference sample
$I_{i,unk}$	measured intensity of element i in the unknown sample
$I_{j,ref}$	measured intensity of element j in the reference sample
$I_{j,unk}$	measured intensity of element j in the unknown sample
J	excitation beam intensity
M_i	molecular mass of the compound containing element i
n	number of identified elements in the unknown sample
N_A	Avogadro constant
N_{av}	atomic density for the average matrix sample
N_i	atomic density of element i
N_{ref}	atomic density of the reference sample
N_{key}	atomic density of the key element
N_{unk}	atomic density of the unknown sample
N_v	number of valence electrons per atom or molecule
Q_{av}	elastic-scattering correction factor for the average matrix sample at the electron energy E_i for the particular Auger-electron or photoelectron peak of interest
Q_i	elastic-scattering correction factor for element i at the electron energy E_i for the particular Auger-electron or photoelectron peak of interest
$Q_i(0)$	elastic-scattering correction factor for element i at emission angle $\alpha = 0$ with respect to the surface normal

$Q_{i,\text{ref}}$	elastic-scattering correction factor for element i in the reference sample
$Q_{i,\text{unk}}$	elastic-scattering correction factor for element i in the unknown sample
R_{av}	backscattering correction factor for the average matrix sample
R_i	backscattering correction factor for element i
$R_{i,\text{ref}}$	backscattering correction factor for element i in the reference sample (these terms are unity for XPS)
$R_{i,\text{unk}}$	backscattering correction factor for element i in the unknown sample (these terms are unity for XPS)
RSF	relative sensitivity factor
$S_{i,\text{At}}$	atomic relative sensitivity factor for element i
$S_{i,\text{Av}}$	average matrix relative sensitivity factor for element i
$S_{i,\text{Ec}}$	elemental relative sensitivity factor for element i in a specified compound
$S_{i,\text{Ep}}$	pure-element relative sensitivity factor for element i
$S_{i,\text{RSF}}$	relative sensitivity factor for element i
$S_{i,\text{E}}$	elemental relative sensitivity factor for element i
$S_{j,\text{RSF}}$	relative sensitivity factor for element j
T	spectrometer response function (SRF)
XPS	X-ray photoelectron spectroscopy
Z	atomic number
Z_{av}	atomic number of the average matrix sample
α	emission angle with respect to the surface normal
θ	angle of incidence of electron beam
$X_{i,\text{ref}}$	atomic fraction of element i in the reference sample
$X_{i,\text{unk}}$	atomic fraction of element i in the unknown sample
$\lambda_{i,\text{ref}}$	electron inelastic mean free path for element i in the reference sample
$\lambda_{i,\text{unk}}$	electron inelastic mean free path for element i in the unknown sample
λ_{av}	electron inelastic mean free path for the average matrix sample
λ_i	electron inelastic mean free path for element i
ρ	density of the solid ($kg \cdot m^{-3}$)

5 General information

It is convenient in many quantitative applications of AES and XPS to utilize relative sensitivity factors (RSFs) for quantitative analyses. Three types of RSF have been used for this purpose: elemental relative sensitivity factors (ERSFs), atomic relative sensitivity factors (ARSFs), and average matrix relative sensitivity