

AS ISO 18115—2006

ISO 18115:2001

ISO 18115:2001/Amd.1:2006

AS ISO 18115—2006

Australian Standard[®]

Surface chemical analysis—Vocabulary



This Australian Standard® was prepared by Committee CH-016, Spectroscopy. It was approved on behalf of the Council of Standards Australia on 20 September 2006. This Standard was published on 20 October 2006.

The following are represented on Committee CH-016:

- Australian Chamber of Commerce
- Australian Institute of Physics
- CSIRO Energy Technology
- Department of Defence (Australia)
- Department of Natural Resources and Mines Qld
- National Association of Testing Authorities Australia
- Queensland Health Scientific Services

Additional Interests:

- Curtin University of Technology
 - La Trobe University
 - University of Newcastle
 - The University of New South Wales
 - The University of Queensland
 - University of South Australia
-

This Standard was issued in draft form for comment as DR 06401.

Standards Australia wishes to acknowledge the participation of the expert individuals that contributed to the development of this Standard through their representation on the Committee and through public comment period.

Keeping Standards up-to-date

Australian Standards® are living documents that reflect progress in science, technology and systems. To maintain their currency, all Standards are periodically reviewed, and new editions are published. Between editions, amendments may be issued.

Standards may also be withdrawn. It is important that readers assure themselves they are using a current Standard, which should include any amendments that may have been published since the Standard was published.

Detailed information about Australian Standards, drafts, amendments and new projects can be found by visiting **www.standards.org.au**

Standards Australia welcomes suggestions for improvements, and encourages readers to notify us immediately of any apparent inaccuracies or ambiguities. Contact us via email at **mail@standards.org.au**, or write to Standards Australia, GPO Box 476, Sydney, NSW 2001.

Australian Standard[®]

Surface chemical analysis—Vocabulary

First published as AS ISO 18115—2006.

COPYRIGHT

© Standards Australia

All rights are reserved. No part of this work may be reproduced or copied in any form or by any means, electronic or mechanical, including photocopying, without the written permission of the publisher.

Published by Standards Australia, GPO Box 476, Sydney, NSW 2001, Australia

ISBN 0 7337 7790 2

PREFACE

This Standard was prepared by the Standards Australia Committee CH-016, Spectroscopy. This Standard is identical with, and has been reproduced from ISO 18115:2001, *Surface chemical analysis—Vocabulary* and its Amendment 1(2006) which has been added to the end of the document.

The objective of this Standard is to ensure that the terms and definitions used in surface analytical techniques describe clearly the same concepts and facilitate the exchange of information by establishing the use of the correct terms and their definitions.

As this Standard is reproduced from an international standard, the following applies:

- (a) Its number appears on the cover and title page while the International Standard number appears only on the cover.
- (b) In the source text ‘this International Standard’ should read ‘this Australian Standard’.
- (c) A full point substitutes for a comma when referring to a decimal marker.

CONTENTS

	<i>Page</i>
INTRODUCTION	iv
1 Scope.....	1
2 Abbreviations	1
3 Format	2
4 Definitions of the surface analysis methods	2
5 Definitions of terms for surface analysis	4
Annex A (Informative) Extract from IEC 60050-111, <i>International Electrotechnical Vocabulary—Chapter 111: Physics and Chemistry</i>	50
Bibliography	52
Alphabetical index of terms in ISO 18115:2001	53
Amendment 1:	
6 Definitions of supplementary terms for surface analysis	58
Alphabetical index of supplementary terms in this Amendment	71

INTRODUCTION

Surface chemical analysis is an important area which involves interactions between people with different backgrounds 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 are 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 meaning 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*, 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.

The terms are given in alphabetical order, classified under three headings:

- Clause 4: Definitions of the surface analysis methods.
- Clause 5: Definitions of terms for surface analysis.
- Clause 6: Amendment 1—Definitions of supplementary 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.

AUSTRALIAN STANDARD

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/m².

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/m² 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/m² 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 α X-rays at 1 486,6 and 1 253,6 eV, respectively. Modern instruments also use monochromated Al K α 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 μ/ρ in the expression $(\mu/\rho)\Delta(\rho x)$ for the fraction of a parallel beam of specified particles or radiation removed in passing through a thin layer of mass thickness $\Delta(\rho x)$ of a substance in the limit as $\Delta(\rho x)$ approaches zero, where $\Delta(\rho x)$ is measured in the direction of the beam

cf. **attenuation length**

NOTE 1 The mass density of the substance is ρ 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 $54,7^\circ$ 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

β

$\langle$ XPS $\rangle$ factor which characterizes the intensity distribution, $L(\gamma)$, of photoelectrons ejected by unpolarized X-rays from isolated atoms in a direction γ 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 μ in the expression $\mu\Delta x$ for the fraction of a parallel beam of specified particles or radiation removed in passing through a thin layer Δx of a substance in the limit as Δx approaches zero, where Δx is measured in the direction of the beam

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 Δx of a substance in the limit as Δx approaches zero, where Δx 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** ^[1]

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

$\langle \text{XPS} \rangle \beta$, 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

$\langle \text{XPS} \rangle$ 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.

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

$\langle \text{AES} \rangle$ **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**.

5.37**Auger transition rate**

quotient of the probability for an **Auger process** by time

5.38**background, inelastic**

intensity distribution in the spectrum for particles originally at one energy but which are emitted at lower energies due to one or more **inelastic scattering** processes

cf. **inelastic scattering background subtraction, Shirley background, Sickafus background, Tougaard background**

NOTE For AES and XPS, the inelastic background associated with a particular Auger electron or photoelectron peak has been approximated by a measured electron energy loss spectrum for which the incident-electron energy is close to the energy of the peak. The Tougaard background is also used. A simpler, but less accurate, inelastic background function is the Shirley background. Simple linear backgrounds have also been used but these are much less accurate, except for the XPS analysis of insulators.

5.39**background, instrumental**

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

5.40**background, Shirley**

⟨AES, XPS⟩ background calculated to fit the measured spectrum at points at higher and lower kinetic energy than the peak or peaks of interest such that the background contribution at a given **kinetic energy** is in a fixed proportion to the total peak area above that background for higher kinetic energies

cf. **Tougaard background**

5.41**background, Sickafus**

⟨AES, XPS⟩ single-term power law background designed to describe the intensity of the **secondary-electron cascade** as a function of electron emission **kinetic energy**

NOTE 1 The measured secondary-electron cascade, for correct application of the Sickafus background, should be the experimentally observed spectrum corrected for the **spectrometer response function** of the measuring instrument.

NOTE 2 The spectrum shape, for a Sickafus background $B_S(E)$, is given by

$$B_S(E) \propto E^{-m}$$

where E is the electron emission kinetic energy and m is a number in the range 1 to 2.

5.42**background signal**

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

cf. **Shirley background, Sickafus background, Tougaard background**

5.43**background, Tougaard**

⟨AES, XPS⟩ intensity distribution obtained from a model for the differential inelastic scattering cross-section with respect to energy loss and the three-dimensional distribution of the emitting atoms in the surface region

cf. **Shirley background**

NOTE 1 A number of classes of atomic distributions may be used together with different differential inelastic scattering cross-sections. The atomic distribution and the inelastic scattering cross-section should be specified.

NOTE 2 The Tougaard background is usually calculated to match the measured spectrum over a wide energy range that excludes the peak region and the spectral region extending to approximately 50 eV less kinetic energy than the peaks of interest. The measured spectrum should be corrected for the **spectrometer response function** of the measuring instrument before calculation of the Tougaard background.

5.44

backscattered electron

⟨AES, EELS⟩ electron originating in the incident beam which is emitted after interaction with the sample

NOTE 1 By convention, an electron with energy greater than 50 eV may be considered as a backscattered electron.

NOTE 2 By convention, the incident beam is often called the **primary beam** and the backscattered electrons are often referred to as the backscattered primary electrons.

5.45

backscattering coefficient

backscattering yield

⟨EIA, RBS⟩ quotient of the number of detected particles in an interval of backscattering energy by that interval and by the number of incident ions

5.46

backscattering energy

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

5.47

backscattering factor

⟨AES⟩ factor defining the increase in the Auger electron current due to additional ionizations in the sample caused by **backscattered electrons** above that arising directly from the primary electrons

NOTE Different usages exist; the factor is commonly the fractional increase, as defined above, and sometimes unity plus that fractional increase. The latter usage is deprecated. For clarity, the particular usage needs to be defined.

5.48

backscattering spectrum

⟨EIA, RBS⟩ plot of backscattering yield versus backscattering energy ^[1]

5.49

backscattering yield

backscattering coefficient

η

⟨AES, EPMA⟩ ratio of the total number of electrons emitted from the sample with energies greater than 50 eV to the total number of electrons incident at a given energy and **angle of incidence**

cf. **secondary-electron yield**, **total secondary-electron yield**, **backscattering factor**

5.50

ball cratering

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

cf. **angle lapping**, **radial sectioning**

5.51

beam convergence angle

angular interval containing all or a specified fraction of the beam in the space prior to or at the focal plane

cf. **beam divergence angle**

NOTE Where the beam is symmetrical, the full or semi-angle may be used. The particular measure of angle needs to be stated.

5.52 beam current

I

quotient of dQ by dt , where dQ is the quantity of electric charge of a specified polarity in the beam passing in the time interval dt

$$I = dQ/dt$$

cf. pulse beam current, average beam current

NOTE For beams in which the current varies with time, the instantaneous and time-averaged beam currents will generally differ. For a pulsed beam, the current when the beam is on may or may not be equal to the d.c. or unpulsed beam current.

5.53 beam current, average

quotient of Q by t , where Q is the quantity of electric charge of a specified polarity in the beam passing in the time interval t

NOTE For beams in which the instantaneous current varies periodically with time, the time interval t is an integral number of periods.

5.54 beam current density

J

(for a parallel beam of charged particles) quotient of dI by dA where dI is the element of beam current incident on an area dA at right angles to the direction of the beam

$$J = dI/dA$$

cf. fluence, flux, dose

NOTE For a convergent or divergent beam, the area dA is replaced by a small sphere of cross-sectional area dA .

5.55 beam current, integrated

total electric charge transported in the beam over a specified time

5.56 beam current, pulse

quotient of Q by t_p where Q is the quantity of electric charge of a specified polarity in the beam passing during the period t_p in which the pulse is on

5.57 beam diameter

(for a particle beam of circular cross-section) full width of the beam at half maximum intensity measured in a plane normal to the beam direction ^[1]

NOTE The beam diameter is usually specified at a given point in space such as the position of the sample.

5.58 beam divergence angle

angular interval containing all or a specified fraction of the beam in the space after the focal plane

cf. beam convergence angle

NOTE Where the beam is symmetrical, the full or semi-angle may be used. The particular measure of angle needs to be stated.

5.59**beam energy**

kinetic energy of the **beam particles**

cf. **beam impact energy, incident-particle energy**

NOTE 1 The energy is usually given in electron volts.

NOTE 2 The beam energy is often taken to be the particle energy on impact at the sample surface. However, where a sample is at a potential other than ground, the **impact energy** of the particles may differ from the beam energy as delivered by an electron or ion gun to the sample environment. In this case, use of the term impact energy avoids confusion.

5.60**beam impact energy**

kinetic energy of the **beam particles** on impact with the sample surface

cf. **beam energy, incident-particle energy**

NOTE 1 For primary ion beams in SIMS, the beam impact energy is given by the difference in electric potential between the ion source, strictly the plasma meniscus, and the sample surface multiplied by the charge on the ion. In some SIMS systems, the **beam energy** is given for the source potential with respect to ground but the sample potential need not be at ground. The impact energy takes account of any sample potential.

NOTE 2 Use of the qualifier "impact" indicates that this is the energy of the particles striking the surface.

5.61**beam particle**

electron, positron, ion, atomic, molecular or cluster species contained in the incident beam

5.62**beam, primary**

directed **flux** of particles or photons incident on a sample

5.63**beam profile**

spatial distribution of the beam **flux** in a plane normal to the beam axis

5.64**binary elastic scattering****elastic scattering**

collision between a moving particle and a second particle in which the total **kinetic energy** and the total momentum are conserved

cf. **inelastic scattering**

NOTE In elastic scattering interactions, the moving particle may be deflected through angles of up to 180°.

5.65**binary elastic scattering peak**

⟨ISS⟩ increase in the spectrometer detection system response above the background level which can be attributed to **binary elastic scattering** of an incident ion by a surface atom of a particular mass ^[1]

5.66**binding energy**

energy that must be expended in removing an electron from a given electronic level to the **Fermi level** of a solid or to the **vacuum level** of a free atom or molecule

5.67**blocking geometry**

⟨EIA, RBS⟩ experimental arrangement wherein the atom rows or planes of a single crystal target are aligned parallel to a vector from the sample to the detector [1]

5.68**Bragg's rule**

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

$$\varepsilon(A_x B_y) = x\varepsilon_A + y\varepsilon_B$$

where $\varepsilon(A_x B_y)$ is the stopping cross-section of the compound, $A_x B_y$, and ε_A and ε_B are the stopping cross-sections of elements A and B, respectively [1]

5.69**bremsstrahlung**

⟨EPMA, XPS⟩ photon radiation emitted from a material due to the deceleration of incident electrons within that material

NOTE 1 The bremsstrahlung radiation has a continuous spectral distribution up to the energy of the incident electrons.

NOTE 2 In XPS, The bremsstrahlung from a conventional X-ray source with an Al or Mg anode leads to a continuous photoelectron background. This radiation may also photoionize inner shells that would be energetically impossible by characteristic Al or Mg K α X-rays. As a result, Auger electron features may appear at negative binding energy values and, in addition, the intensities of other Auger electron features may be greater than if the inner shell vacancies had been created only by the characteristic X-rays. The bremsstrahlung-excited Auger electron features can be helpful in determining the various **Auger parameters** needed to identify chemical states.

5.70**cascade mixing**

a diffusion-like process in which atoms of material are moved randomly by energy deposited by incident particles slowing down in the sample surface region

cf. **atomic mixing, collision cascade, knock-on, recoil implantation**

NOTE 1 If atomic mixing and knock-on effects are not significant, the measured sputter depth profile of a **delta layer** will be asymmetric on account of cascade mixing since the surface moves through the sample as it is sputtered. The initial internal profile produced will be Gaussian, however until significant delta material has been lost through the sample surface.

NOTE 2 If cascade mixing is the only significant mixing process, the centroid of the measured distribution will lie at the true delta position (after any shift in the depth scale arising from pre-equilibrium effects has been corrected).

NOTE 3 In the **dilute limit**, the measured depth profile for the delta layer will have an exponential tail because any internal atom has an equal probability of being moved deeper or shallower and there is thus an indefinitely persistent but decaying concentration in the near-surface region. The presence of this tail often leads to the belief that there is a directional **knock-on** process at work. True knock-on effects have rarely if ever been observed, and are probably not significant as causes of sputter profile distortion.

5.71**channelling**

preferential motion of energetic particles along certain axial or planar directions of a crystalline solid as the particles move through the sample

NOTE The potentials of the individual atoms of the solid combine to reduce the scattering of the energetic particles from these directions.

5.72**characteristic electron energy losses**

(AES, EELS, XPS) **inelastic scattering** of electrons in solids that produces a non-uniform energy loss spectrum determined by the characteristics of the material

cf. **plasmon**

NOTE 1 The most probable **characteristic losses** arise from excitation of valence electrons. For some solids (for example, non-transition metals), inelastic scattering is dominated by plasmon excitations. For other solids, the inelastic scattering may be due to a combination of plasmon excitation and single valence-electron excitations, and these excitations may not be distinguishable. Inelastic scattering can also occur through the excitation of core level electrons when this is energetically possible.

NOTE 2 The characteristic energy losses are most prominent in the energy loss range 0 eV to 100 eV.

NOTE 3 Characteristic electron energy loss peaks are often observed in association with other peaks in a spectrum (e.g. Auger electron peaks, photoelectron peaks, and the peak arising from elastic scattering of primary electrons).

5.73**characteristic X-rays**

photons emitted by ionized atoms and having a particular distribution in energy and intensity characteristic of the atomic number and chemical environment of the atom ^[1]

NOTE 1 In XPS, the term is applied to the X-ray source used to excite photoelectrons in the sample.

NOTE 2 In EPMA, characteristic X-rays emitted from the sample are detected and analysed to give information on the composition of the sample.

5.74**charge modification**

alteration of the amount or the distribution of charge at a sample surface

5.75**charge neutralization**

maintenance at a fixed potential, usually near neutrality, of the surface of a non-conducting or poorly conducting sample material under bombardment by primary particles or photons

NOTE Charge neutralization may be accomplished by bombarding the surface with electrons or, more rarely, ions or photons.

5.76**charge referencing**

(AES, XPS) method by which the **charging potential** of a sample is determined in order to correct the measured energies so that those energies correspond to a sample with no surface change

cf. **adventitious carbon referencing**

NOTE Charge referencing is often conducted using **adventitious carbon referencing** or by **gold decoration**.

5.77**charging potential**

electrical potential of the surface region of an insulating sample caused by irradiation

NOTE Different charging potentials may occur on different areas or at different depths in a sample arising from sample inhomogeneities or non-uniform intensity of the incident flux of radiation

5.78**chemical effects**

(AES, EELS, EPMA, XPS) change in the shape of a measured spectrum, or in the peak energy for an element, arising from chemical bonding

5.79**chemical shift**

⟨AES, EELS, EMPA, XPS⟩ change in **peak energy** arising from a change in the chemical environment of the atom

5.80**collision cascade**

sequential energy transfer between atoms in a solid as a result of bombardment by an energetic species [1]

cf. **atomic mixing**, **cascade mixing**, **knock-on**, **recoil implantation**

5.81**compositional depth profile****CDP**

chemical or atomic composition measured as a function of distance normal to the surface

5.82**constant ΔE mode****constant analyser energy mode****CAE mode****fixed analyser transmission mode****FAT mode**

mode of **electron energy analyser** operation that varies the electron retardation but keeps the **pass energy** constant in the energy dispersive portion of the analyser

NOTE This mode is often used in XPS to maintain a high and constant energy resolution throughout the spectrum.

5.83**constant $\Delta E/E$ mode****constant retardation ratio mode****CRR mode****fixed retardation ratio mode****FRR mode**

mode of **electron energy analyser** operation that varies the retarding potential so that the **pass energy** in the energy dispersive portion of the analyser is a constant fraction of the original **vacuum level** referenced **kinetic energy**

NOTE This mode is often used in AES to improve the **signal-to-noise ratio** for high-energy emitted electrons at the expense of spectral resolution.

5.84**Coster-Kronig transition**

⟨AES, EPMA, XPS⟩ **Auger process** involving an electron from the same principal shell as the initial vacancy

cf. **Auger transition**, **super Coster-Kronig transition**

EXAMPLES $L_1L_2M_5$; $M_1M_2N_5$.

5.85**counts**

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

NOTE The counts may be representative, one-for-one, with the particles being detected (in the absence of **dead time** losses in the counting measurement), in which case they follow Poissonian statistics (unless other **noise** sources are present) or they may simply be proportional to the number of particles being detected. The type of measure needs to be clearly stated.

5.86**crater depth**

average depth of the region of a crater from which the measured signal is derived

NOTE 1 The crater is generally formed by ion bombardment in **sputter depth profiling** and, in this case, may be different from the thickness of sample material removed by sputtering due to dilation of the **altered layer**.

NOTE 2 The crater depth may be modified by the formation of a reacted layer (e.g. an oxide) following any exposure to the atmosphere or other environments.

5.87

crater edge effect

signals from the crater edge which often originate from depths shallower than the central region of the crater formed in **depth profiling**

5.88

cross-section

(for a specified target entity and for a specified reaction or process produced by incident charged or uncharged particles of specified type and energy) quotient of probability of reaction or process for the target entity by the incident-particle **fluence** ^[2]

NOTE 1 Cross-sections are often expressed as an area per target entity (atom, molecule etc.) for the relevant process.

NOTE 2 A cross-section of σ per atom for the removal of particles from a given state in a beam will lead to a reduction dN in the number of N of particles in that state in a distance dx given by the relation:

$$dN = N\sigma n dx$$

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

Integration leads to the relation:

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

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

5.89

cross-section, elastic scattering

cross-section for binary elastic scattering

5.90

cross-section, elastic scattering, differential

quotient of the **cross-section for elastic scattering** into a particular infinitesimal solid angle far from the target by that infinitesimal solid angle

NOTE The differential elastic scattering cross-section is related to the elastic scattering cross-section, σ_e , by

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

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

5.91

cross-section, enhanced elastic

(EIA, RBS) **cross-section** of an atom for elastic scattering that is greater than the **Rutherford cross-section** due to partial penetration of a nucleus in the sample by the incident particle

5.92

cross-section, inelastic scattering

(AES, EELS, EMPA, XPS) cross-section for **inelastic scattering** by an electron traversing a material

5.93

cross-section, ionization

cross-section for a process that will produce, in an atom, a vacancy in a previously occupied shell

NOTE 1 A total ionization cross-section refers to removal of an electron from any atomic shell or sub-shell of an atom.

NOTE 2 A partial or sub-shell ionization cross-section refers to removal of an electron from a specified shell or sub-shell of the atom.

NOTE 3 A partial ionization cross-section may be expressed per electron in a shell or sub-shell or for the total number of these electrons in a shell or sub-shell of the particular atom.

NOTE 4 An atom may have multiple vacancies following an initial ionization or as the result of subsequent Auger or **Coster-Kronig** processes.

5.94

cross-section, nuclear reaction

⟨EIA⟩ cross-section at a given beam energy and emission direction of the detected product for a particular nuclear reaction per atom

NOTE This cross-section is usually expressed per atom as an area in units of barns; one barn = 10^{-28} m².

5.95

cross-section, photoionization

total ionization **cross-section** for an incident photon of a given energy interacting with a material to produce one or more photoelectrons from all sub-shells that are energetically accessible

cf. **ionization cross-section, sub-shell photoionization cross-section**

5.96

cross-section, Rutherford

⟨RBS⟩ **elastic scattering cross-section** calculated using classical mechanics

cf. **elastic scattering cross-section, enhanced elastic cross-section**

NOTE The resulting cross-section formula was first derived by Rutherford.

5.97

cross-section, stopping

⟨EIA, RBS⟩ quotient of the rate of energy loss of a particle with distance along its trajectory in a sample by the atomic density of sample atoms for an infinitesimal sample thickness

NOTE 1 This stopping cross-section is usually expressed in units of eV·m²/atom and not an area per atom as is customary for **cross-sections**.

NOTE 2 The atomic density is sometimes taken as the number density, N , and sometimes as the mass density, ρ , so that the units will be eV·m²/atom or eV·m²/kg. The stopping cross-section ε is thus given either by

$$\varepsilon \equiv (1/N)(dE/dx)$$

or by

$$\varepsilon \equiv (1/\rho)(dE/dx)$$

where dE/dx is the rate of loss of energy E with distance x along the particle trajectory.

NOTE 3 Older texts may be found with the stopping cross-section given in keV·cm²/gm and in many other forms.

5.98

cross-section, sub-shell photoionization

cross-section for an incident photon interacting with a material to produce a one or more photoelectrons from a given sub-shell

cf. **photoionization cross-section**

NOTE Photoionization from one sub-shell may lead to **shake-up** or **shake-off** of electrons from other shells.

5.99

cross-section, transport

σ_{tr}

quotient of the fractional momentum loss of a particle incident on the sample arising from elastic scattering by the areic density of the sample atoms, for an infinitesimally thin sample

NOTE 1 This **cross-section** is expressed as an area per atom.

NOTE 2 The cross-section for the loss of any momentum, however small, is simply the **elastic scattering cross-section**. By contrast the transport cross-section is a measure of the probability of the loss of a substantial fraction of the initial momentum, analogous to **stopping cross-section** which is a measure of the probability of the loss of a substantial energy.

NOTE 3 Transport cross-section is related to **differential elastic scattering cross-section**, $d\sigma_e(\Omega)/d\Omega$, by

$$\sigma_{tr} = 2\pi \int_0^\pi \frac{d\sigma_e(\Omega)}{d\Omega} (1 - \cos\theta) \sin\theta d\theta$$

where θ is the angle of scattering.

5.100

cross-sectioning

sample preparation in which the sample is cleaved, cut or polished in a plane perpendicular to the **interface** under study, so that associated compositional differences or gradients may be observed in that plane

5.101

dead time

time per pulse for which a pulse counting system is unavailable for further counting

5.102

dead time, extended

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

5.103

dead time, multidetector

effective **dead time** of the whole detector, treating it as a single detector

5.104

dead time, non-extended

dead time for a system where the pulse lengths are not extended by extra pulses arriving during the dead time associated with earlier pulses

5.105

decay length

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

cf. **attenuation length**

5.106

decay length, average emission function

negative reciprocal slope of the logarithm of a specified exponential approximation to the **emission depth distribution function** over a specified range of depths, as determined by a straight-line fit to the emission depth distribution function plotted on a logarithmic scale versus depth on a linear scale^[1]

5.107

decay length, deep emission function

asymptotic value of the **emission function decay length** for increasing depths from the surface