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Surface chemical analysis — Fundamental approaches to determination of lateral resolution and sharpness in beam-based methods

Analyse chimique des surfaces — Approche fondamentale pour la détermination de la résolution latérale et de la netteté par des méthodes à base de faisceau

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Foreword

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This second edition cancels and replaces the first edition (ISO/TR 19319:2003), which has been technically revised.

Introduction

Surface-analytical techniques such as SIMS, AES and XPS enable imaging of surfaces. The most relevant parameter of element or chemical maps and line scans is the lateral resolution, also called image resolution.1) Therefore well defined and accurate procedures for the determination of lateral resolution are required. Those procedures together with appropriate test specimen are basic preconditions for comparability of results obtained by imaging surface-analytical methods and performance tests of instruments as well. This Technical Report is intended to serve as a basis for the development of International Standards.

Nowadays there is some confusion in the community in the understanding of the term "lateral resolution". Definitions originating from different fields of application and different communities of users can be found in the literature. Unfortunately they are inconsistent in many cases. As a result, values of "lateral resolution" published by manufacturers and users having been derived by using different definitions and/or determined by different procedures cannot be compared to each other. It is the intention of this Technical Report to basically describe different approaches for the characterization of lateral resolution including their interrelations.

The term resolution was introduced with respect to the performance of microscopes by Ernst Abbe.[1] Later on it was applied to spectroscopy by Lord Rayleigh.[2] It is based on the diffraction theory of light and the original definition of lateral resolution as "the minimum spacing at which two features of the image can be recognised as distinct and separate" is in common use in the light and electron microscopy communities as documented in the standard ISO 22493:2008.[3]

However, in the surface analysis community a very different approach, the "knife edge method", is the most popular one for the determination of lateral resolution. This method is based on evaluation of an image or of a line scan over a straight edge. Here lateral resolution is characterized by parameters describing the steepness of the edge spread function ESF. The standard "ISO 18516:2006 Surface Chemical Analysis – Auger electron spectroscopy and X-ray photoelectron spectroscopy – Determination of lateral resolution"[4] is limited to this approach. But the ESF and corresponding rise parameters $D_{x-(1-x)}$ are more related to image sharpness than to lateral resolution which refers to two separated features.

The reason why the original meaning of resolution is not commonly implemented in the common practice in surface analysis is the lack of suitable test specimens having the required features in the sub-µm range. However, recently a new type of test specimen was developed featuring a series of flat square-wave gratings characterized by chemical contrast and different periods.[5,6] Such test specimens may enable an implementation of the original definition of lateral resolution into practical approaches in surface chemical analysis.

Having solved the problem of availability of appropriate test specimens another problem has to be solved: The establishment of a criterion for whether two features are separated or not. The Rayleigh criterion[2] was developed for diffraction optics and its application in imaging surface analysis is not straightforward. The Sparrow criterion[7] defines a resolution threshold exclusively by the existence of a minimum between two maxima. Actually, for practical imaging in surface analysis, noise is a relevant feature especially at the limit of resolution. Therefore the Sparrow criterion will fail to solve the problem. The solution is to develop a resolution criterion relying on the detection of a minimum between two features but additionally considering noise effects.

The lateral resolution of imaging systems is strongly related to a number of functions describing the formation of images:

— the modulation transfer function,

— the contrast transfer function,

— the point spread function,

1) The term "image resolution" is used in the microscopy community whereas in the surface analysis community the term "lateral resolution" is common practice to distinguish it from "depth resolution".

— the line spread function and

— and the edge spread function.

Those functions may be utilized to describe the performance of optical instruments and instruments used for imaging in surface analysis as well. In particular the contrast transfer function has been used successfully for the benefit of the determination of lateral resolution of imaging instruments in surface analysis.

Section 4 of this report describes the basics of procedures for the analysis of images of stripe patterns, narrow stripes and step transitions. A comparison of all procedures related to lateral resolution and sharpness is given in 4.1.7.

Section 5 of the report describes physical factors affecting lateral resolution, analysis area and sample area viewed by the analyser in Auger electron spectroscopy and X-ray photoelectron spectroscopy. Section 6 of the report gives guidance on the determination of sample area viewed by the analyser in applications of Auger electron spectroscopy and X-ray photoelectron spectroscopy.

Surface chemical analysis — Fundamental approaches to determination of lateral resolution and sharpness in beam-based methods

1 Scope

This Technical Report describes:

a) Functions and their relevance to lateral resolution:

   1) Point spread function (PSF) — see 4.1.1

   2) Line spread function (LSF) — see 4.1.2

   3) Edge spread function (ESF) — see 4.1.3

   4) Modulation transfer function (MTF) — see 4.1.4

   5) Contrast transfer function (CTF) — see 4.1.5.

b) Experimental methods for the determination of lateral resolution and parameters related to lateral resolution:

   1) Imaging of a narrow stripe — see 4.2

   2) Imaging of a sharp edge — see 4.3

   3) Imaging of square-wave gratings — see 4.4.

c) Physical factors affecting lateral resolution, analysis area and sample area viewed by the analyser in Auger electron spectroscopy and X-ray photoelectron spectroscopy — see Clauses 5 and 6.

2 Terms and definitions

For the purposes of this document, the following terms and definitions apply.

2.1
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

[SOURCE: ISO 18115:2010, definition 5.8]

2.2
contrast transfer function
CTF
ratio of the image contrast to the object contrast of a square-wave pattern as a function of spatial frequency

Note 1 to entry: In this document the contrast transfer function CTF has been used also with an abscissa expressed in terms of w_{LSF}/P and is called the generalized contrast transfer function in those cases (cf. 4.4.3.2). w_{LSF} is the full width at half maximum of the line spread function LSF

Note 2 to entry: In transmission electron microscopy and other phase sensitive methods the term contrast transfer function is used with a different meaning considering amplitude as well as phase information.

2.3
cut-off frequency of the contrast transfer function
lowest spatial frequency at which the contrast transfer function CTF equals to zero

Note 1 to entry: In this document the spatial frequency at which the contrast transfer function CTF equals the threshold of resolution under consideration of noise (cf. 4.4.3.3) is called effective cut-off frequency of the contrast transfer function.

2.4
edge spread function
ESF
normalized spatial signal distribution in the linearized output of an imaging system resulting from imaging a theoretical infinitely sharp edge

[SOURCE: ISO 12231:2012, definition 3.43]

2.5
effective cut-off frequency
see cut-off frequency of the contrast transfer function, Note 1 to entry

2.6
effective lateral resolution
minimum spacing of two stripes of a square-wave grating at which the dip of signal intensity between two maxima of the image is at least 4 times the reduced noise σ_{NR}

2.7
generalized contrast transfer function
see **contrast transfer function**, Note 1 to entry

2.8
image contrast
c_i
$c_i = (I_{max}-I_{min})/(I_{max}+I_{min}) = \Delta I/2\ I_{mean}$ (Michelson contrast), where I_{max}, I_{min} and I_{mean} are signal intensities in the image

Note 1 to entry: Other definitions (not used in this document) include: difference in signal between two arbitrarily chosen points of interest (P_1, P_2) in the image field, normalized by the maximum possible signal available under the particular operating conditions, $c_i = |S_2 - S_1| / S_{max}$ (ISO 22493:2008, definition 5.3).

Note 2 to entry: With respect to aperiodic patterns the Weber contrast $c = (I - I_b)/I_b$ is used to quantify the contrast between a feature with the signal intensity I and the background signal intensity I_b.

Note 3 to entry: With respect to periodic object patterns, the terms contrast and modulation often are used synonymously.

2.9
image resolution
minimum spacing at which two features of the image can be recognised as distinct and separate

[SOURCE: ISO 22493:2008, definition 7.2]

2.10
lateral resolution
minimum distance between two features (in this document the period of a square wave grating) which can be imaged in that way, that the dip between two maxima is at least 4 times the **reduced noise**σ_{NR} (cf. 4.4.2.3)

Note 1 to entry: This definition is in accordance with the definition of image resolution given in ISO 22493:2008.

Note 2 to entry: This definition is different from the definition of lateral resolution given in ISO 18115:2010.

2.11
linear system
system whose response is proportional to the level of input signals

[SOURCE: ISO 9334:1995, definition 3.1]

2.12
line spread function
LSF
normalized spatial signal distribution in the linearized output of an imaging system resulting from imaging a theoretical infinitely thin line

[SOURCE: ISO 12231:2012, definition 3.94]

2.13
modulation
m
measure of degree of variation in a sinusoidal signal

$$m = (I_{max} - I_{min})/(I_{max} + I_{min})$$

[SOURCE: ISO 9334:1995, definition 3.17]

2.14
modulation transfer function MTF
ratio of the image modulation to the object modulation as a function of spatial frequency

[SOURCE: ISO/IEC 19794-6:2011, definition 4.7]

2.15
noise
time-varying disturbances superimposed on the analytical signal with fluctuations leading to uncertainty in the signal intensity

Note 1 to entry: An accurate measure of noise can be determined from the standard deviation of the fluctuations. Visual or other estimates, such as peak to peak noise in a spectrum or in a line scan, may be useful as semiquantitative measures of noise.

[SOURCE: ISO 18115:2010, definition 5.315]

Note 2 to entry: By averaging over $S_{PP}/4$ data points of the line scan over a square-wave grating the standard deviation of noise σ_N can be reduced by a factor of $(S_{PP}/4)^{1/2}$. $\sigma_{NR} = (4/S_{PP})^{1/2}\sigma_N$ is called **reduced noise** in this document (cf. 4.4.2.3). S_{PP} means number of sampling points per period.

2.16
object pattern
spatial distribution of a sample property seen by the imaging instrument

[SOURCE: ISO 9334:1995, definition 4.1]

2.17
optical transfer function
OTF
frequency response, in terms of spatial frequency, of an imaging system to a sinusoidal object pattern and Fourier transform of the imaging system's point spread function

[SOURCE: ISO 9334:1995, definition 3.8]

2.18
point spread function
PSF
normalized distribution of signal intensity in the image of an infinitely small point

[SOURCE: ISO 9334:1995, definition 3.5]

2.19
reduced noise
see **noise**, Note 2 to entry

2.20
Rose criterion
condition for an average observer to be able to distinguish small features in the presence of noise, which requires that the change in signal for the feature exceeds the noise by a factor of at least three

[SOURCE: ISO 22493:2008, definition 5.3.7]

2.21
sample area viewed by the analyser
two-dimensional region of a sample surface measured in the plane of that surface from which the analyser can collect an analytical signal from the sample or a specified percentage of that signal

2.22
sampling points per period
S_{PP}
grating period divided by sampling step width

Note 1 to entry: For the case of 3-stripe gratings the image of the grating may have a smaller period than the object grating (cf. 4.4.1.1). In this case it must be explained whether the grating period of the object or the image is considered.

2.23
signal-to-noise ratio
$R_{S/N}$
ratio of the signal intensity to a measure of the total **noise** in determining that signal

[SOURCE: ISO 18115:2010, definition 5.427]

2.24
spatial frequency
reciprocal of the period of a periodic object pattern (grating)

3 Symbols and abbreviated terms

AES	Auger electron spectroscopy
c_i	image contrast
c_o	object contrast
$(c_i / c_o)_{ThR}$	c_i/c_o at the threshold of resolution
CTF	contrast transfer function
d	distance between two narrow stripes
D	dip between two maxima
d_{gr}	distance between two consecutive gratings

D_{LSF}	data distance of the MTF calculated by Fourier transform
D_{ThR}	dip at the threshold of resolution
$D_{x-(100-x)}$	ESF steepness parameter giving the distance between points of well-defined intensities x and 100-x (e.g. 20 % to 80 %) of the profile over a straight edge
DNR	dip-to-noise ratio
erf	error function
ESF	edge spread function
F_r	fit range
FWHM	full width at half maximum
G	gap between two stripes
G(x)	Gaussian function
i(x,y)	normalized intensity distribution of measured signals in the image
I_i	incident beam current (in AES)
I_{max}	maximum value of signal intensity in the image of a 3-stripe-grating (A-B-A)
$I_{max\,l}$	signal intensity of the left maximum in the image of a 3-stripe-grating (A-B-A)
$I_{max\,r}$	signal intensity of the right maximum in the image of a 3-stripe-grating (A-B-A)
I_{min}	signal intensity of the minimum in the image of a 3-stripe-grating (A-B-A)
I_{pll}	intensity of the lower plateau of constant concentration
I_{plu}	intensity of the upper plateau of constant concentration
$J_A(r)$	intensity distribution of detected Auger electrons as a function of the radius r
$J_{Ab}(r)$	intensity distribution of detected Auger electrons that were created by backscattered
$J_{Ai}(r)$	intensity distribution of detected Auger electrons that were created by the incident beam
k	spatial frequency
k_S	steepness parameter of the logistic function
L	length
L(x)	Lorentzian function
L_{pl}	Length of a plateau of constant concentration
LSF	line spread function
m	modulation
m_i	image modulation
m_o	object modulation
M_{LSF}	length range of measured LSF values

MTF	modulation transfer function
o(x,y)	object pattern
OTF	optical transfer function
P	grating period
P_0	period of the largest non-resolved grating
P_1	period of the first (finest) resolved grating
P_2	period of the second resolved grating
P_{int}	period at $R_{D/RN}$ = 4 determined by interpolation between P_0 and P_1
P_{ext}	period at $R_{D/RN}$ = 4 determined by extrapolation with P_1 and P_2
PSF	point spread function
PSV1	type 1 Pseudo-Voigt function
PSV2	type 2 Pseudo-Voigt function
q	grading factor of consecutive grating periods $q = P_{n+1}/P_n$
R	backscattering factor (in AES)
r	radius from the centre of the incident electron beam on the sample surface (in AES)
r_e	effective lateral resolution
$R_{D/RN}$	ratio of dip-to-reduced-noise
R_{LSF}	length range where LSF data are used for Fourier transform
$R_{S/N}$	signal-to-noise ratio
r_{max}	upper limit of integration in Formula (65)
s	mean deviation of w_{LSF} determined by a fitting procedure
S_w	sampling step width
S_{pp}	sampling points per period as a variable
spp	dimension unit of the variable S_{PP}
SIMS	Secondary Ion Mass Spectrometry
u	uncertainty of a quantity
U	expanded uncertainty of a quantity
U_c	combined expanded uncertainty of a quantity
w	full width at half maximum of a peak function
w_G	full width at half maximum of the Gaussian part of a type 2 Pseudo-Voigt function
w_{im}	full width at half maximum of the upper plateau of constant concentration in an image of

w_L	full width at half maximum of the Lorentzian part of a type 2 Pseudo-Voigt function
w_{LSF}	full width at half maximum of the line spread function
w_S	width of a stripe in the object pattern
x, x'	length variable
XPS	X-ray photoelectron spectroscopy
y, y'	length variable
Δr	lateral resolution
Δr (50)	lateral resolution determined from a 25% to 75% intensity change in a line profile over a straight edge
η	Lorentzian fraction of a Pseudo-Voigt function
σ_b	Gaussian parameter describing the radial distribution of backscattered electrons (in AES)
σ_i	Gaussian parameter describing the radial distribution of the incident electron beam (in AES)
σ_N	standard deviation of noise
σ_{NR}	standard deviation of reduced noise

4 Determination of lateral resolution and sharpness by imaging of stripe patterns

4.1 Theoretical background

4.1.1 Image formation and the point spread function (PSF)

The imaging process describes the formation of an image as a result of the interaction between an object and an imaging system. The object may be characterized by the object pattern o(x,y). This is determined by a distribution of a certain parameter, for instance a concentration of an element, in the object plane (x, y) and the relation of this parameter to the respective signal intensity seen by the imaging instrument. The imaging system is represented by its point spread function (PSF). The PSF(x-x',y-y') is the normalized intensity distribution of measured signals in the image i(x',y') related to a point at position (x,y) in the object pattern o(x,y).

For linear systems (cf. terms and definitions) the image is formed by the superposition of all intensity distributions produced in the image plane by each individual point of the object pattern o(x,y).[8] This is mathematically described by the convolution integral

$$\mathrm{i}(x',y') = \int_{-\infty}^{+\infty}\int \mathrm{o}(x,y)\,\mathrm{PSF}(x'-x,y'-y)\,\mathrm{d}x\mathrm{d}y \quad (1)$$

This convolution integral can be written as

$$\mathrm{i}(x,y) = \mathrm{o}(x,y) \otimes \mathrm{PSF}(x,y) \quad (2)$$

where $\otimes$ denotes the convolution operation. Formulae (1) and (2) reveal that the image is a weighted sum of point spread functions emerging from every point of the object. Figure 1 illustrates the image formation and the influence of the PSF on the image quality in terms of sharpness.

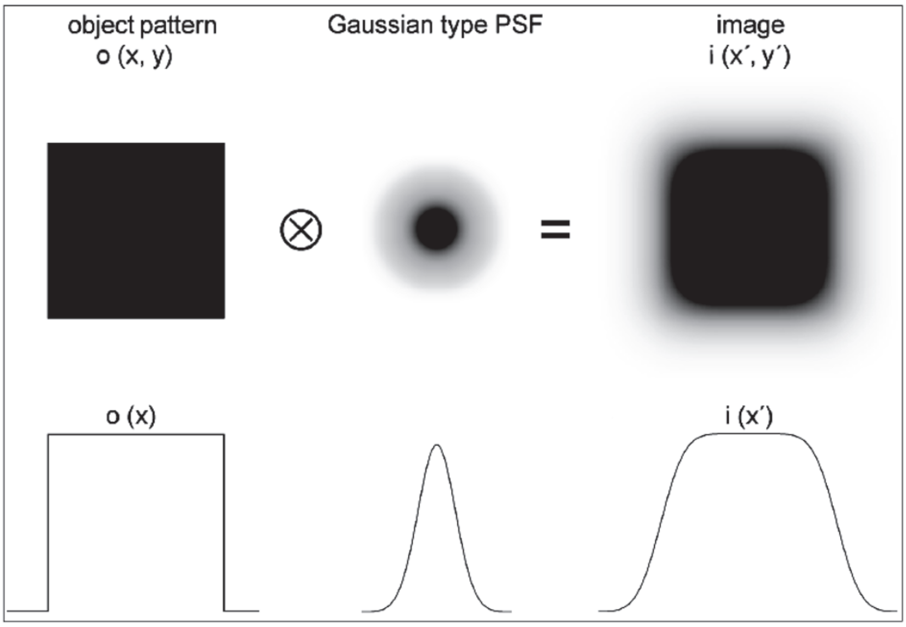

Figure 1 — Top: Imaging of a square simulated by the convolution of the square with a Gaussian PSF where ⊗ denotes the convolution operation. Bottom: X-cuts of object, PSF and image, respectively

In the example given in Figure 1 the dimension of the object and the PSF are of the same order of magnitude. However, for practical applications, two borderline cases of imaging are of particular interest:

1. If the FWHM of the PSF is small compared to the smallest details of the imaged object, then the convolution yields an image that is very similar to the original object. In that case the imaging process (Figure 2a) delivers sharp images of the object.

2. If the FWHM of the PSF is large compared to the imaged object, then the convolution yields the PSF (Figure 2b). The latter case can be exploited to determine the PSF without a deconvolution procedure.

   The PSF describes the performance of an imaging instrument with respect to lateral resolution and the sharpness of images obtained. The smaller the FWHM of the PSF the better is the lateral resolution.

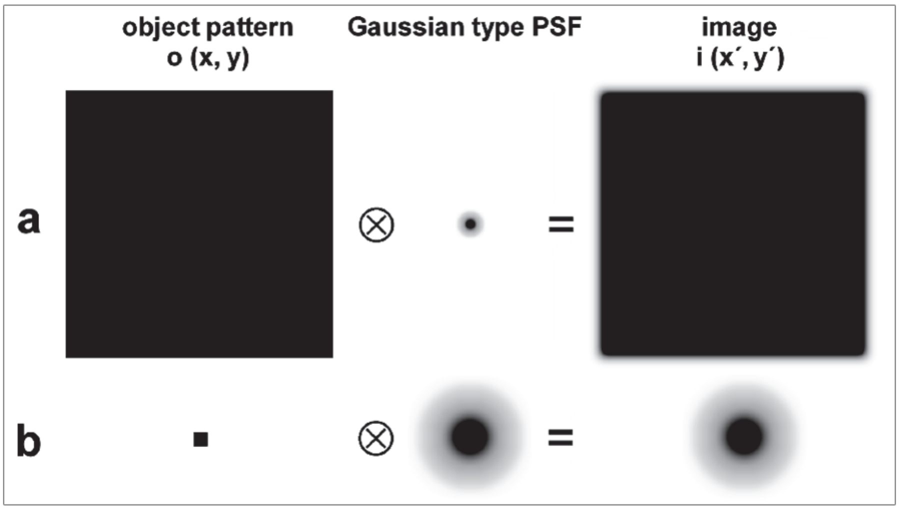

Figure 2 — Two borderline cases of imaging: a) The object is large compared to the FWHM of the PSF. This case is ideal for imaging. b) The object is small compared to the FWHM of the PSF. This case is ideal for the determination of the PSF

4.1.2 The line spread function (LSF)

The LSF is the normalized intensity distribution in the image of a narrow line and yields a one-dimensional description of image quality. According to the model of image formation described above (Figure 1) the LSF corresponds to the convolution of the PSF with an infinitely narrow line, mathematically described by the Dirac delta function δ(x):

$$\mathrm{LSF}(x) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{PSF}(x', y)\delta(x - x')\mathrm{d}x'\mathrm{d}y \tag{3}$$

$$= \int_{-\infty}^{+\infty} \mathrm{PSF}(x, y)\mathrm{d}y \tag{4}$$

The LSF is generally different from a cross section through the two-dimensional PSF. In Figure 3 this is demonstrated for the top hat distribution. Only in the case of a PSF represented by a two-dimensional Gaussian distribution the LSF is identical to the corresponding one-dimensional distribution:

$$\mathrm{G}(x) = \frac{I_0}{\sigma\sqrt{2\pi}} \exp\left(-(x - x_0)^2 / 2\sigma^2\right) \tag{5}$$

The LSF approach is more often used for the determination of lateral resolution than the PSF approach and the full width at half maximum (FWHM) of the LSF is often used as a measure of lateral resolution. However, with the availability of well-defined nanoscaled pointlike objects, the PSF approach may become relevant in the future, too. When a narrow line is imaged, a considerable number of line scans can usually be added by appropriate software tools and the LSF information is obtained at reasonable signal-to-noise ratios.

Finally it should be mentioned that the LSF is not necessarily a Gaussian shaped function. Other shapes as Lorentzian, Voigt function, etc., are possible (cf. 4.2.1). Therefore two imaging instruments having LSFs with the same FWHM but with different shapes will differ in the lateral resolution which can be achieved (this effect will be demonstrated in 4.4.3.1).

4.1.3 The edge spread function (ESF)

The ESF is the intensity distribution in the image of an edge (step transition) measured in the direction perpendicular to that of the edge. The ESF is the integral of the LSF

$$\mathrm{ESF}(x) = \int_{-\infty}^{x} \mathrm{LSF}(x')\mathrm{d}x' \tag{6}$$

The ESF may be determined by a convolution of the PSF with a step function.

The distance between points of well defined relative intensity (e.g. 12 %–88 %, 16 %–84 %, 20 %–80 % or 25 %–75 %) in an ESF is often taken as a measure of lateral resolution. For a Gaussian LSF the distance between the 12 % and 88 % intensity points (indicated in Figure 4) corresponds to its FWHM.

