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

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National foreword

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TECHNICAL REPORT

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2013-03-15

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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ISO/TR 19319 was prepared by Technical Committee ISO/TC 201, *Surface chemical analysis*, Subcommittee SC 2, *General procedures*.

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

$c_i = (I_{\max} - I_{\min}) / (I_{\max} + I_{\min}) = \Delta I / 2 I_{\text{mean}}$ (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 $R_{\text{D/RN}} = 4$ determined by interpolation between P_0 and P_1
P_{ext}	period at $R_{\text{D/RN}} = 4$ 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
$R_{\text{D/RN}}$	ratio of dip-to-reduced-noise
R_{LSF}	length range where LSF data are used for Fourier transform
$R_{\text{S/N}}$	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
$\Delta r (50)$	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

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

This convolution integral can be written as

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

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.

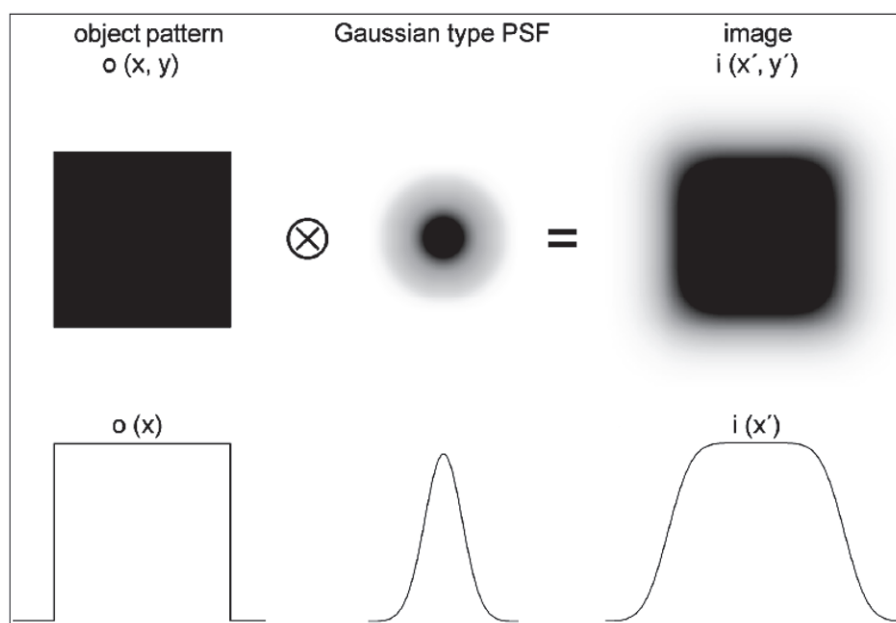


Figure 1 — Top: Imaging of a square simulated by the convolution of the square with a Gaussian PSF where $\otimes$ denotes the convolution operation. Bottom: X-cuts of object, PSF and image, respectively

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.

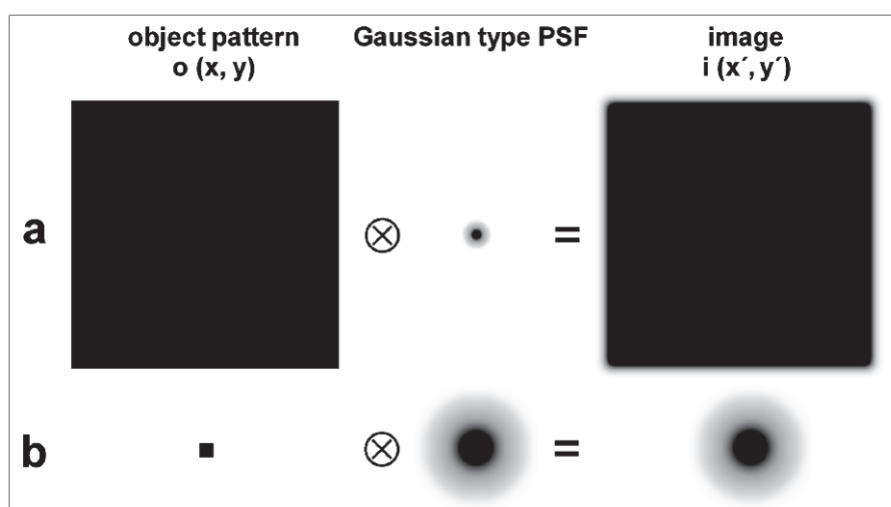


Figure 2 — Two borderline cases of imaging: a) The object is large compared to the FWHM of the PSF. This case is ideal for imaging. b) The object is small compared to the FWHM of the PSF. This case is ideal for the determination of the PSF

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 $\delta(x)$:

$$\text{LSF}(x) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \text{PSF}(x', y) \delta(x - x') dx' dy \quad (3)$$

$$= \int_{-\infty}^{+\infty} \text{PSF}(x, y) dy \quad (4)$$

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:

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

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

$$\text{ESF}(x) = \int_{-\infty}^x \text{LSF}(x') dx' \quad (6)$$

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.

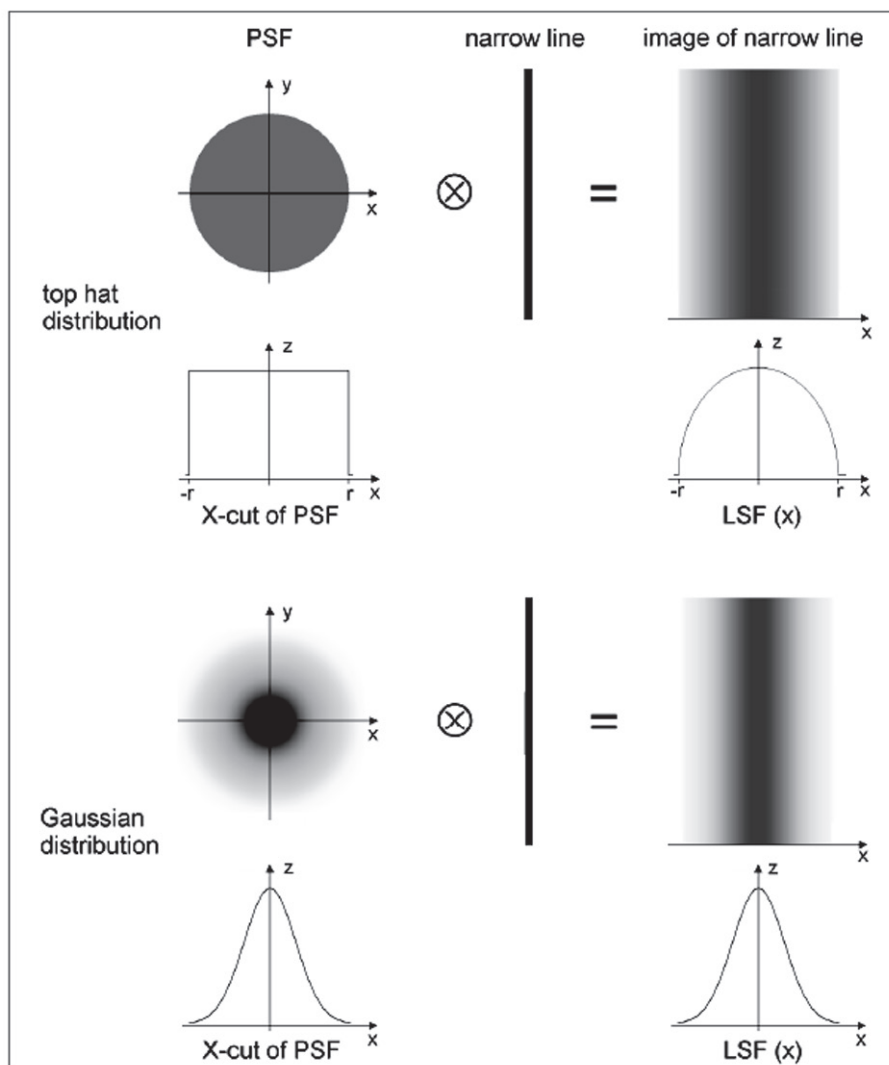


Figure 3 — Determination of the LSF by imaging of a narrow line. Different types of PSF were convoluted with a narrow line. The z-axis denotes the signal intensity within the images (from [9])

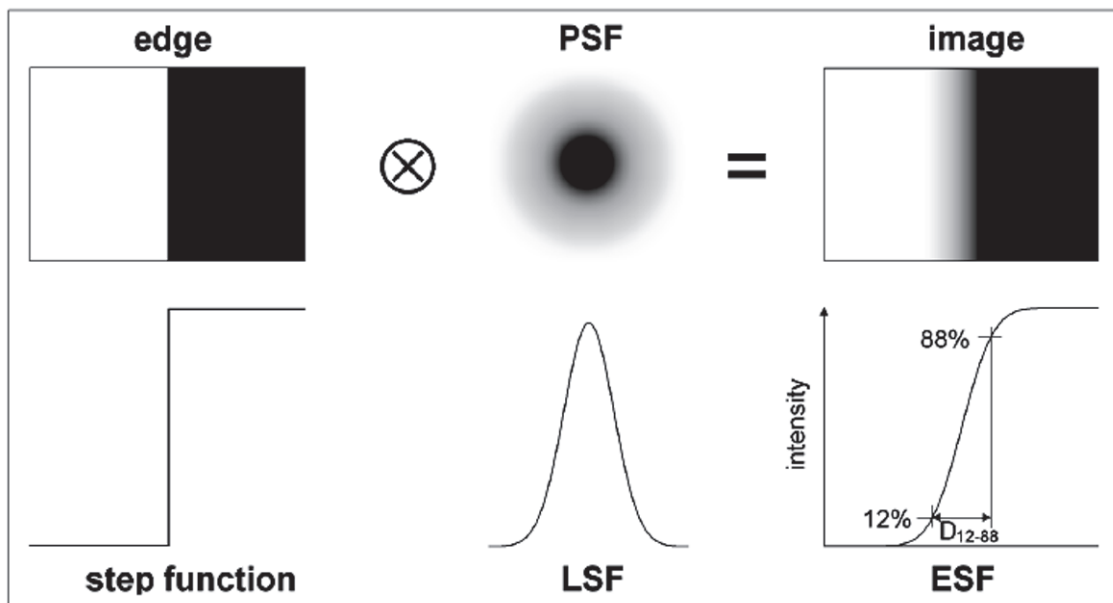


Figure 4 — Determination of the ESF by imaging of an edge. The value D_{12-88} is used as a measure of lateral resolution

4.1.4 The modulation transfer function (MTF)

The concept of the optical transfer function (OTF) was developed to characterize the performance of imaging systems.^[8,10] It was adapted from electronic and communication engineering to optical imaging and is based on the transfer of sinusoidal signals. “The optical transfer function (OTF) is the frequency response, in terms of spatial frequency (cf. terms and definitions), of an optical system to sinusoidal distributions of light intensity in the object plane”^[10]. “The part of OTF describing the reproduction of contrast is called the modulation transfer function (MTF), while the phase component is called the phase transfer function (PTF)”^[8]. Both parts of the OTF may be determined by imaging a sine wave grating. With respect to surface analytical methods, only the MTF is of interest.

The modulation of periodic patterns in objects and images is defined as

$$m = (I_{\max} - I_{\min}) / (I_{\max} + I_{\min}) \quad (7)$$

where $I_{\max}$ is the maximum value of a periodic structure and $I_{\min}$ is the minimum value between two maxima (cf. [Figure 5](#)).

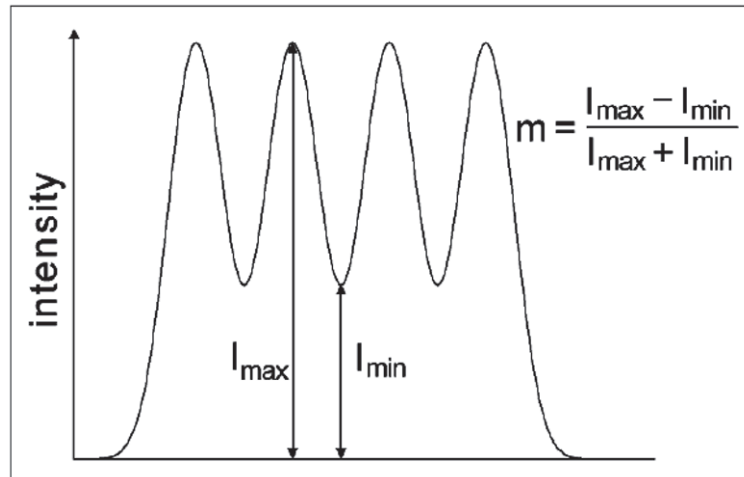


Figure 5 — Definition of modulation m

The MTF describes the transfer of the object modulation m_o to the image modulation m_i as a function of spatial frequency k

$$\text{MTF}(k) = m_i/m_o \quad (8)$$

where k is the reciprocal of the period of a sine wave grating. The object modulation m_o is based, for instance, on differences in sample composition and it can be determined from the respective image profile as outlined in [4.4.1.3](#).

An ideal imaging instrument is characterized by $m_i = m_o$ and correspondingly $\text{MTF} = 1$ for all k values. In reality imaging is always characterized by a decreasing image modulation m_i vs. increasing spatial frequency ([Figure 6](#)). Therefore the MTF can be used to describe the performance of an imaging instrument. The MTF is directly related to its lateral resolution.

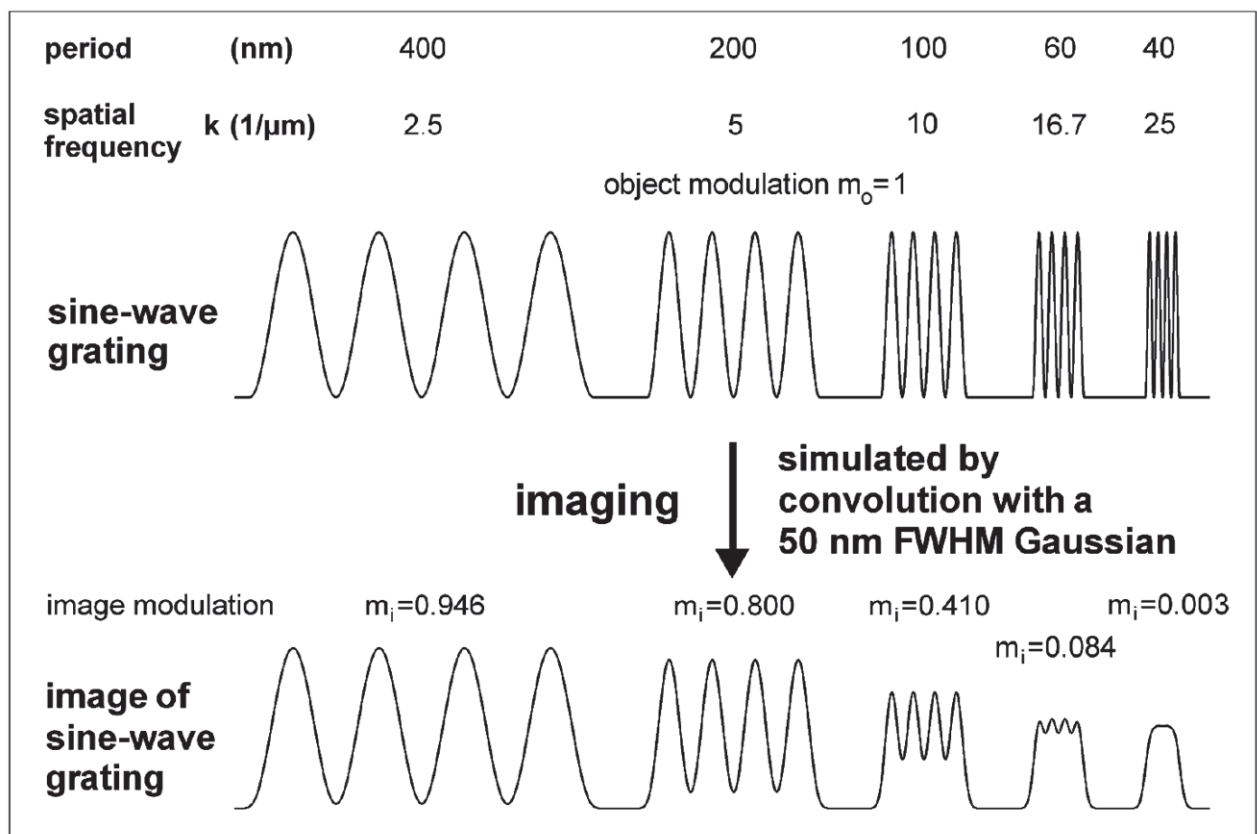


Figure 6 — Imaging of sine wave gratings with different periods and the transfer of modulation from object to image

Another definition of the optical transfer function OTF is based on the fact, that the OTF is the Fourier transform (FT) of the point spread function P

$$\text{OTF}(k, l) = \text{FT}[\text{PSF}(x, y)] = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \text{PSF}(x, y) \exp[-i2\pi(xk + yl)] dx dy \quad (9)$$

where k and l are spatial frequency variables associated with the space coordinates (x, y) , respectively. The OTF is a complex function and the MTF is the normalized modulus of the OTF. For the one-dimensional case (and only this will be treated below) the MTF is given by the Fourier transform of the line spread function (LSF)

$$\text{MTF}(k) = |\text{OTF}(k)| = \int_{-\infty}^{\infty} \text{LSF}(x) \exp(-i2\pi xk) dx / \int_{-\infty}^{\infty} \text{LSF}(x) dx \quad (10)$$

A narrow LSF in position space yields a wide MTF in spatial frequency space, and vice versa. The Fourier transform of a Gaussian distribution is again Gaussian and therefore a Gaussian LSF yields a Gaussian MTF. [Figure 7](#) demonstrates that both methods of calculating the MTF, Fourier transformation of the LSF and determination of m_i from the image of a sine wave grating, yield exactly the same values of the MTF.

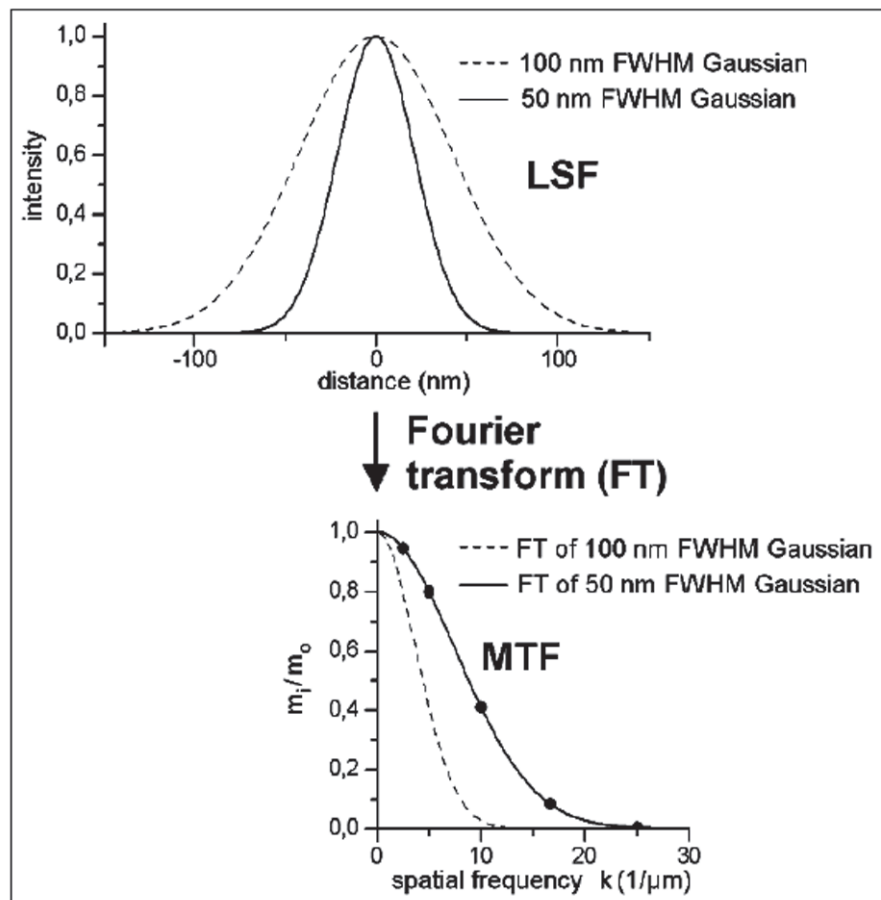


Figure 7 — Calculation of the modulation transfer function (MTF) by Fourier transform of the line spread function (LSF). The black dots are m_i/m_0 values taken from [Figure 6](#)

4.1.5 The contrast transfer function (CTF)

Optimal samples for a determination of the lateral resolution of beam-based imaging methods of surface analysis have a flat surface and a high material contrast. In the sub-100 nm range, this requirement is fulfilled by square-wave gratings, whereas flat sine-wave gratings are not available. Furthermore, the sharp contrast at the edges of a square-wave grating enables the determination of the LSF and ESF. For this reason we describe the determination of lateral resolution (cf. 4.4) using this kind of grating.

In analogy to the modulation m of sine-wave gratings the contrast of square-wave gratings is defined by $c = (I_{\max} - I_{\min}) / (I_{\max} + I_{\min})$. The variation of contrast with spatial frequency is described by the contrast transfer function

$$\text{CTF}(k) = c_i/c_0 \quad (11)$$

where c_i and c_0 are the contrast of image and object pattern, respectively (cf. terms and definitions). In [Figure 8](#) simulation results of the imaging of square-wave gratings and sine-wave gratings are displayed for high and medium resolution and at the limit of resolution as well. The imaging system is represented here by a Gaussian LSF with 50 nm FWHM. In all cases the contrast c_i in the image of a square-wave grating is higher than the modulation m_i in the image of the sine-wave grating. If the grating period is large compared to the FWHM of the imaging system's LSF (300 nm period grating), the intensity in the image of the square-wave grating drops to zero between the strips of the grating providing $c_i = 1$, whereas this is principally not the case for the sine-wave grating. A plateau of the CTF ($c_i/c_0 = 1$) at low spatial frequencies for square-wave gratings appears accordingly. Imaging of sine-wave gratings yields for a Gaussian LSF a Gaussian MTF (cf. [Figures 7](#) and [9](#)).

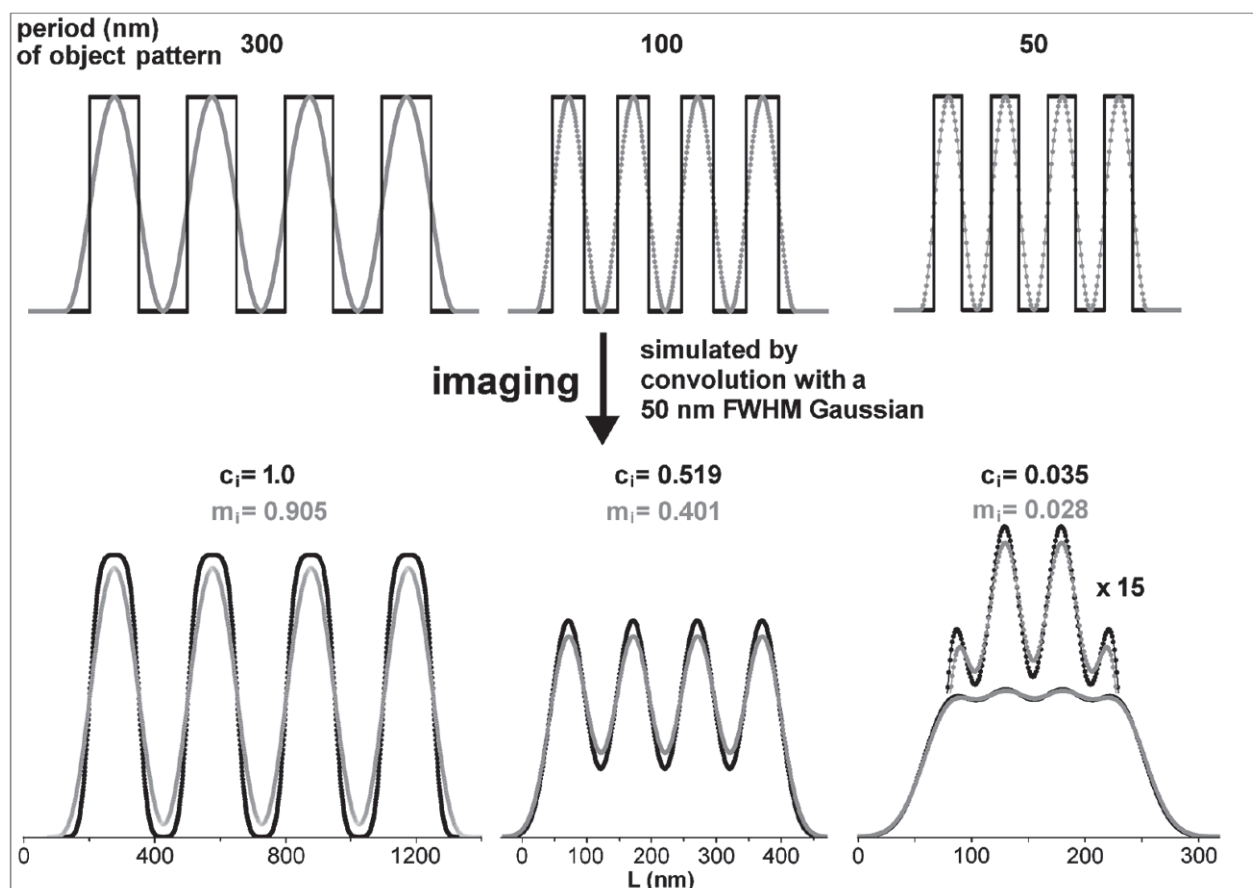


Figure 8 — Imaging of square-wave gratings (black lines) and sine-wave gratings (grey lines) of different periods. c_i and m_i are contrast and modulation in the image of a square-wave and sine-wave grating, respectively. Note the different length scales

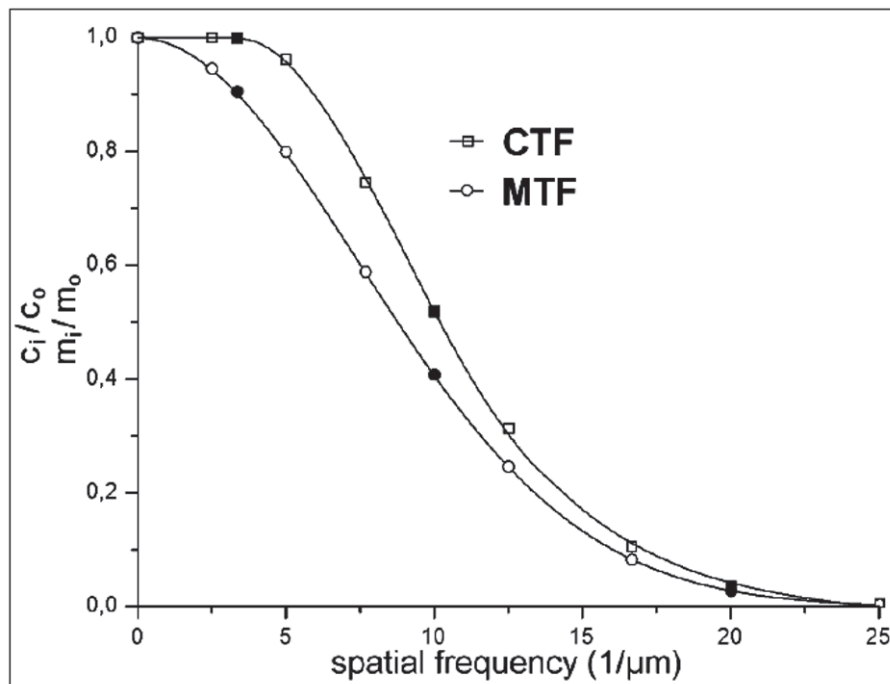


Figure 9 — CTF and MTF determined from images of square-wave gratings and sine-wave gratings, respectively. The imaging system is characterized by a 50 nm FWHM Gaussian LSF. The black symbols correspond to values taken from images displayed in [Figure 8](#)

4.1.6 Classical resolution criteria

The most commonly used resolution criterion in microscopy is the Rayleigh criterion: “Two point sources are just resolved if the central maximum of the intensity diffraction pattern produced by one point source coincides with the first zero of the intensity diffraction pattern produced by the other”[2]. It is an empirical estimate of resolution and corresponds to a decrease of intensity (dip) of 19 % (rectangular aperture) or 26.4 % (radial aperture) from the intensity of the two maxima. The threshold of resolution defined by the Rayleigh criterion reflects rather the performance of visual inspection than the sensitivity of modern instruments with sophisticated detectors. Because the Rayleigh criterion needs a rather clear separation of features (expressed by the depth of the dip), it leads to a resolution which is worse in comparison to resolutions obtained by more appropriate criteria.

The Sparrow criterion[7] defines the lowest resolution threshold that is possible in principle: the appearance of a dip between two maxima of signal intensity. In practical imaging noise prevents the detection of a very small dip between two maxima. As a consequence the resolution determined according to the Sparrow criterion is unrealistically high. Three grating profiles are resolved in [Figure 10](#) according to the Sparrow criterion and only one grating profile is resolved according to the Rayleigh criterion.

The Rayleigh criterion, the Sparrow criterion and other so-called classical resolution criteria[11] are related to the pointspread function of the imaging instrument and do not take into account measurement conditions such as noise and sampling step width. All classical criteria do not cover object contrast issues. Therefore they give rather a theoretical limit of resolution and their application in imaging surface analysis is not straightforward. The application of the Rayleigh criterion and the Sparrow criterion in surface analysis has been discussed in Ref. [12] but they do not play a role in practical surface analysis.

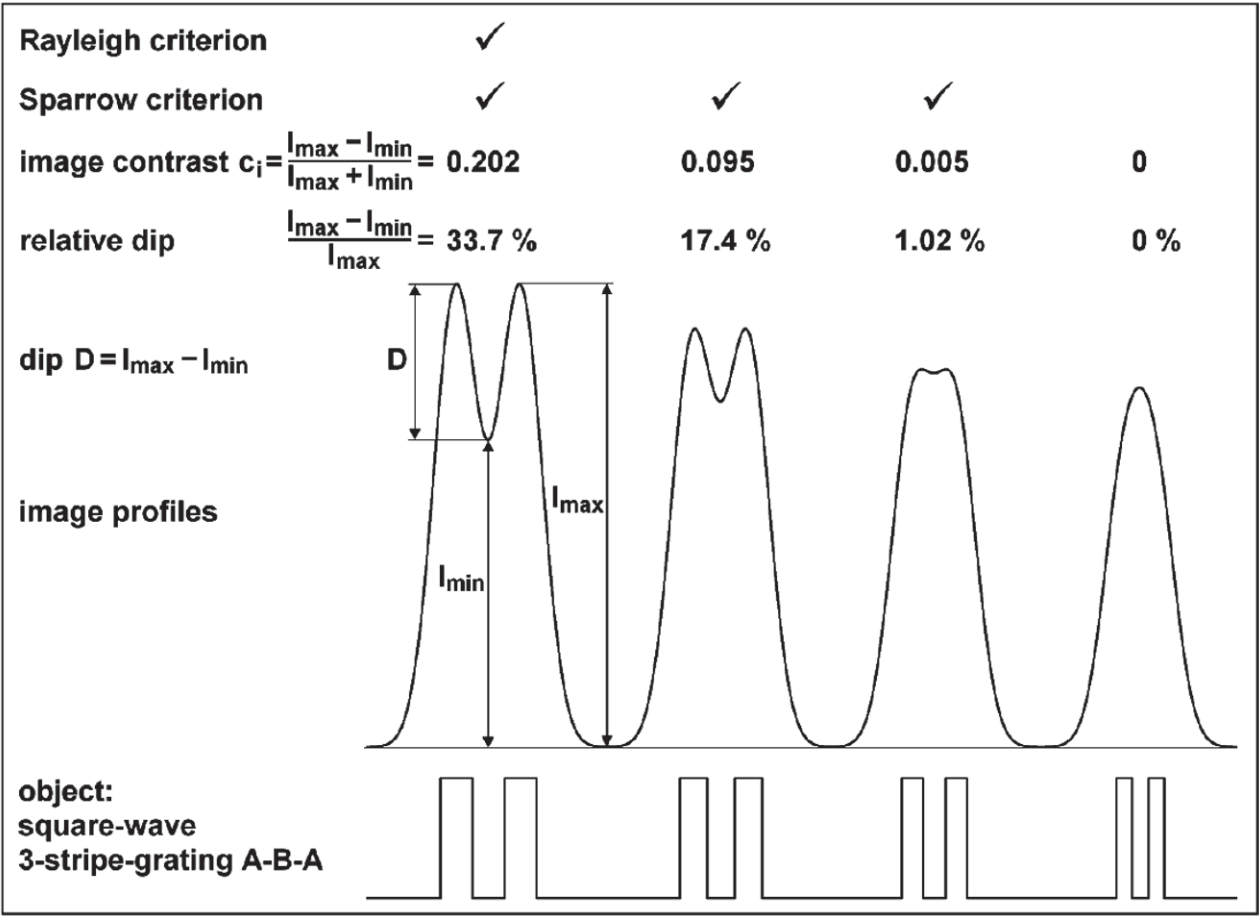


Figure 10 — Application of the Rayleigh criterion and the Sparrow criterion to simulated image profiles over square-wave gratings with different periods

4.1.7 Comparison of functions, parameters and methods related to effective lateral resolution and sharpness

See [Tables 1, 2](#) and [3](#).

Table 1 — Summary of essential results of the methods related to effective lateral resolution

Feature or function	Method of determination	Relation to effective lateral resolution	Advantages	Disadvantages	Subclause
Effective lateral resolution, r_e	Visual determination of r_e from an image of a series of square-wave gratings	Period of the finest resolved grating corresponds to r_e	Real time procedure without any data treatment	Subjective decision whether a grating is resolved or not Large uncertainty of r_e at large values of the grading factor q	4.4.2 4.4.4
Effective lateral resolution, r_e	Determination of dip-to-reduced-noise ratios $R_{D/RN}$ from a linescan over three square-wave gratings, calculation of r_e from the intersection of $R_{D/RN}$ (P) with $R_{D/RN} = 4$ according to Formula (39)	Calculated value of r_e is based on the resolution criterion (37)	Criterion-based calculation of r_e High accuracy of r_e also at large values of the grading factor ($q \leq 1.8$)	Numerical evaluation of noise and dips from a linescan over three gratings	4.4.2 4.4.4
Effective cut-off frequency of the CTF	Determination of the intersection between CTF and $(C_1/C_0)_{ThR}$	r_e corresponds to the reciprocal of the effective cut-off frequency of the CTF	Criterion based method for the determination of r_e	Time-consuming evaluation of noise and dips from a linescan over a series of gratings	4.4.3.3

Table 2 — Summary of essential results of the methods related to sharpness

Feature or function	Method of determination	Relation to sharpness	Advantages	Disadvantages	Subclause
CTF (contrast transfer function)	Linescan over a series of square-wave gratings, image contrast as function of spatial frequency	Describes sharpness over the whole range of spatial frequencies	Response of an imaging system over the whole range of spatial frequencies	Time-consuming numerical evaluation of noise and dips from a linescan over a series of gratings	4.1.5 4.4.3
LSF (line spread function)	Linescan over a narrow stripe	LSF describes the sharpness of an image	Simple procedure of measurement		4.1.2 4.2.1–4.2.5
FWHM of LSF, w_{LSF}	Linescan over a narrow stripe, determination of FWHM	Measure of sharpness of an image	Simple procedure	Shape of the LSF is not considered	4.2.1–4.2.5
MTF (modulation transfer function)	LSF from linescan over a narrow stripe MTF by Fourier transform of LSF	Describes sharpness over the whole range of spatial frequencies	Response of an imaging system over the whole range of spatial frequencies	Tails of LSF have to be measured with high accuracy Noise affects the spectrum of spatial frequencies	4.1.4 4.2.6
ESF (edge spread function)	Linescan over a straight edge (step transition) covering the 0% and 100% levels of signal intensity	ESF describes the sharpness of an image	Simple procedure	For long-tailed LSFs the 0% and 100% levels of ESF may be not covered by measurement	4.1.3 4.3
D_{12-88} , D_{16-84} , D_{20-80} ESF rise parameters	Linescan over a straight edge (step transition) covering the 0% and 100% levels of signal intensity	Measure of sharpness of an image	Simple procedure	0% and 100% levels of ESF may be not covered by measurement, then $D_{x-(1-x)}$ may be underestimated	4.1.3 4.3

Table 3 — Requirements for test samples

Feature	Method of determination	Type of sample	Required sample properties	Subclause
Effective lateral resolution r_e	Visual determination of r_e from an image of a series of square-wave gratings	Series of chemical square-wave gratings A–B–A (materials A and B) with graded grating periods P	Grating factor $q = P_{n+1}/P_n$ of grating periods P : Optimum: $1.2 \leq q \leq 1.5$ Calculation according to Formula (39): $q \leq 1.7$ Optimum distance d_{gr} between two consecutive gratings: General: $1.5 P \leq d_{gr} \leq 3 P$ Gaussian LSF: $P \leq d_{gr} \leq 2 P$ Expanded ($k=2$) uncertainty of certified grating periods: $U(P) \leq 10 \%$	4.4.1.1 4.4.1.2 4.4.4
	Calculation of r_e from the intersection of R_D/R_N (P) with $R_D/R_N = 4$ according to Formula (39)			
	Determination of r_e as the reciprocal of the effective cut-off frequency of the CTF			
Line spread function, LSF FWHM of the LSF, w_{LSF} Modulation transfer function, MTF	Linescan over a narrow stripe	Narrow stripe	Stripe width w_s to ensure $\Delta w_{LSF} < 10 \%$: Gaussian LSF: $w_s \leq 0.6 w_{LSF}$ Lorentzian LSF: $w_s \leq 0.4 w_{LSF}$ Stripe distance d to ensure $\Delta w_{LSF} < 6 \%$: Gaussian LSF: $d \geq 2.5 w_{LSF}$ Lorentzian LSF: $d \geq 5 w_{LSF}$	4.2.2 4.2.7
	Linescan over a straight edge (step transition) covering the 0% and 100% levels of signal intensity	Chemical edge: material A–material B with extended lower (A) and upper (B) plateaus Spatial edge: vacuum–material A	Plateau lengths L_{pl} to ensure $\Delta D_{x-(1-x)} < 10 \%$: Gaussian LSF: $L_{pl} \geq 2 w_{LSF}$ Lorentzian LSF: $L_{pl} \geq 40 w_{LSF}$	4.3.3 4.3.5

4.2 Determination of the line spread function and the modulation transfer function by imaging of a narrow stripe

The line spread function (LSF) (cf. 4.1.2) determined by imaging a narrow stripe (defined in 4.2.2) may be used to characterize the quality of an image and the performance of an imaging instrument^[13] because its width w_{LSF} and shape substantially determine the lateral resolution of the image (cf. 4.4.3.1). w_{LSF} is related to lateral resolution but in general it is not the lateral resolution. Its value may differ substantially from the lateral resolution (cf. 4.4.3.3). The LSF may be obtained directly from the measured profile over a narrow stripe or by fitting the measured profile with a model function as outlined in 4.2.3.

4.2.1 Model functions for the LSF

The transverse intensity distribution in light and particle beams can be described by different model functions.^[14] The most frequently used function is the two-dimensional Gaussian function. According to Formula (4) and Figure 3 (cf. 4.1.2) the LSF is also a Gaussian function (normal distribution) for these probe beams

$$G(x) = y_0 + \frac{I_0}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-x_0)^2}{2\sigma^2}\right) \quad (12)$$

where σ is the standard deviation of the normal distribution, x_0 is the centre position, y_0 is the background intensity and I_0 is the total intensity expressed as the area under the curve. The full width at half maximum (FWHM) of $G(x)$ is

$$w = [2 \ln(2)]^{1/2} \times 2\sigma = 1.1774 \times 2\sigma \quad (13)$$

The Gaussian function describes the intensity distribution within a beam which is formed by an ideal lens system. However, in reality the LSF may deviate from Gaussian shape. Therefore other model functions are considered, too. One option is a combination of Gaussian functions with different widths (cf. 5.2.2 and^[14-16]) as shown in Figure 11.

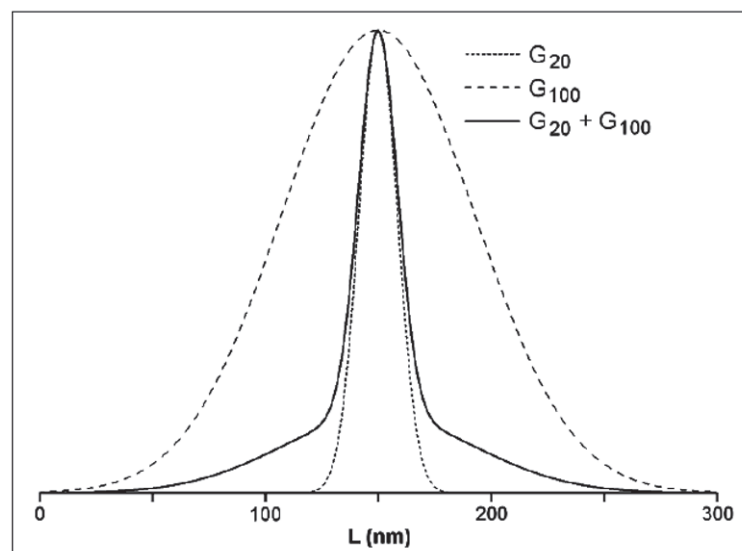


Figure 11 — Two Gaussian functions G with different widths and the sum of these functions. The functions are normalized to the same height. FWHM values in nm are given as indices

The Lorentzian function $L(x)$ is well known in spectroscopy, because it is the resonance function of the harmonic oscillator and fits the shape of spectral lines of atoms. It can be used also for fitting LSFs with

extended tails (Figure 12), which may occur due to lens aberration^[17] and/or particle scattering within the sample. It is defined by

$$L(x) = y_0 + \frac{2 \times I_0 \times w}{\pi [4(x - x_0)^2 + w^2]} \quad (14)$$

where w is the FWHM of the function, x_0 is the centre position, y_0 is the background intensity and I_0 is the total intensity (area under the curve).

The Pseudo-Voigt function is a weighted sum of Gaussian and Lorentzian functions. The type 1 Pseudo-Voigt function (cf. Figure 12) is a linear combination of a Lorentzian function and a Gaussian function with the same FWHM denoted by w and weighted by a factor η :

$$PSV1 = y_0 + I_0 [\eta L(x, x_0, w) + (1 - \eta) G(x, x_0, w)] \quad (15)$$

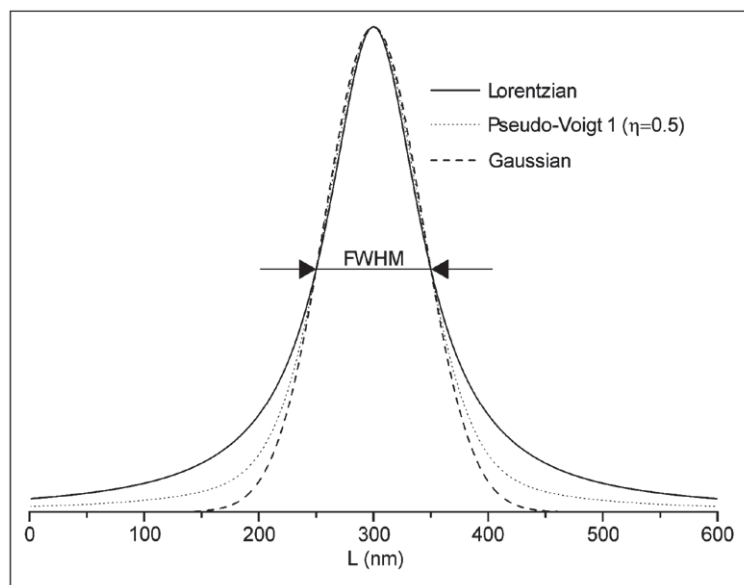


Figure 12 — Gaussian function, Lorentzian function and type 1 Pseudo-Voigt function having the same FWHM of 100 nm. The functions are normalized to the same height

The type 2 Pseudo-Voigt function is a linear combination of a Lorentzian function and a Gaussian function with different widths w_L and w_G :

$$PSV2 = y_0 + I_0 [\eta L(x, x_0, w_L) + (1 - \eta) G(x, x_0, w_G)] \quad (16)$$

A great variety of LSF shapes (Figure 13) can be simulated by a type 2 Pseudo-Voigt function.

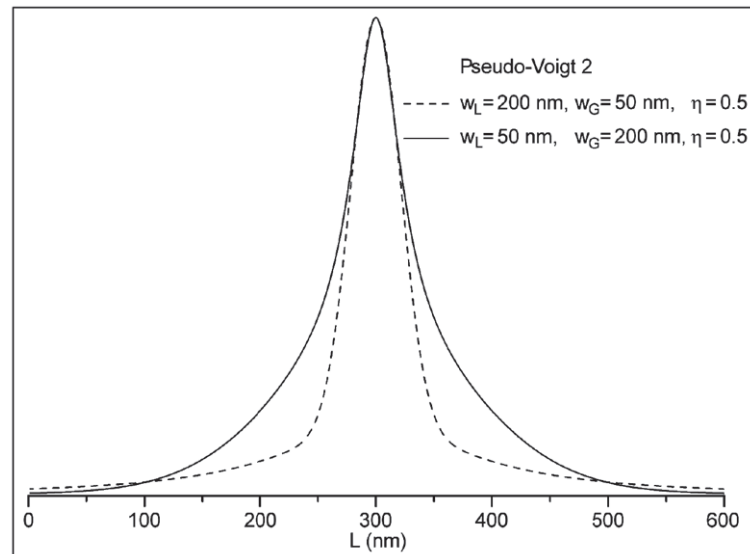


Figure 13 — Type 2 Pseudo-Voigt functions with different combinations of w_L and w_G . The functions are normalized to the same height

4.2.2 What is a narrow stripe?

A stripe may be called narrow if its width w_s is small compared to the full width at half maximum of the LSF w_{LSF} characterizing the imaging system used. In this case a profile across the image of the stripe reveals that LSF. If w_s is not small compared to w_{LSF} , then the FWHM of the image profile increases with increasing width of the stripe. This effect is demonstrated by a simulation displayed in [Figure 14](#), where stripe images are simulated by convolution with a Gaussian LSF.

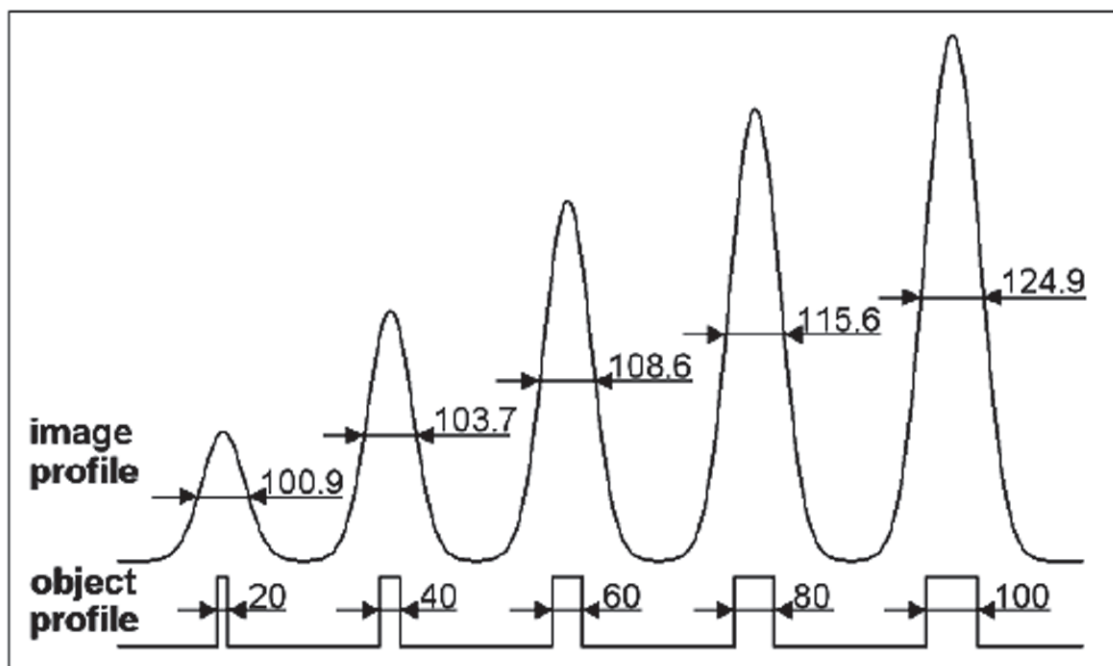


Figure 14 — Imaging of a series of stripes simulated by convolution with a Gaussian LSF with $w_{LSF} = 100$ nm. The values given in the image profiles are the FWHM in nm

The deviation of w_{LSF} taken from the image profile from the true value of $FWHM_{LSF}$ is displayed as a function of w_s/w_{LSF} in Figure 15.

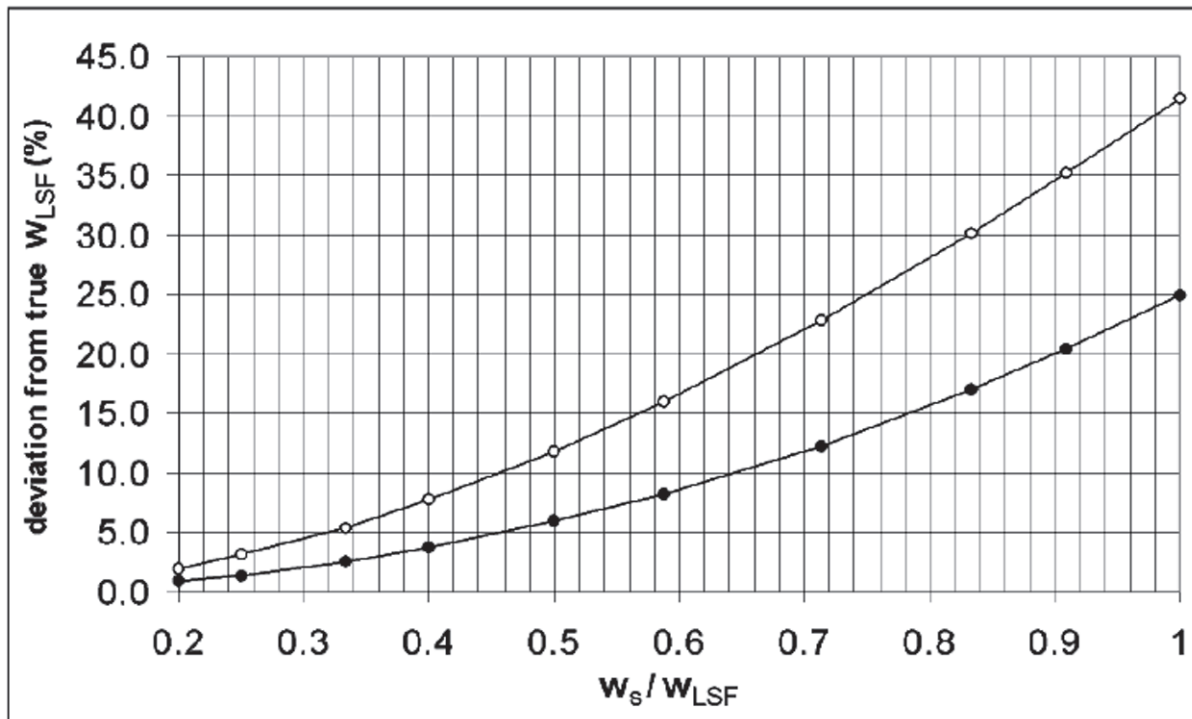


Figure 15 — Deviation of the FWHM of the profile of an imaged stripe from w_{LSF} as function of the ratio w_s/w_{LSF} . Black dots: Gaussian LSF; Open circles: Lorentzian LSF

The shape of the image profile is also influenced by the stripe width w_s . For small values of the ratio w_s/w_{LSF} , e.g. 0.2 as displayed by the left image profile in Figure 14, the image profile may be fitted by the LSF shape function with a slightly increased FWHM. For $w_s/w_{LSF} = 1$ as displayed by the right image profile in Figure 14, the shape of the image profiles differs from that of the LSF. Figure 16 shows the best fits of image profiles for the $w_s/w_{LSF} = 1$ case. The image profile created with a Gaussian LSF shows only a small deviation from Gaussian shape, whereas the profile created with a Lorentzian LSF deviates considerably from Lorentzian shape.

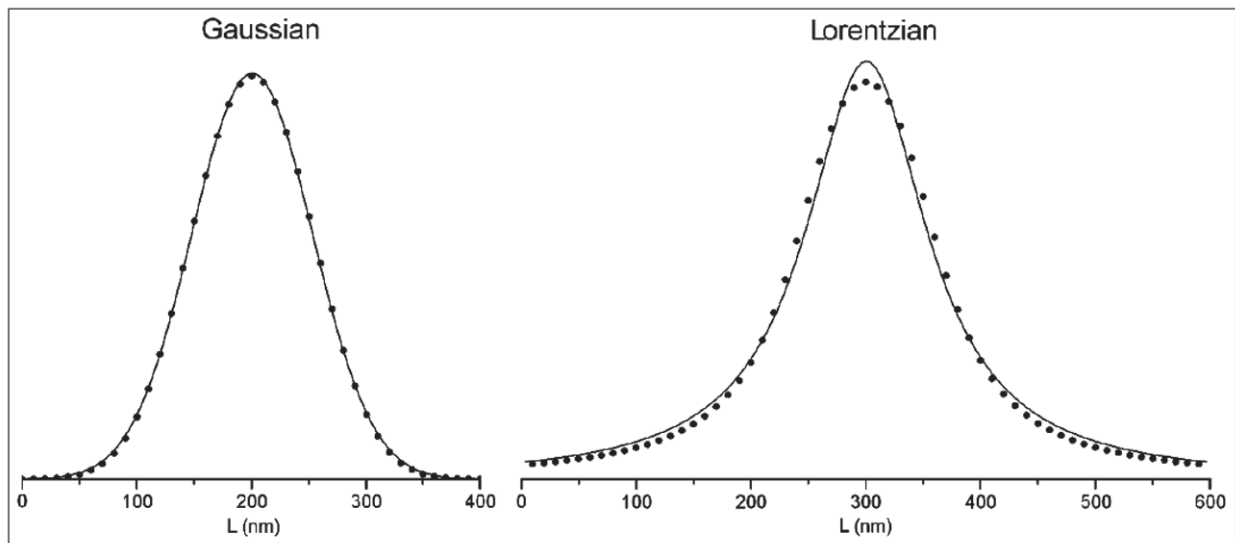


Figure 16 — Image profiles (black dots) over a 100 nm wide rectangular stripe simulated by convolution with 100 nm wide Gaussian and Lorentzian LSFs revealing the deviations from the principal shape of the LSF. Lines show the best fit with a Gaussian and Lorentzian, respectively

4.2.3 The effect of signal-to-noise ratio and sampling step width on LSF determination

For sufficiently high signal-to-noise ratios $R_{S/N}$ the LSF and its full width at half maximum w_{LSF} can be obtained directly from the measured profile over a narrow stripe. This simple situation is displayed in [Figure 17](#), left panel, top. However, experimental data can be also analysed by fitting with more or less appropriate LSF model functions ([Figure 17](#), left panel, middle and bottom).

The low $R_{S/N}$ case is given in [Figure 17](#), right panel. Here shape and w_{LSF} have to be determined by fitting experimental data with a peak shape model function. Depending on the model function, the w_{LSF} can be taken either directly from the respective fit parameter results ([Figure 17](#), middle row) or from the fitted curve ([Figure 17](#), lower row). In any case the background signal y_0 must be determined carefully outside the stripe profile.

The profiles given in [Figure 17](#) were created by the convolution of a narrow stripe with a type 2 Pseudo-Voigt function. Indeed, for the high $R_{S/N}$ case a fit with that type of function yields a better result (smaller χ^2) than a fit with a Lorentzian. In the low $R_{S/N}$ case the values of χ^2 are very similar for both functions but a fit with a Lorentzian yields a smaller deviation of w_{LSF} from the value of the implemented type 2 Pseudo-Voigt model function. The latter result is accidental and caused by noise which has broadened the stripe profile.

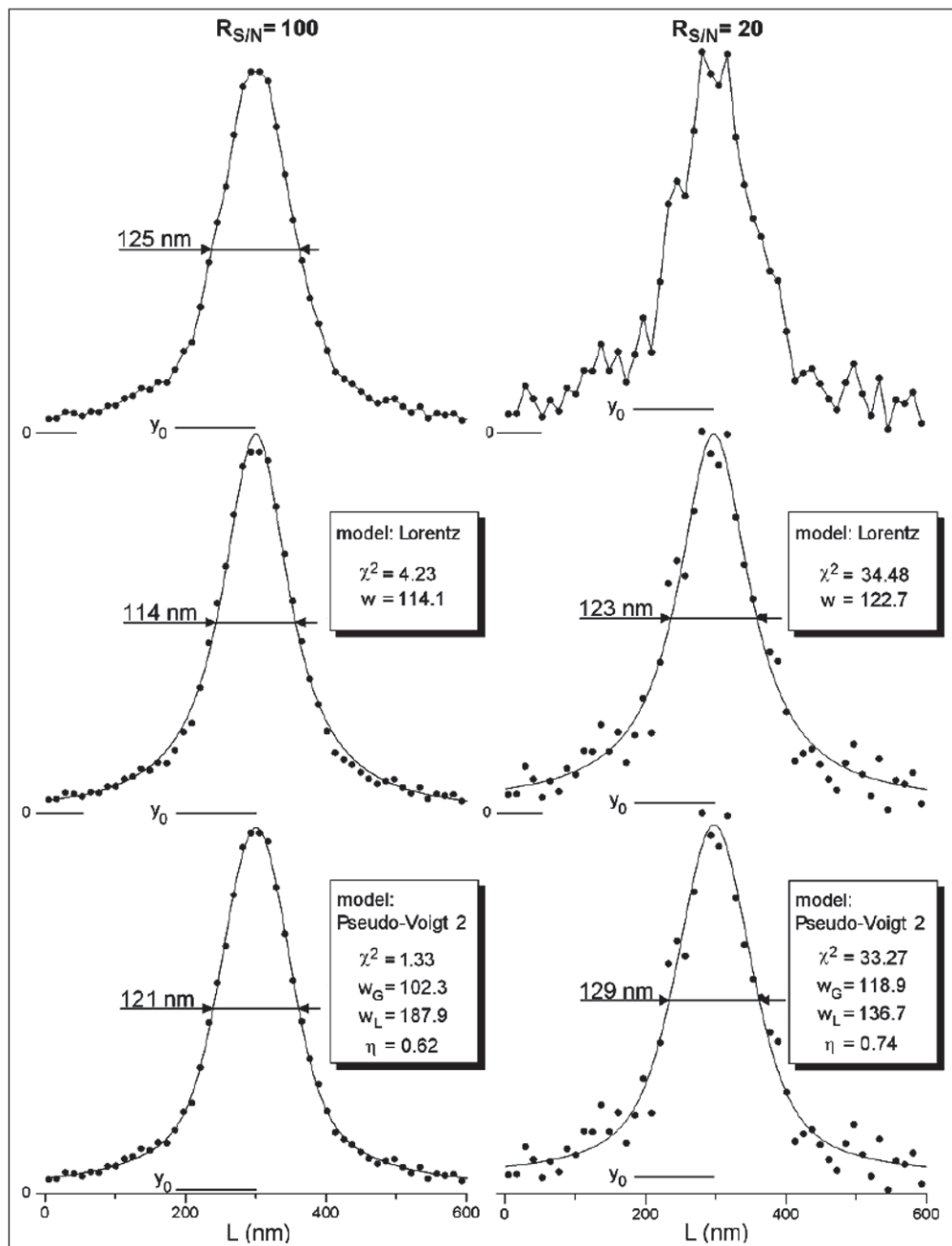


Figure 17 — Determination of w_{LSF} from a simulated image profile of a narrow stripe at different $R_{S/N}$ levels ($R_{S/N} = I_{max}/\sigma_N$, where σ_N is the standard deviation of noise). Data points (black dots) represent a measured profile simulated by convolution of a 20 nm wide stripe with a type 2 Pseudo-Voigt function (PSV2, $w_G = 100$ nm, $w_L = 200$ nm, $\eta = 0.6$, cf. 4.2.1) and subsequent addition of two different noise levels. The FWHM of the PSV2 function is 118.4 nm, the FWHM of the convolution without noise is 119.7 nm. Upper row: raw data; Middle row: Profiles fitted with a Lorentzian; Lower row: Profiles fitted with a PSV2 function. y_0 is the background signal and χ^2 is a measure of the quality of the fit

The quality of the determination of the LSF and its width w_{LSF} depends on the sampling step width used for the measurement of the profile. Especially but not only at low signal-to-noise ratios $R_{S/N}$, the uncertainty of w_{LSF} increases with decreasing number of sampling points, i.e. increasing sampling step width. This effect is demonstrated by fitting LSFs for simulated image profile data at different $R_{S/N}$ levels. The random nature of noise was taken into account in this simulation by adding different sets of Gaussian

noise to a Gaussian profile with $w_{LSF} = 30$ nm representing the image profile. To establish data sets with different sampling step widths the number of data points was reduced simply by removing data points.

All w_{LSF} values obtained by fitting Gaussian profiles with different sets of Gaussian noise ($R_{S/N} = 10$) and a variation of sampling step widths are summarized in [Figure 18](#). Step width and number of sampling points, both normalized to $w_{LSF} = 30$ nm of the original noise-free Gaussian profile are given at the abscissa.

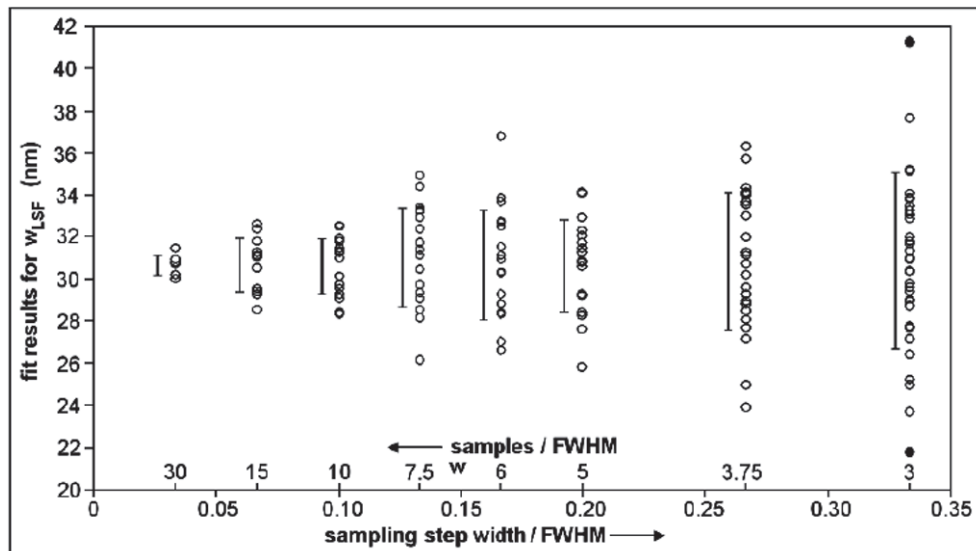


Figure 18 — Dispersion of w_{LSF} data determined for simulated Gaussian profiles at $R_{S/N} = 10$ and different sampling step widths. The noise-free Gaussian profile has a FWHM of 30 nm. The bars denote the standard deviations. Both black dots at 3 samples/FWHM denote extreme values of w_{LSF} obtained from profiles which are displayed in the upper row of [Figure 19](#)

[Figure 19](#) (top line) shows the largest positive and negative deviations, respectively, of fitted w_{LSF} data from the original FWHM = 30 nm noise-free Gaussian profile. Strong noise ($R_{S/N} = 10$) and large step width (10 nm corresponding to only three data points per w_{LSF}) cause deviations up to 38 % in those cases.

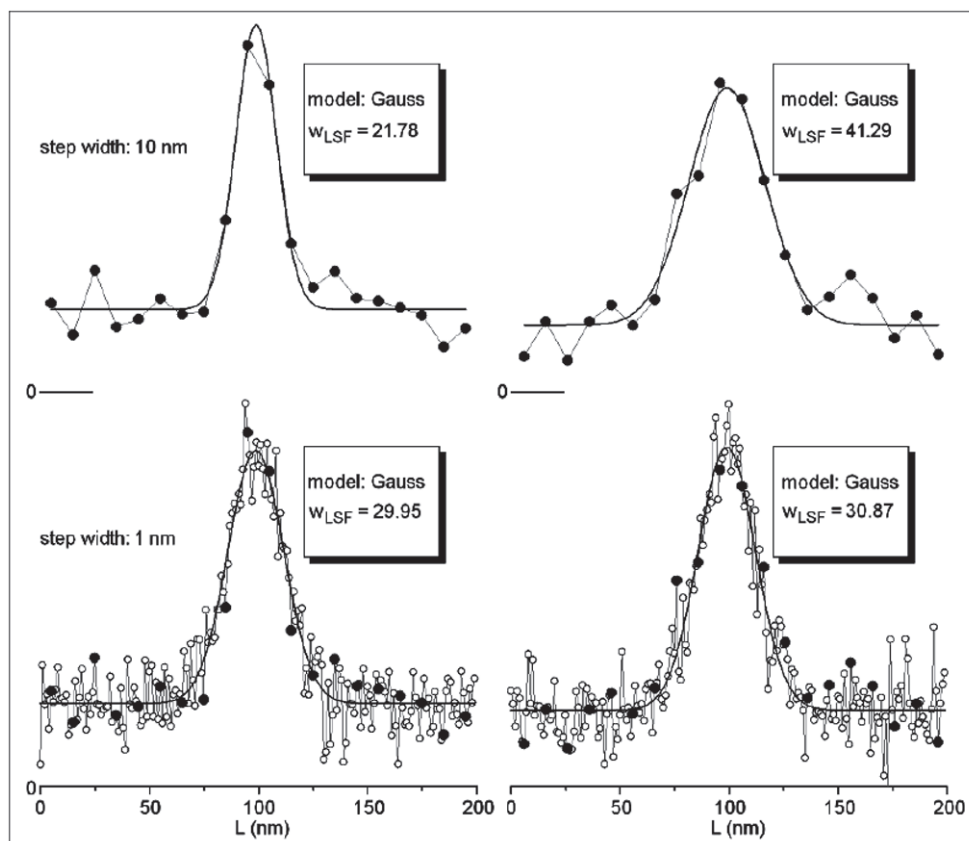


Figure 19 — Fits of Gaussian profiles (30 nm FWHM) superimposed by different sets of Gaussian noise providing $R_{S/N} = 10$. Those profiles simulate an image profile across a narrow stripe at different step widths of sampling. Dots are data points (connected by a fine line). Fitted profiles are displayed by bold lines. w_{LSF} results are given in the boxes. Top: Narrowest and widest profile from 36 profiles at a sampling step width of 10 nm. Bottom: Profiles with a sampling step width of 1 nm which were created with the same sets of Gaussian noise as the profiles given in the upper row. The black dots denote the data points of the reduced data sets in the upper row

[Figure 20](#) shows the largest deviations of w_{LSF} obtained from fitting of different profiles with different levels of noise and two sampling step widths. The variability of w_{LSF} data vs. sampling step width is much stronger for noisy profiles ($R_{S/N} = 10$) than for those with medium ($R_{S/N} = 30$) or low ($R_{S/N} = 100$) levels of noise.

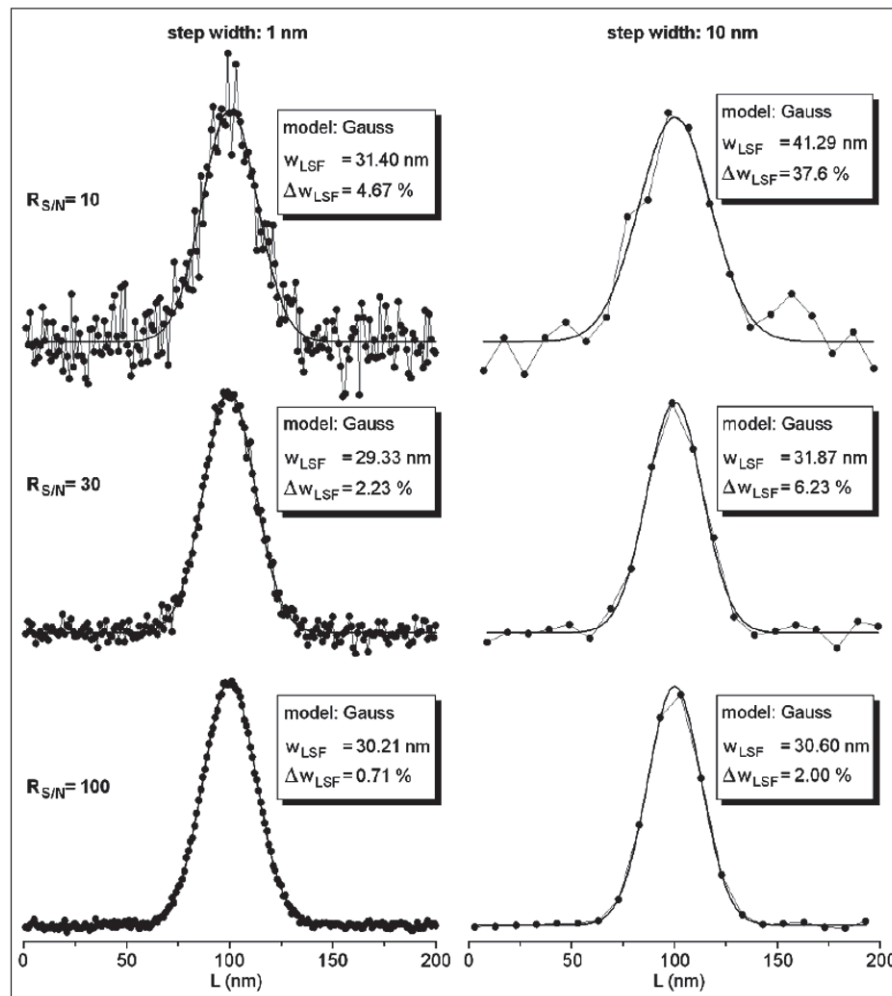


Figure 20 — Largest positive or negative deviations of fitted w_{LSF} from the FWHM of the original noise-free profile (30 nm) for different sampling step widths and $R_{S/N}$ levels

The accuracy of w_{LSF} determined by fitting of noisy stripe profiles depends on $R_{S/N}$ as well as sampling step width. As a measure of accuracy of the fitting procedure a mean deviation

$$s = \sqrt{\frac{1}{(n-1)} \sum_{i=1}^n \left[(w_{LSF})_i - (w_{LSF})_t \right]^2} \quad (17)$$

was calculated, where $(w_{LSF})_i$ is one of n results of the fitting procedure and $(w_{LSF})_t$ is the true FWHM of the noise-free Gaussian profile. The deviation s is a little different from the standard deviation given by bars in [Figure 18](#) because the fitting results were related to the true value of $(w_{LSF})_t$ and not to the arithmetic mean of w_{LSF} . As a result s includes, besides the statistical error, also possible systematic deviations of the fitting procedure. Therefore it is a measure of precision and trueness of the fitting procedure. [Figure 21](#) shows the relative deviation $s/(w_{LSF})_t$.

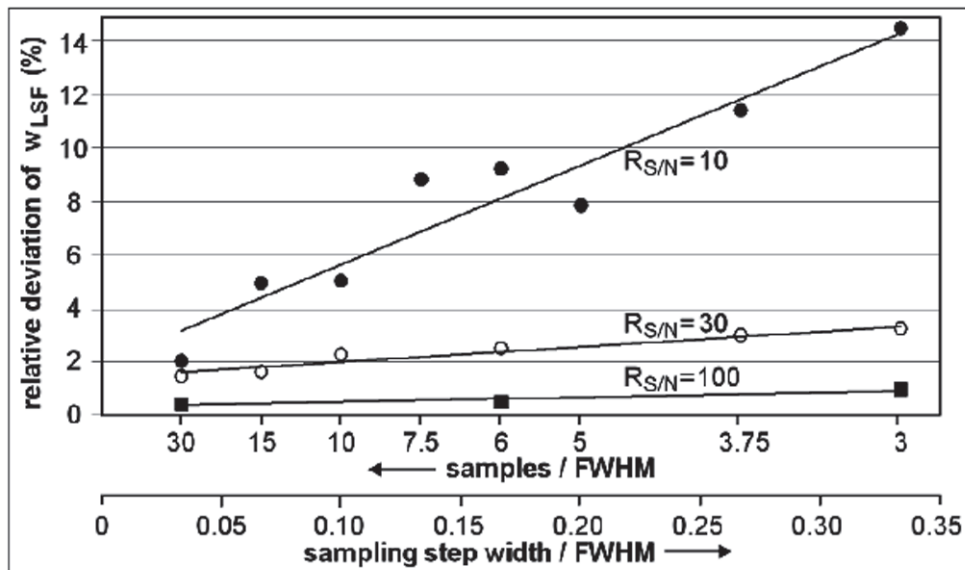


Figure 21 — Relative deviation $s \cdot 100/(w_{LSF})_t$ of fitted w_{LSF} data as a function of sampling step width for different values of $R_{S/N}$. The values for $R_{S/N} = 10$ are calculated from the values shown in [Figure 18](#)

4.2.4 The effect of smoothing on LSF determination from a noisy image profile

For low $R_{S/N}$ levels, the LSF and its width w_{LSF} cannot be taken directly from the measured profile over a narrow stripe (cf. 4.2.3). In many cases smoothing may be attractive to enable the simple direct approach of LSF and w_{LSF} determination. When the measured profile over the narrow stripe is formed by a sufficient number of sampling points different kinds of smoothing procedures may be applied. The application of such smoothing procedures has been discussed in detail with respect to spectroscopic data[18]–[20].

[Figure 22](#) displays a noisy profile and its smoothing by three different methods which are implemented in the ORIGIN™ software.[21] An important smoothing parameter is the smoothing interval which determines the number of data points considered at one step of the smoothing routine. With increasing smoothing intervals noise will be reduced more efficiently, but the profile becomes flattened and broadened. Therefore, it is necessary to find the optimum smoothing interval. [Figure 22](#) shows, that adjacent averaging has the lowest suitability for smoothing noisy profiles of imaged narrow stripes, because it broadens the profile more than the other methods. Better results can be obtained by using Savitzky-Golay smoothing and fast Fourier transform (FFT) filter smoothing. Results optimized in terms of smoothing intervals are displayed in [Figure 23](#). w_{LSF} values obtained directly from the smoothed data points and those determined from a fit of the smoothed profile differ by less than 5 % from the value determined from a fit of the unsmoothed profile.