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TECHNICAL SPECIFICATION

Nanotechnologies – Description, measurement and dimensional quality parameters of artificial gratings

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IEC Central Office
3, rue de Varembé
CH-1211 Geneva 20
Switzerland

Tel.: +41 22 919 02 11
Fax: +41 22 919 03 00
info@iec.ch
www.iec.ch

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NANOTECHNOLOGIES – DESCRIPTION, MEASUREMENT AND DIMENSIONAL QUALITY PARAMETERS OF ARTIFICIAL GRATINGS

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Technical specifications are subject to review within three years of publication to decide whether they can be transformed into International Standards.

IEC 62622, which is a technical specification, has been prepared within the joint working group 2 of IEC technical committee 113 and ISO technical committee 229.

The text of this technical specification is based on the following documents:

Enquiry draft	Report on voting
113/133/DTS	113/143/RVC

Full information on the voting for the approval of this technical specification can be found in the report on voting indicated in the above table. In ISO, the standard has been approved by 16 member bodies out of 16 having cast a vote.

This publication has been drafted in accordance with the ISO/IEC Directives, Part 2.

The committee has decided that the contents of this publication will remain unchanged until the stability date indicated on the IEC web site under "http://webstore.iec.ch" in the data related to the specific publication. At this date, the publication will be

- transformed into an International Standard,
- reconfirmed,
- withdrawn,
- replaced by a revised edition, or
- amended.

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INTRODUCTION

Artificial gratings play an important role in the manufacturing processes of small structures at the nanoscale as well as characterization of nano-objects.

For example, in high volume manufacturing of semiconductor integrated circuits by means of lithography techniques, grating patterns on the photomask and the silicon wafer are optically probed and the resulting optical signal is analyzed and used for relative alignment purposes of mask to wafer in the different lithographic production steps in the wafer-scanner production tools. In semiconductor manufacturing as well as in other manufacturing processes requiring high positioning accuracy at the nanoscale, often length or angular encoder systems based on artificial gratings are used to provide position feedback of moving axes. Another area of application for artificial gratings in nanotechnology is their use as calibration standards for high resolution microscopes, like scanning probe microscopes, scanning electron microscopes or transmission electron microscopes which are necessary tools for the characterization of nanoscale structures.

The quality of the artificial gratings used for position feedback generally influences the achievable accuracy of alignment systems or positioning systems in manufacturing tools. This also holds for the application of artificial gratings as standards for calibration of image magnification of high resolution microscopes, where the quality of the grating plays an important role in the achievable calibration uncertainty of the standard and thus for the attainable measurement uncertainty of the microscope.

This technical specification concentrates on specifying quality parameters, expressed in terms of deviations from nominal positions of grating features, and provides guidance on the application of different categories of measurement and evaluation methods to be used for calibration and characterization of artificial gratings

NANOTECHNOLOGIES – DESCRIPTION, MEASUREMENT AND DIMENSIONAL QUALITY PARAMETERS OF ARTIFICIAL GRATINGS

1 Scope

This technical specification specifies the generic terminology for the global and local quality parameters of artificial gratings, interpreted in terms of deviations from nominal positions of grating features, and provides guidance on the categorization of measurement and evaluation methods for their determination.

This specification is intended to facilitate communication among manufacturers, users and calibration laboratories dealing with the characterization of the dimensional quality parameters of artificial gratings used in nanotechnology.

This specification supports quality assurance in the production and use of artificial gratings in different areas of application in nanotechnology. Whilst the definitions and described methods are universal to a large variety of different gratings, the focus is on one-dimensional (1D) and two-dimensional (2D) gratings.

2 Normative references

The following documents, in whole or in part, are normatively referenced in this document and are indispensable for its application. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO/IEC 17025, *General requirements for the competence of testing and calibration laboratories*

ISO/TS 80004-1:2010, *Nanotechnologies – Vocabulary – Part 1: Core terms*

3 Terms and definitions

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

3.1 Basic terms

3.1.1
feature
region within a single continuous boundary, and referred to a reference plane, that has a defining physical property (parameter) that is distinct from the region outside the boundary

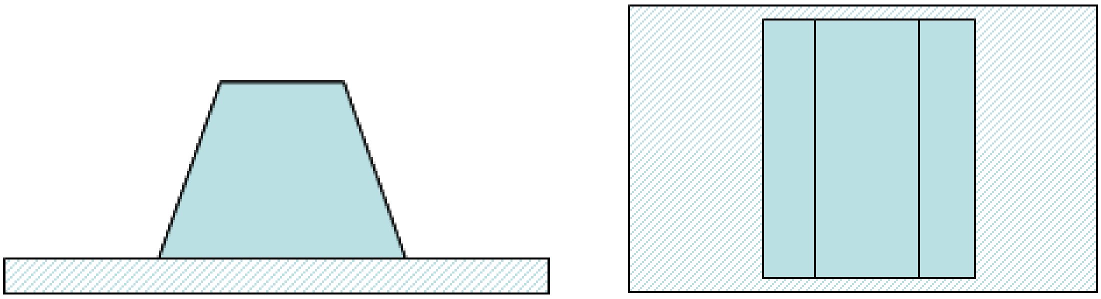

Figure 1 – Example of a trapezoidal line feature on a substrate

EXAMPLE In Figure 1 a feature with a trapezoidal cross-section on a substrate is shown.

Note 1 to entry: This definition is adapted from [1][1] (SEMI P35 (5.1.5 feature (lithographic)).

Note 2 to entry: In general, a feature is a three-dimensional object. It can also be a nano-object (defined in ISO/TS 80004-1:2010, 2.5). It can have different shape, e.g. it can be a dot, a line, a groove, etc. It might be symmetric or non–symmetric. It can have the same material properties as the substrate or different ones. It can be located on the surface of a substrate or within the substrate (sometimes called "buried feature").

Note 3 to entry: In [2] the term 'geometrical feature' is generally defined as point, line or surface.

3.1.2
reference plane
user-defined plane approximating the surface of a substrate and containing a feature coordinate system

Note 1 to entry: This definition is adapted from [1].

3.1.3
feature coordinate system
coordinate system
Cartesian coordinate system defined by the reference plane as x-y plane, the x-axis defined by the main grating direction and the origin defined by a suitable, specified reference position

Note 1 to entry: Often, the position of a particular feature is chosen as the origin of the coordinate system, e.g. the first feature in a 1D grating, or the lower left feature in a 2D grating.

Note 2 to entry: In other cases, the origin can also be defined from an analysis of the positions of all features of interest, e.g. the mean value of all positions in the x-direction for a 1D grating. In the case of a 2D grating the origin can also be defined by a least squares regression fit over all measured x- and y-positions of all features of the 2D grating allowing translation of the origin and rotation of the whole 2D grating (so-called multi-point alignment). In these cases the origin of the feature coordinate system no longer corresponds to a particular feature.

Note 3 to entry: The origin can also be chosen as the position of a specified alignment feature or auxiliary feature within the reference plane.

Note 4 to entry: In case of angular gratings the feature coordinate system can favorably be defined as a polar coordinate system: r, φ or a cylindrical coordinate system: r, φ, z.

3.1.4
feature pattern
set of features, specified by number, type, and positions of features

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1 Numbers in square brackets refer to the Bibliography.

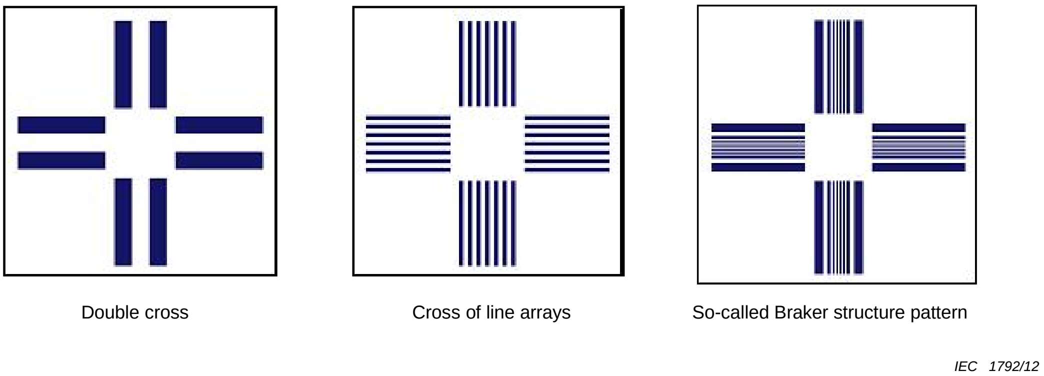


Figure 2 – Examples of feature patterns

EXAMPLE Figure 2 shows examples of different types of feature patterns.

Note 1 to entry: Different kinds of features can be arranged differently in a set to form feature patterns. These can be rather simple e.g. a single cross structure as a combination of two orthogonal line features, complex like, e.g. a double cross-structure or a line array or even more complex, e.g. irregularly spaced line features.

3.1.5
feature position

x_i, y_i, z_i

coordinates describing the position of a prescribed point of the i^{th} feature of a number *N* of features projected onto the reference plane relative to a specified coordinate system

Note 1 to entry: For 1D gratings the x-positions of the features are primarily of interest assuming the direction of the grating, i.e. the direction in which the number of grating features per unit length is maximal, is the x-direction, whereas for 2D gratings their x- and y-positions are of interest. In both cases, their z-positions are usually of minor interest, assuming the *reference plane* is already well aligned to the axes of the measurement instrument.

Note 2 to entry: Depending on the chosen criterion for the feature position evaluation (see Note 3), the measured feature position is dependent on the interaction of the measurement instrument used with the feature characteristics, like its shape, size and material properties.

Note 3 to entry: The determination of the feature position is often based on the analysis of a microscopic image of the feature. The microscope image signals can be analyzed in different ways to determine the feature position. Mostly the centre position of the feature is of interest which can be determined, e.g. by calculation of the centroid or by determination of the mean value between the position of the left and the right edge of the feature.

Note 4 to entry: If only parts of the feature are of interest, e.g. the edge position of a line feature, the determination of the position of the respective edge(s) should be based only on the parts of the feature that are of interest.

Note 5 to entry: The above definition for the feature position can also be applied to a feature pattern.

Note 6 to entry: If angular gratings are analyzed, it is favorable to express the feature position in polar coordinates *r, φ* or in cylindrical ones *r*, *φ*, *z.*

3.1.6
distance between features

d

difference of the feature positions determined on equivalent or homologous feature characteristics in the direction of interest

Note 1 to entry: The distance *d* between two consecutive features, *i* and *i*-1, in the x-direction is:

$$d = \text{abs}\,(x_i - x_{i-1})$$

Note 2 to entry: The distance *d* between two consecutive features in the reference x,y plane generally is:

$$d = [(x_i - x_{i-1})^2 + (y_i - y_{i-1})^2]^{0,5}$$

Note 3 to entry: The distance *d* between two consecutive features at the positions x_i, y_i, z_i and x_{i-1}, y_{i-1} z_{i-1} in the general case is:

$$d = [(x_i - x_{i-1})^2 + (y_i - y_{i-1})^2 + (z_i - z_{i-1})^2]^{0,5}$$

Note 4 to entry: Usually the distance between features is of interest for the centre positions of the features. In some cases however the distance can also be of interest for positions on the feature edges.

3.2 Grating terms

3.2.1
grating
periodically spaced collection of identical features

Note 1 to entry: In [3], which provides a vocabulary of diffractive optics, a grating is defined as a "periodic spatial structure for optical use" (3.3.1.2). In this technical specification, gratings are not restricted to optical use only.

Note 2 to entry: Often gratings show a ratio of the distance between neighboring identical features to their size that is close to one. However, the definition is not restricted to these cases and also includes so-called sparse gratings and thus in principle line scales, too.

Note 3 to entry: Although this technical specification is primarily addressing periodic gratings, the definition of grating quality parameters should also be applicable to non-periodic gratings, like chirped gratings (3.3.5.2) as far as possible. Limitations might occur in particular for spatial filtering approaches of feature position data.

Note 4 to entry: Sometimes a grating can be divided into several sub-gratings having different features.

3.2.2
pitch
p
distance between neighboring features of a grating

Note 1 to entry: Often, the feature centre positions are used to determine the pitch. In some cases, however, also the distance between equivalent edges of a pair of features is used to determine the pitch values.

Note 2 to entry: This definition is in alignment with the definition for pitch as specified in [1] (5.1.14).

3.2.3
nominal pitch
p_{nom}
intended pitch value, indicated in the specification of a grating

3.2.4
number of grating features
N_{f}
result of a summation over all identical features of the grating in the direction of interest

Note 1 to entry: The number of grating features can be different in the different directions for 2D and three-dimensional (3D) gratings. The total number of features in 2D and 3D gratings is the product of the number of grating features along the 2 or 3 different directions (e.g. dots in the case of 1D features).

3.2.5
mean pitch
p_{m}
average pitch value determined over all identical features of the grating

Note 1 to entry: The mean pitch is not necessarily the arithmetic mean pitch, but any statistically characteristic pitch.

Note 2 to entry: If all feature positions of the grating are known, the mean pitch of a grating can be determined by a linear least squares regression fit of all measured feature positions $x_{i,\,\mathrm{m}}$ to the nominal feature positions $x_{i,\,\mathrm{nom}}$. If the uncertainties of the measured feature positions are equal, a standard linear regression fit can be applied. In case of a variation of the uncertainties u_{xi} of the measured feature positions $x_{i,\,\mathrm{m}}$, a weighted linear regression fit should be applied, using the inverse variances as weights ($w_i = 1/(u_{xi})^2$). The resulting slope m of the regression line (yielding values for slope m and intercept b) can be used to calculate the mean pitch value $p_{\mathrm{m}} = m \cdot p_{\mathrm{nom}}$ taking into account the position information of all features of the grating.

Note 3 to entry: The mean pitch of a grating is often also called the period length or grating constant *Λ* of the grating.

Note 4 to entry: For an ideal grating, the values for the mean pitch, the local pitch and the pitch for all neighboring features are identical. For real gratings, however, the values would be different, depending on the quality of the grating and the different length ranges over which the local pitch value will be evaluated. In addition, the capability of measurement methods to determine the different pitch values on non-ideal gratings is different. The measurement methods, therefore, can be classified in different groups, see 3.5.

Note 5 to entry: If the boundary length of a grating L_b (3.2.8) and the number of grating features N_f (3.2.4) are known, an approximation to the mean pitch can be determined by the equation: $p_m = L_b / (N_f - 1)$; $N_f \geq 2$. The same pitch value results if the arithmetic mean value of all pitch values over all neighboring features is calculated. In the sum $\Sigma^{Nf-1}_{i=1} (x_{i+1} - x_i) / (N_f - 1)$ for calculation of the arithmetic mean value of all pitch values of a grating all feature position values x_i cancel out except for the first and last feature. In both cases the resulting approximation of the mean pitch value is based on the positions of the first and the last feature in the grating only and thus less representative of the whole grating than the mean pitch determined by a linear regression fit [4].

3.2.6
local pitch

$\boldsymbol{p_{loc} (x_c, l_r)}$

average pitch value determined over a defined length range l_r of a grating centered around a defined feature position x_c

EXAMPLE If a local pitch p_{loc} of a nominally 1 mm long 1D grating with 100 nm nominal pitch is evaluated around a central position at x_c = 400 µm over a length range l_r of 20 µm, the resulting local pitch should be expressed as: p_{loc} (400 µm, 20 µm) or p_{loc} (4001, 201) if expressed in number of features of the grating.

Note 1 to entry: The local pitch can also be defined over a specified number of features N_r centered around a specified feature with index N_c. In this case the notation for the local pitch is: $p_{loc} (N_c, N_r)$.

3.2.7
nominal length of grating

$\boldsymbol{L_{nom}}$

intended length of a grating, indicated in the specification of the grating

Note 1 to entry: The length of a grating is defined in the direction of the grating, i.e. the direction in which the number of grating features per unit length is maximal.

3.2.8
boundary length of grating

$\boldsymbol{L_b}$

distance between the first and the last feature of a grating

Note 1 to entry: The center to center distance is the default case.

3.2.9
characteristic length of grating

$\boldsymbol{L_c}$

length of a grating, based on the mean pitch and the number of grating features

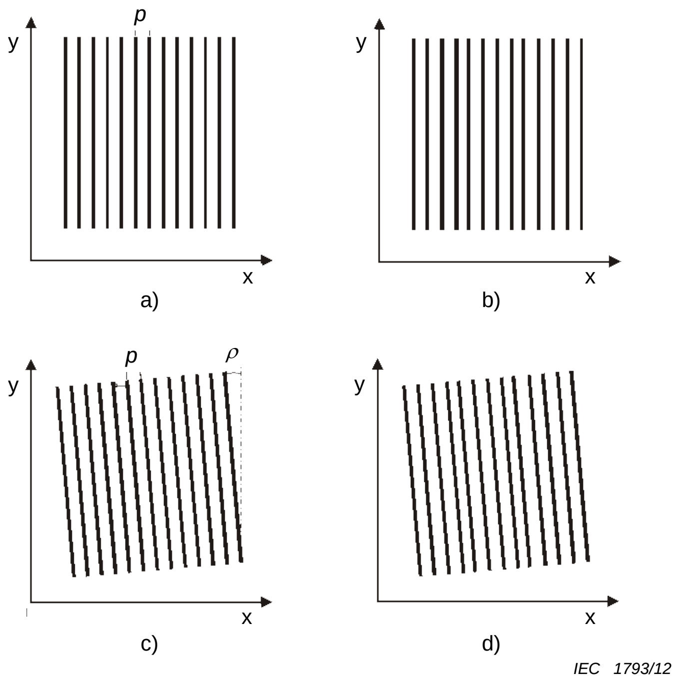
$$L_c = p_m \cdot (N_f - 1)$$

Note 1 to entry: For an ideal grating the nominal length, the boundary length and the characteristic length values of a grating are identical. For real gratings, however, they are different.

3.3 Grating types

3.3.1
1D grating

grating in which features are repeated in only one direction within the reference plane



Pitch *p* is defined in the direction of the grating.

a) ideal 1D grating;

b) 1D grating with local pitch variation;

c) ideal 1D grating with misalignment by angle ρ to the instrument axes x and y;

d) 1D grating with local pitch variation and misalignment to instrument axes.

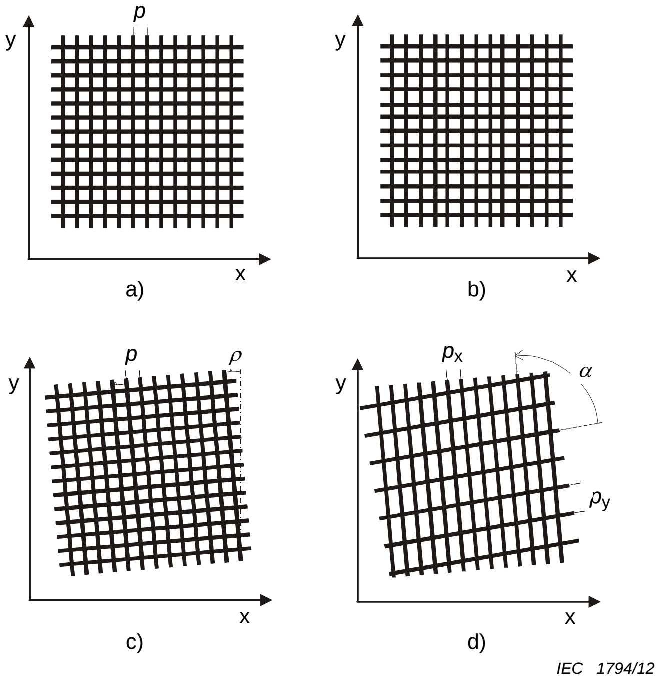
Figure 3 – Examples of 1D line gratings

EXAMPLE Figure 3 shows examples of 1D line gratings.

Note 1 to entry: 1D gratings are also denoted as one-dimensional gratings.

Note 2 to entry: According to the Note 2 to entry of 3.2.1 a line scale can be understood as a sparse 1D grating, too.

3.3.2
2D grating
grating in which features are repeated in two, non-parallel directions within the reference plane



Pitches p_x and p_y are defined in the directions of the grating:

a) ideal 2D grating;

b) 2D grating with local pitch variation in both directions;

c) ideal 2D grating with misalignment by angle ρ to the instrument axes x and y;

d) 2D grating with deviation from orthogonality ($\alpha \neq 90$ °), different pitch values and misalignment to instrument axes x and y.

Figure 4 – Example of 2D gratings

EXAMPLE Figure 4 shows examples of 2D gratings

Note 1 to entry: Often the two directions are nominally orthogonal to each other, e.g. along the x- and y-direction.

Note 2 to entry: 2D gratings are also denoted as two-dimensional gratings.

Note 3 to entry: The deviation from orthogonality of the 2D grating can be described as in 3.4.13 and [5].

3.3.3
3D grating
grating in which features are repeated in three, non-parallel directions, containing the reference plane

Note 1 to entry: Often the three directions are nominally orthogonal to each other, e.g. along the x-, y- and z-direction.

Note 2 to entry: 3D gratings are also denoted as three-dimensional gratings.

Note 3 to entry: An example of a 3D grating is a 3D photonic crystal.

3.3.4
angular grating
grating which extends along a circular direction within the reference plane

Note 1 to entry: In most cases the angular gratings extend over the full angular range of 2π rad (360 °), i.e. the first and the last feature of the angular grating are neighboring features.

Note 2 to entry: Angular gratings are also denoted as radial gratings.

3.3.5
complex grating
grating characterized by more than one nominal pitch value in the direction of interest

3.3.6
double pitch grating
complex grating characterized by two different nominal pitch values in the direction of interest

3.3.7
chirped grating
complex grating characterized by an intended, monotonic variation of pitch values in the direction of interest

Note 1 to entry: Monotonic variation means that the pitch values always increase, or decrease, along the direction of interest.

3.4 Grating quality parameter terms[2]

3.4.1
deviation in boundary length
$\boldsymbol{\delta L_b}$
difference between the measured boundary length and the nominal length

$$\delta L_b = L_{b,\,m} - L_{nom}$$

where

$L_{b,\,m}$ is the measured boundary length;

L_{nom} is the nominal length.

3.4.2
relative deviation in boundary length
$\boldsymbol{\delta L_{b,\,rel}}$
deviation in boundary length relative to the nominal length

$$\delta L_{b,\,rel} = \delta L_b / L_{nom}$$

3.4.3
deviation in characteristic length
$\boldsymbol{\delta L_c}$
difference between the measured characteristic length and the nominal length

$$\delta L_c = L_{c,\,m} - L_{nom}$$

where

$L_{c,\,m}$ is the measured characteristic length;

L_{nom} is the nominal length.

Note 1 to entry: The parameter deviation in characteristic length δL_c is a quality parameter of a grating. In some applications, however, the characteristic length L_c of a grating is only of secondary interest; δL_c is of minor importance in these cases.

3.4.4
relative deviation in characteristic length
$\boldsymbol{\delta L_{c,\,rel}}$
deviation in characteristic length relative to the nominal length

---

2 The definitions of grating deviations in 3.4 provide grating quality parameters, which can be determined for every type of grating. However, the impact of these grating quality parameters can be of varying importance for different applications.

$\delta L_{c,\,rel} = \delta L_c / L_{nom}$

3.4.5
deviation in feature position
δx_i
difference between the measured feature position and the nominal feature position, based on the nominal pitch

$\delta x_i = x_{i,\,m} - p_{nom} \cdot (i - 1)$

where

$x_{i,\,m}$ is the measured feature position of the i^{th} feature in a grating – oriented along the x-direction;

p_{nom} is the nominal pitch of the grating.

Note 1 to entry: This definition assumes a grating with one nominal pitch value. It can be extended, however, also to complex gratings, like e.g. chirped gratings, provided all the nominal feature positions are specified.

Note 2 to entry: If the orientation of the grating features is in other directions, the definition can be adapted accordingly, i.e. δy_i, δz_i.

Note 3 to entry: In case of angular gratings over 360 °, the sum over all deviations in angular feature positions $\delta\alpha_i$ always is zero because the circular angle 2π rad (360 °) is a natural, invariable and error-free angle standard. This fact is the basis of application of error separation techniques, which allow for determining the deviations in angular feature position of angular gratings with very small uncertainties in the nanoradian range [6].

3.4.6
relative deviation in feature position
$\delta x_{i,\,rel}$
deviation in feature position relative to the nominal feature position

$\delta x_{i,\,rel} = \delta x_i / (p_{nom} \cdot (i - 1))$

where

δx_i is the deviation in feature position of the i^{th} feature in a grating;

p_{nom} is the nominal pitch of the grating.

3.4.7
feature position deviation from linearity
$\delta x_{i,nl}$
difference between the measured feature position and the calculated feature position, based on the measured mean pitch

$\delta x_{i,\,nl} = x_{i,\,m} - (p_m \cdot (i - 1) + b)$

where

$x_{i,m}$ is the measured feature position of the i^{th} feature in a grating;

p_m is the measured mean pitch of the grating;

b is the intercept of a linear least squares regression line, determined according to 3.2.5, Note to entry 2.

Note 1 to entry: As a result of the mean pitch definition, the sum over all feature position deviation from linearity values of a grating is zero.

3.4.8
relative feature position deviation from linearity
$\delta x_{i,nl,\,rel}$
feature position deviation from linearity relative to the nominal feature position

$\delta x_{i,\,nl,\,rel} = \delta x_{i,\,nl} / (p_{nom} \cdot (i - 1))$

where

$\delta x_{i,\text{ nl}}$ is the feature position deviation from linearity of the i^{th} feature in a grating;

p_{nom} is the nominal pitch of the grating.

3.4.9
peak-to-valley deviation from linearity
$\delta L_{\text{nl,P-V}}$
difference of the maximum and the minimum value or range of the feature position deviations from linearity of all grating features

$$\delta L_{\text{nl, P-V}} = \delta x_{i,\text{nl, max}} - \delta x_{i,\text{nl, min}}$$

where

$\delta x_{i,\text{nl, max}}$ is the maximum of all feature position deviations from linearity;

$\delta x_{i,\text{nl, min}}$ is the minimum of all feature position deviations from linearity.

3.4.10
relative peak-to-valley deviation from linearity
$\delta L_{\text{nl,P-V, rel}}$
peak-to-valley deviation from linearity relative to the nominal length of a grating

$$\delta L_{\text{nl, P-V, rel}} = \delta L_{\text{nl, P-V}} / L_{\text{nom}}$$

where

$\delta L_{\text{nl, P-V}}$ is the peak-to-valley deviation from linearity;

L_{nom} is the nominal length of a grating.

3.4.11
rms deviation from linearity
$\delta L_{\text{nl, rms}}$
square root of the arithmetic mean of the squares of the feature position deviation from linearity over all N_{f} features of the grating

$$\delta L_{\text{nl, rms}} = [\Sigma^{\text{Nf}}_{i=1} (\delta x_{i,\text{nl}})^2 / N_{\text{f}}]^{0,5}$$

where

$\delta x_{i,\text{nl}}$ is the feature position deviation from linearity of the i^{th} feature in a grating;

N_{f} is the number of grating features.

3.4.12
relative rms deviation from linearity
$\delta L_{\text{nl, rms, rel}}$
rms deviation from linearity relative to the nominal length of a grating

$$\delta L_{\text{nl, rms, rel}} = \delta L_{\text{nl, rms}} / L_{\text{nom}}$$

where

$\delta L_{\text{nl, rms}}$ is the rms deviation from linearity over all features of the grating;

L_{nom} is the nominal length of a grating.

3.4.13
deviation from orthogonality
$\delta \alpha_{\text{ortho}}$
deviation from $\pi/2$ rad (90°) of the nominally orthogonal directions of 2D or 3D gratings

Note 1 to entry: The term squareness is often also used as a synonym for orthogonality.

3.4.14
filtered grating deviation terms
$\delta X_Y^F(\lambda_c, P)$
any grating deviation term as defined in 3.4, however determined on the basis of filtered values of the deviations in feature positions

$\delta X_Y^F(\lambda_c, \beta, P)$

where

- *X* is a general symbol to be replaced by one of the defined quantities in 3.4 for a particular case;
- *Y* is a general subscript symbol to be replaced by one of the defined indices in 3.4 for a particular case;
- *F* is a general superscript symbol to be replaced by a suitable term which unequivocally describes the characteristics of the filter algorithm applied for the analysis of the deviations in feature position of a grating;
- λ_c is a parameter which describes the critical filter length of the applied filter;
- β is an additional (optional) parameter to describe the filter characteristics;
- *P* is a parameter describing which spectral parts of the filtered data are to be analyzed. P can either be LP for low-pass, HP for high-pass or BP for band-pass data.

EXAMPLE 1 If the deviations in feature position δx_i of a grating are analyzed after an arbitrary filter algorithm F with wavelength λ_c and high-pass characteristic has been applied to the original data, the filtered deviations in feature position are denoted by $\delta x_i^F(\lambda_c, , \text{HP})$.

EXAMPLE 2 If the relative rms deviation from linearity$\delta L_{\text{nl, rms, rel}}$ of a grating is of interest in case a linear profile filter with Gaussian low-pass filter characteristics and an assumed cut-off wavelength of 80 nm is applied to the original data, the filtered relative rms deviation from linearity should e.g. be denoted as $\delta L_{\text{nl, rms, rel}}^{\text{FPLG}}$ (80 nm, , LP) (FPLG stands for Filter Profile Linear Gaussian).

Note 1 to entry: Clause 5 discusses the different classes of existing filter algorithms applicable to grating deviation terms in more detail.

3.5 Measurement method categories for grating characterization

3.5.1
global methods
GM
measurement methods which probe the grating of interest as a whole

Note 1 to entry: Examples of grating characterization methods which belong to the GM category are given in Clause 5 and in Clause A.2.

Note 2 to entry: Global methods sometimes are also called integral methods.

3.5.2
local methods
LM
measurement methods which probe the grating in a small region of interest only and which do not offer a sufficient displacement metrology capability to link the information from subsequent measurements of the grating phase-coherently

Note 1 to entry: Examples of grating characterization methods which belong to the LM category are given in Clause 5 and in Clause A.2.

3.5.3
hybrid methods
HM
measurement methods which probe the grating in a small region of interest and which in addition allow to link the information from subsequent measurements over the whole grating phase-coherently by use of suitable displacement metrology

Note 1 to entry: Examples of grating characterization methods which belong to the HM category are given in Clause 5 and in Clause A.2.

4 Symbols and abbreviated terms

AFM	atomic force microscopy
CCD	charge-coupled device
DOE	diffractive optical element
DUV	deep ultraviolet
EUV	extreme ultraviolet
GM	global method
GPS	geometrical product specifications
HM	hybrid method
HR-OM	high resolution optical microscopy
IR	infrared
LER	line edge roughness
LM	local method
LWR	line width roughness
OD	optical diffraction
OM	optical microscopy
SEM	scanning electron microscopy
SPM	scanning probe microscopy
TEM	transmission electron microscopy
Vis	visible spectrum

5 Grating calibration and quality characterization methods

5.1 Overview

Artificial gratings play an important role in the manufacturing as well as characterization of structures on the nanoscale. The use of the term nanoscale shall conform to ISO/TS 80004-1:2010, 2.1 where it is defined as "size range from approximately 1 nm to 100 nm". In this Clause 5 different categories of measurement methods for grating calibration and characterization of grating quality are given. Guidance is provided to choose a measurement method category which best fits the requirements set for the characterization in terms of global and local quality parameters of a particular grating.

5.2 Global methods

The category of global methods comprises measurement methods, which probe the grating of interest as a whole. All of the methods in this category are based on the use of electromagnetic radiation, mainly but not exclusively in the optical region, with a known wavelength to probe the whole grating. The measurement of the reflected, diffracted or transmitted light is then analyzed to extract information about the dimensional grating parameters. A short description of some global methods follows below.

In diffractometry the grating under test is illuminated by monochromatic light which extends over the size of the grating. The diffracted light is then analyzed with respect to the diffraction angle. Often, the diffracted light is measured in the Littrow configuration, i.e. the direction of the negative first order diffracted beam is parallel to the direction of the incoming beam and also more than one optical wavelength is used [7]. In most cases, the direction of the diffracted beam is measured by means of a rotary table and a photo detector or CCD device serves to measure the beam intensity. A diffractometer usually measures the diffraction angles of the diffracted beams only, from which the mean pitch of a grating can be determined with very small uncertainty. However, it usually does not provide information about local pitch variations of the grating. The radiation bandwidth and the lack of full spatial and temporal coherence of lasers are to be given due consideration in the diffractometry results.

In scatterometry, the intensity and polarization of optical radiation diffracted by a grating, sometimes in addition to the diffraction angles (as in diffractometry), is measured, and used to extract information about the geometrical characteristics of the grating as well as the optical material properties of the grating [8]. Different types of scatterometers exist, namely those with variation of wavelength of the incoming radiation only but no variations between the directions of incoming beam and detector (spectral scatterometry), those with measurement of diffracted intensities at different diffraction angles for monochromatic incoming radiation only (goniometric scatterometry) or a combination of both [9]. Scatterometry measurements which do not probe the non-specularly diffracted radiation have substantially reduced sensitivity to a grating's pitch in exchange for high sensitivity to feature dimensions. Scatterometry is applied in different parts of the wavelength spectrum, from IR over Vis to DUV and EUV and thus allows one to analyze a broad spectrum of different gratings with largely varying pitch values.

To make full use of the information measured by scatterometry the measurement results are usually backed up by appropriate simulations of the diffraction spectra by means of rigorous optical diffraction calculations. In this way, the measured spectra can be compared with simulated spectra, which are calculated for some model geometries of the grating topography. By variation of model parameters a close correlation with the measured spectra can be obtained. In addition to the mean pitch of the grating, also variations of the pitch values over the grating can be inferred along with information about the mean height, width and sidewall angle of the grating features [10].

Another example of a global measurement method for grating characterization is the use of Fizeau interferometry with the grating being arranged in Littrow configuration [11]. In this configuration, the interferometer is sensitive to the wavefront distortions caused by the pitch variations of the grating within the aperture, thus the local pitch variation of the grating can be determined by this method.

The common advantage of the global methods is that they allow measurements to be performed over the whole grating quickly. It is possible to obtain very small uncertainties for the determination of the mean pitch with a comparatively simple optical setup (diffractometry). Other optical configurations allow for determining local pitch variations in case these variations occur over length ranges which are larger than the lateral resolution of the setup (Fizeau interferometer). To determine a larger set of dimensional parameters of interest of a grating (pitch, pitch variation and in addition height, width, sidewall angle of features) from the analysis of the measured diffraction signal from the grating in a dedicated (scatterometer) setup requires the application of complex rigorous optical modeling approaches.

5.3 Local methods

The category of local methods comprises measurement methods, which allow a small region of the grating to be probed and which do not offer a sufficient displacement metrology capability to link the phase information from subsequent measurements of the grating signal coherently. In order to determine the phase difference of the periodic grating signals measured in subsequent images taken at two different sites of a grating, the relative displacement of the grating sample to the microscope in between the two images has to be determined with high precision (phase-coherent link).

Examples of local methods are all types of high resolution microscopy methods, which image a part of a grating within the field of view defined by the chosen magnification of the microscope. Typical microscopy methods applied for the characterization of gratings include SPM including AFM, SEM, TEM, and OM.

Within the field of view, the local methods are able to measure the local pitch of the grating and also possible pitch variations. To determine the mean pitch of the grating and to estimate the variation of the local pitch over the whole grating using local methods, repeated measurements at different locations of the grating have to be carried out using the microscope.

A common advantage of the local methods is that they provide information on individual feature qualities like feature parallelism, line edge roughness and defects as well as the local pitch within the field of view. Due to the limited field of view, the measurement uncertainty of the local methods for the mean pitch usually is larger in comparison to the global methods. Also the measurement speed for a complete characterization of gratings is relatively low, in particular for the SPM methods.

5.4 Hybrid methods

The category of hybrid methods comprises measurement methods which probe the grating in a small region of interest and which in addition link the information from subsequent measurements over the whole grating in a phase-coherent way by use of suitable displacement metrology.

Like the local methods, the hybrid methods are characterized by application of high resolution microscopy for measurements on individual grating features, but are combined with a high accuracy positioning system that enables to determine the displacements of the grating between subsequent positioning, and imaging steps with an accuracy that allows a phase-coherent stitching of the grating intensity signals in the different fields of view.

In this sense, the hybrid methods combine the advantages of the local methods (ability to characterize individual feature quality) and the global methods (determination of the mean pitch over the whole grating with small uncertainties). They also have the capability to detect phase jumps in the periodicity of the grating. However, the hybrid methods require high accuracy positioning and displacement metrology systems in addition to high resolution microscopes.

An example of a hybrid system based on an SEM and a laser-controlled positioning stage which was used for characterization of a 2D grating with 100 nm nominal pitch is given in [12] and is also discussed in Clause A.2. In reference [13] the calibration of the mean pitch and the linearity deviations of two gratings with a ratio of nominal pitch values of 1:4 by a hybrid calibration method and their application to serve as a 1:4 magnification standard for lithography lenses are described. The results of a bilateral comparison on a grating standard with nominally 25 nm pitch by means of hybrid methods, in this case so-called metrological SPM, are given in reference [14]. It should also be mentioned here that calibrations of line scales are also based on the application of hybrid methods.

5.5 Comparison of methods

Table 1 shows a compilation of the characteristics of the different measurement methods and categories for grating calibration and grating characterization. This table in combination with the descriptions given in 5.2 to 5.4, information in the references and Clause A.2 provide guidance in choosing a suitable characterization method or set of characterization methods for a specified set of requirements for the qualification of a grating.

Table 1 – Comparison of different categories for grating characterization methods

Method category	Method type	Ability to measure mean pitch with small uncertainty	Ability to measure local pitch variation	Ability to measure feature dimen-sions on individual features	Ability to measure feature dimen-sions on grating features	Meas. speed	Complexity of measurement setup and measurement effort	Complexity of data analysis
Global methods	Diffractometry	++	--	--	--	++	low	medium
Global methods	Scatterometry: – goniometric – spectral	 ++ o	 + -	 -- --	 ++ ++	 + ++	 high medium	 very high very high
Global methods	Fizeau inter-ferometry in Littrow config-uration	o	+	-		++	high	medium
Local methods	Optical mi-croscopy	-	+	+	+	o	low	low
Local methods	SPM	-	++	++	++	-	medium	medium
Local methods	SEM	-	++	++	+	o	high	medium
Local methods	TEM	--	++	++	++	--	very high	high
Hybrid methods	Based on HR-OM, SEM, SPM, TEM	++	++	++	++	 o - --	very high	high

Symbol legend:

++ very good;

\+ good;

o satisfactory;

\- poor;

-- insufficient

5.6 Other deviations of grating features

5.6.1 General

In the definitions of grating deviation terms in Clause 3 it was assumed that the grating features only showed deviations from their nominal positions in the direction of the grating. Other parameters which also influence the grating quality and limit the measurement uncertainty of gratings are listed below. In this technical specification, these additional influences are just mentioned but not discussed and analyzed in detail.

5.6.2 Out of axis deviations

5.6.2.1 General

These are deviations which extend perpendicular to the direction of the grating. If, for example, the intended direction of a 1D grating is the x-direction, the out of axis deviations are in y-direction.

5.6.2.2 Non-parallel line features

If the line features are not parallel over the entire grating, there will be a dependence of the measurement results for the deviations in feature position on the chosen measurement area along the lines. If the deviations from the parallel orientation of the line features change over the grating, these deviations will result in an increased variation of local pitch values.

5.6.2.3 Curved line features

If the line features are curved over the entire grating, there will be a dependence of the measurement results for the deviations in feature position on the chosen measurement area along the lines. If the deviations from the ideal shape of the line features change over the grating, these deviations will result in an increased variation of local pitch values.

5.6.3 Out of plane deviations

5.6.3.1 General

These are deviations which extend perpendicular to the plane of the grating. If, for example, the intended orientation of a 1D or 2D grating is in the x-y plane, the out of plane deviations are in the z-direction, perpendicular to the x-y plane.

5.6.3.2 Topography of the features

A change of the height of the features over the grating might have only a minor influence on the grating quality parameters defined in Clause 3. However, the influence of height variations has to be analyzed individually for the different measurement methods applied for grating characterization.

5.6.3.3 Topography of the substrate

Effects of topography changes $z(x,y)$ on measured deviations in feature position, e.g. due to the bending of a kinematically mounted substrate by gravity forces are well-known from line scale metrology, see e.g. [15]. These substrate bending effects also have to be taken into account properly for analysis of the measurement results of linear and angular encoders.

5.6.4 Other feature deviations

5.6.4.1 General

In this subclause 5.6.4 the remaining influences on grating quality and measurement uncertainty of grating parameters due to size, shape and material variations of the features are discussed.

5.6.4.2 Line edge roughness and line width roughness

Line edge roughness (LER) describes the deviations of a line feature contour from an ideal straight line. Line width roughness (LWR) describes the deviations of the local widths of a line feature from an ideal constant value. For decreasing line feature widths, the relative importance of LER and LWR is increasing and becomes a major issue for further progress in lithography [16]. Both effects result in a dependence of the measurement results for the deviations in feature position on the chosen measurement area along the lines and in addition in an increased variation of local pitch values.

5.6.4.3 Changing material properties

Changing material properties of the grating features or of the substrate will affect the measurement results for the feature position and the mean pitch. However, the magnitude of this influence is dependent on the measurement technique used for characterization of the grating and can thus not be estimated in a general way.

5.7 Filter algorithms for grating quality characterization

For the characterization of the quality of gratings it is often necessary to apply suitable filter algorithms to the original measurement data of feature position deviations. For example one might be primarily interested in the high frequency variations (small spatial wavelength) of the feature position deviations for one application, whereas in another application the position deviations with larger spatial wavelengths might be of interest, while the higher frequency deviations could be efficiently suppressed by a filter with low-pass characteristics.

Standardized filter algorithms for the evaluation of deviations in feature positions of artificial gratings do not yet exist. The evaluation of measurement data of feature position deviations shows some similarities to the analysis of surface texture profile data. In surface texture metrology, a series of documents on filtration of areal (3D) as well as profile (2D) surface texture data already exists and will be developed further. ISO/TS 16610-1:2006 [17] provides guidance on the series of documents on filtration and classification of different filter algorithms. In reference [18] an overview on the historical developments as well as recent trends of filtration within the GPS framework of ISO standards is given. If profile filter algorithms from the field of surface texture are applied to the analysis of feature position deviations, their designation should follow those specified in ISO/TS 16610-1:2006.

It has not yet been fully investigated which of the standardized profile filters of surface texture metrology (linear filters (Gaussian, spline, spline wavelet), morphological filters and robust filters) can also be applied for the analysis of deviations in feature positions of artificial gratings in a meaningful way. Moreover, profile filter algorithms developed for purposes other than surface texture metrology could in principle also be applied for the analysis of feature positions of artificial gratings.

An example of a simple moving average phase-correct filter to remove the waviness in a profile of position deviation data is given in [4]. In reference [19] a multipoint linear error compensation scheme is described, which allows the impact of encoder errors in position control applications to be reduced. In Clause A.2 examples of measured grating feature position deviations are shown, which have been evaluated by application of a spline filter.

For the evaluation of data of the feature positions of artificial gratings the applied filter algorithms should offer the following capabilities: no sensitivity to end effects (in case the whole grating has to be analyzed), determination of spectral content of data in terms of characteristic wavelengths or wavelength bands (high-pass, band-pass, low-pass filter), phase-correct filtering, sensitivity to detect phase jumps in the position data, robustness to outliers, applicability for feature position deviations at the nanoscale, ability to be applied also on complex gratings.

NOTE Phase jumps can occur if the grating was manufactured by a sequential method, which is based on repositioning of the substrate and subsequent stitching of writing areas on the substrate. Phase jumps are difficult to detect, but can be critical for the application of the grating.

6 Reporting of grating characterization results

6.1 General

The reporting of the results of the characterizations of artificial gratings shall conform with ISO/IEC 17025. This standard also defines general requirements for an adequate documentation of the results of a calibration.

In addition to necessary information about the name and address of the calibration laboratory as well as the client, the date of receipt of the specimen, the date(s) of the calibration and the issue of report, the calibration report shall also provide sufficient information about specimen details, the calibration procedure (instrument details, operating conditions, software used, validation), and the measurement results including their uncertainties. In the following, the last requirements are exemplified by the characterization of artificial gratings and the determination of their quality parameters.

6.2 Grating specifications

The calibration report should contain the necessary information about the grating to be characterized:

- manufacturer of the grating (if available);
- type of the grating (1D, 2D, 3D, angular, complex);
- nominal pitch(es) of the grating p_{nom};
- nominal length(s) of the grating L_{nom};
- type (line, square, dot, etc.), material, nominal width and height of the grating features;
- substrate material of the grating;
- any alignment features to be used for orientation of the grating.

6.3 Calibration procedure

The calibration report should contain the necessary information about the measurement instrument and procedure used for characterization of the grating:

- measurement category (GM, LM, HM);
- description of measurement instrumentation used for calibration;
- traceability of the measurement;
- calibration procedure (description, number of repeat measurements, etc.);
- operating conditions.

6.4 Grating quality parameters

The calibration report should contain the necessary information about the measurement results of the grating quality parameters and their uncertainties. It shall be clarified between the client and the calibration laboratory beforehand which of the grating quality parameters defined in 3.4 are of importance for the application of the grating by the client and thus have to be determined. The following list compiles some of the grating quality parameters:

- measured mean pitch p_m (optional: measured local pitch values p_{loc});
- deviation in boundary length δL_b;
- deviation in characteristic length δL_c:
- peak-to-valley deviation from linearity $\delta L_{nl,P-V}$;
- rms deviation from linearity $\delta L_{nl, rms}$;
- relative deviations of the quality parameters, i.e. deviations in relation to L_{nom};
- filtered quality parameters.

Annex A
(informative)

Background information and examples

A.1 Background information on length traceability at the nanoscale

Nanotechnology covers a broad spectrum of different applications at the nanoscale. The term nanoscale itself is defined in ISO/TS 80004-1:2010, 2.1 as the "size range from approximately 1 nm to 100 nm", i.e. it refers to the SI unit of length.

Since 1983, the SI unit of length, the meter, is defined as the length of the path travelled by light in vacuum during a time interval of 1/299 792 458 of a second. It follows that the speed of light is exactly 299 792 458 m/s and that the unit of length depends on the unit of time, the second.

There are different possibilities for the realization of the unit of length on the basis of this definition. Two methods are applied for this purpose:

a) measurement of the travelling time of light or other type of electromagnetic radiation, a method which is mainly applied for measurement over longer distances, e.g. in geodesy, astronomy or satellite based navigation systems; and
b) use of interferometric techniques with known laser radiation (e.g. nominal 633 nm for the HeNe laser), which realizes a length measurement based on the analysis of the intensity modulation of the interferometer signals which in turn depends on the wavelength of light in the chosen environment of the interferometer.

The latter method thus offers a very direct way of traceability to the definition of the length unit with corresponding small uncertainties and is therefore widely used in different measurement and production machines. Different laser radiations are recommended for the realization of the meter, as described in the Mise en pratique [20].

However, the variation of the laser wavelength with the parameters of air, like temperature, pressure, humidity and residual gas composition can be disadvantageous, if the smallest uncertainties for length measurements under ambient conditions are required. In addition, the cost of laser interferometer equipment also has to be taken into account. It can thus be explained that alternative approaches for length metrology are also followed, and these are often based on the use of artificial or natural gratings, which – if calibrated – serve as length standards or material measures of length.

In [3] a grating is defined as a "periodic spatial structure for optical use" and serves as a basic component of different types of diffractive optical elements (DOE), which use diffraction of optical radiation as their operating principle. Different realizations of DOE are addressed by the definitions of amplitude DOE, phase DOE, transmission DOE, reflection DOE and active DOE. An example of a technical realization of an active DOE is an acousto-optical modulator, in which acoustic standing waves generate features within the material which diffract incoming light in a defined way. Throughout this technical specification, however, gratings are not restricted to optical use only.

Artificial gratings play an important role in the manufacturing as well as the characterization processes of structures on the nanoscale. For example, in high volume manufacturing of semiconductor integrated circuits by means of lithography techniques, grating structures are used for alignment purposes of photomask to silicon wafer in the different lithographic production steps in the wafer-scanner production tools. Here double patterning lithography currently puts new requirements on grating and feature placement characterization methods. The smallest structure size on the wafer today is already below 30 nm and overlay tolerances of a few nanometers have to be achieved during manufacturing of integrated circuits.

Another field of application for artificial gratings in nanotechnology is their use as the calibration standards for high resolution microscopy techniques, which are necessary tools for characterization of structures at the nanoscale. Here the manufacturing and characterization of high quality grating calibration standards with sub-100 nm pitch are current challenges. There are already several normative documents published or under development that describe the use of grating based physical standards for calibration of image magnification of different types of high resolution microscopes like TEM in [21], SEM in [22], SPM in [23] or optical microscopy in [24].

However, in all of the above-mentioned documents [21], [22], [23] and [24], the grating standards are assumed to be ideal in the sense that possible deviations of the grating structures from their nominal values are not taken into account. In Clause 5 different types of instruments for grating calibration and determination of deviations in feature positions are categorized and described. Moreover, guidance is given to assist in the selection process of a measurement category in alignment with the grating quality requirements set for a particular application of a grating.

In addition to artificial gratings also natural crystal lattices can be used as length standards in nanotechnology, provided the measurement method allows resolving the lattice structure, like e.g. transmission electron microscopy or x-ray diffraction. Due to its good availability and high purity, the silicon single crystal material plays an important role in nanometrology. The distance between Si atomic lattice planes is in the sub-nm range ($d_{220} \approx 0{,}192$ nm) [25] and from this it follows that the Si atomic lattice is an interesting, intrinsic reference for length metrology at the nanoscale. It has been frequently used, for example, as a magnification standard for high resolution TEM images.

Surface and volume natural crystalline lattices are well-defined structures and have been dealt with in crystallography, solid state physics and surface science for many decades, see Annex B for an overview on 2D and 3D Bravais lattices. In the context of this technical specification, crystal lattices may be considered as natural gratings in contrast to the artificial gratings. Moreover, artificial gratings which would not show any deviations from the feature positions from their nominal values could be described with the terminology developed for crystal lattices.

In incremental length or angle encoder measurement systems, artificial linear or angular gratings are used as references for translational or rotational relative motions. The readout of the encoder systems depends on the details of the optical design, but in general the length information is deduced from the signals of the reading heads, which are based on the period length of the artificial grating structures. These types of measurement systems sometimes are also called “grating interferometers”. An example of a “grating interferometer” which makes use of a natural grating is the so-called x-ray interferometer, which analyses the variations of x-ray intensity signals when an x-ray is diffracted at a system of two fixed and one moveable thin lamella in a special kind of interferometer made of single crystal material, like e.g. silicon. [26]

It is instructive to compare the grating structures of magnification standards and of length encoder systems with classical length standards based on graduations, i.e. line scales. Line scales have traditionally been used as length standards and they still play an important role in the metrological infrastructure of today. There are nowadays outdated normative documents for line scales that explicitly deal with the deviations of the positions of graduation lines [27] (in German: Teilungsfehler).

In legal metrology there is the recommendation OIML R 98 which deals with specifications and classification of high-precision line measures of length [28]. For the accuracy classes 0 to 3 maximum permissible manufacturing errors for the distances between any two marks of a line measure are specified in µm between ± (0,5 + 0,5 L) and ± (5 + 5 L), where L is the numerical value of the nominal length of the interval between those two marks in meters. Line measures of class M (metrological class) are measures of high stability for which the manufacturing errors are not specified but are measured and indicated in a certificate.

Under the auspices of the CCL, the Consultative Committee for Length of the CIPM (Comité international de poids et mesures, International Committee for Weights and Measures), international comparisons on 1D gratings [29] as well as 2D gratings [5] and high precision graduated line scales of 280 mm length [30] were performed in recent years. These first series of international comparisons in the field of dimensional nanometrology provided valuable information on the existing measurement capabilities of the National Metrology Institutes (NMIs) to support the emerging field of nanotechnologies.

A.2 Examples of application and characterization of artificial gratings in nanotechnology

Artificial gratings are used in several applications in the field of nanotechnology. In some of these applications, the total length of the grating has to be close to the nominal total length value, especially when these gratings serve as length material standards as in length encoder systems or magnification standards for high resolution microscopy methods. In other fields of application, the total length is of secondary interest, but the nonlinearity deviations should be as small as possible, as determined on all (filter) length scales of interest.

Example 1: Grating based length encoder system (L_{nom} = 280 mm)

An example of an artificial grating used as a length material standard is shown below. In Figure A.1 one measurement result of a measurement comparison of three partners using vacuum length comparators on a length encoder system which was used as a transfer standard is shown [31]. The transfer standard consists of a 1D (phase) grating with nominally 512 nm pitch and 256 nm feature line width which extends over 280 mm on a Zerodur substrate. An interferometric reading head is moved relatively over the grating and offers an optical resolution of displacement measurement of 128 nm, which – after electronic interpolation by a factor of 4 096 – provides a displacement measurement resolution of about 30 pm. Such type of high resolution length encoder systems are widely used in different high precision manufacturing processes for axes position feedback, including applications in manufacturing on the nanoscale.

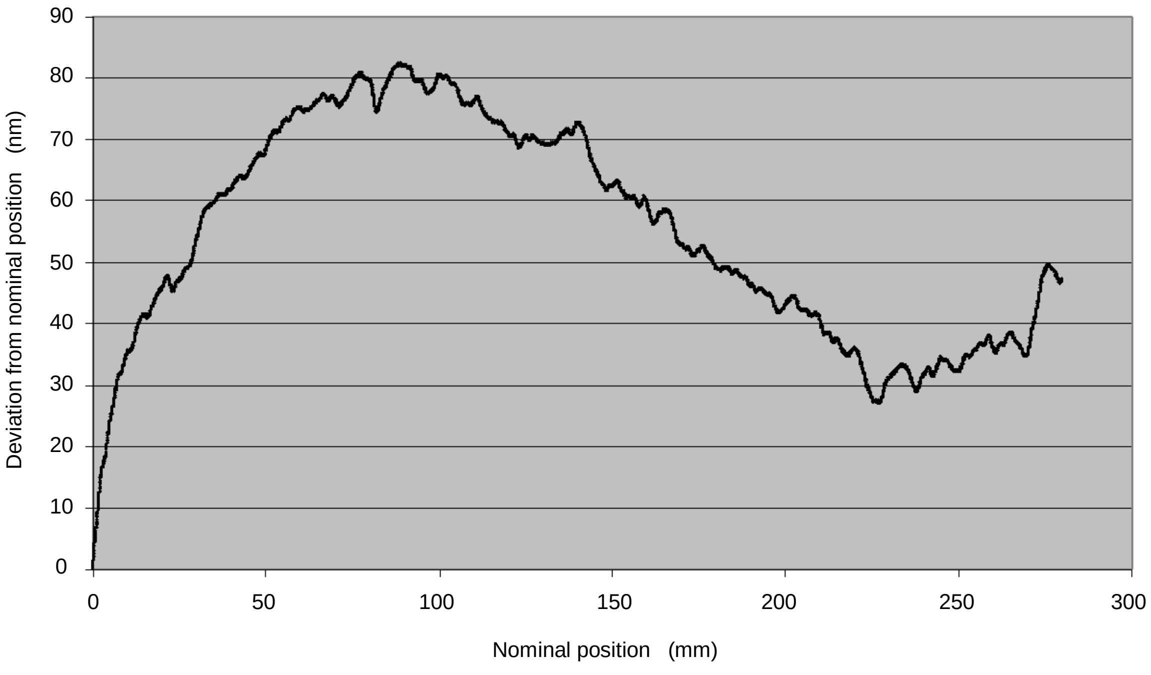


Figure A.1 – Result of a calibration of a 280 mm length encoder system which was used as a transfer standard in an international comparison [31]

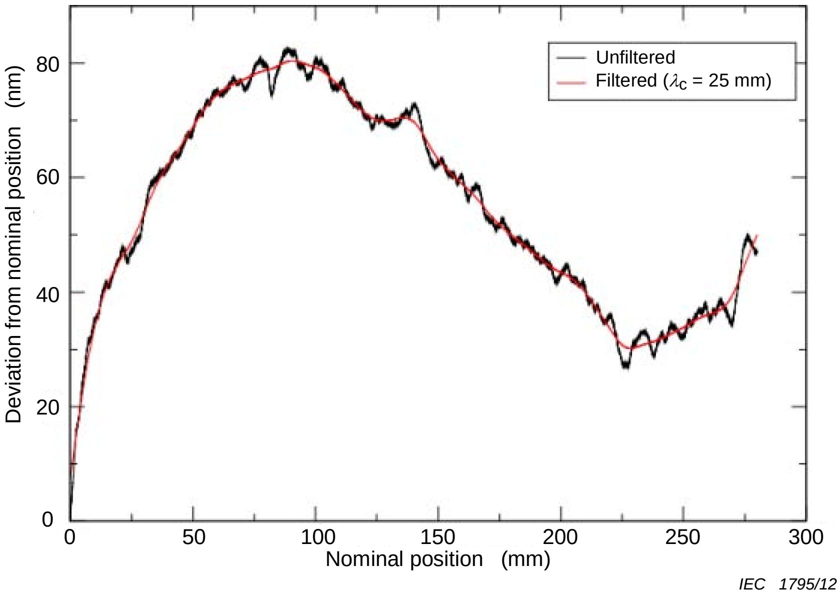


Figure A.2 – Filtered (linear profile Spline filter with λ_c = 25 mm) results of Figure A.1

An analysis of the data in Figure A.1 and A.2 with respect to the determined quality parameters of the grating is given in Table A.1. The high-pass filtered data (unfiltered data – low-pass filtered data) are analyzed for the linearity deviation quality parameters only.

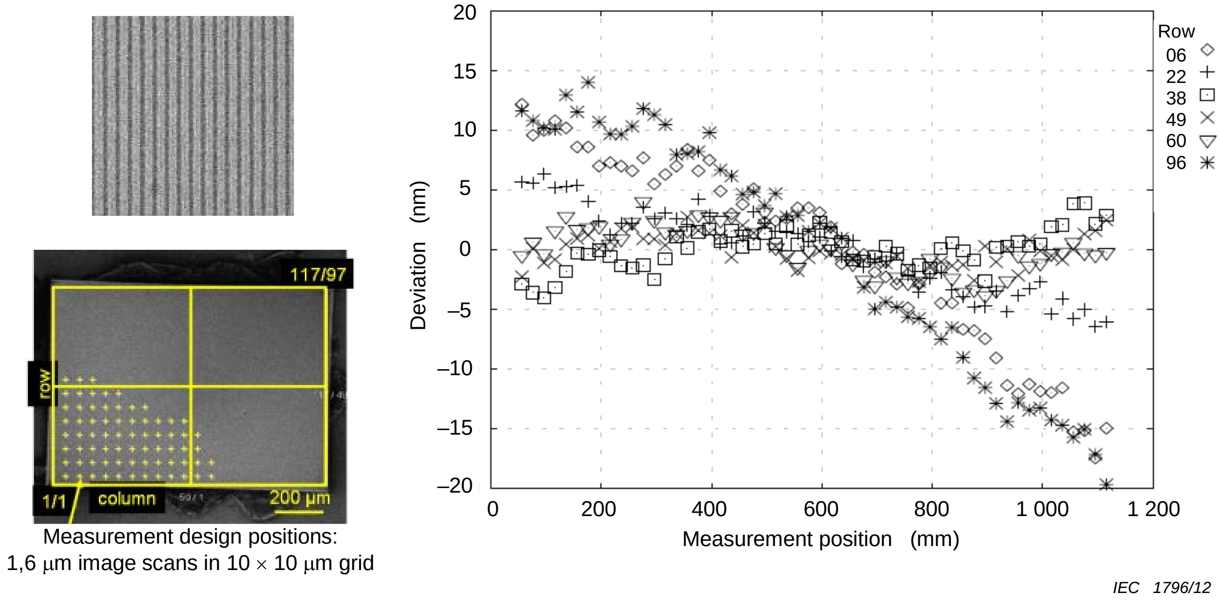
Table A.1 – Grating quality parameters of the grating in Figures A.1 and A.2

Grating quality parameters: **Grating from Figure A.1 with L_{nom} = 280 mm and p_{nom} = 512 nm**	**Measurement results (unfiltered)**	**Measurement uncertainties (*k* = 2)**	**Measurement results (filtered: Spline (25 mm, β = *0*, LP)**	**Measurement uncertainties (*k* = 2)**	**Measurement results (filtered: Spline (25 mm, β = *0*, HP)**	**Measurement uncertainties (*k* = 2)**
Measured mean pitch p_m (in nm)	511,999 95	0,000 01	511,999 95	0,000 01		
Deviation in boundary length δL_b (in nm)	47	5	43	5		
Relative deviation in boundary length $\delta L_{b, rel}$	$1{,}7 \cdot 10^{-7}$	$1{,}8 \cdot 10^{-8}$	$1{,}5 \cdot 10^{-7}$	$1{,}8 \cdot 10^{-8}$		
Deviation in characteristic length δL_c (in nm)	-28	5	-28	5		
Relative deviation in characteristic length $\delta L_{c, rel}$	$-1{,}0 \cdot 10^{-7}$	$1{,}8 \cdot 10^{-8}$	$-1{,}0 \cdot 10^{-7}$	$1{,}8 \cdot 10^{-8}$		
Peak-to-valley deviation from linearity $\delta L_{nl,P-V}$ (in nm)	91	4	82	4	4	4

Grating quality parameters: **Grating from Figure A.1 with L_{nom} = 280 mm and p_{nom} = 512 nm**	**Measurement results (unfiltered)**	**Measurement uncertainties (*k* = 2)**	**Measurement results (filtered: Spline (25 mm, β = *0*, LP)**	**Measurement uncertainties (*k* = 2)**	**Measurement results (filtered: Spline (25 mm, β = *0*, HP)**	**Measurement uncertainties (*k* = 2)**
Relative peak-to-valley deviation from linearity $\delta L_{nl,P\text{-}V,\ rel}$	$3{,}3 \cdot 10^{-7}$	$1{,}4 \cdot 10^{-8}$	$2{,}9 \cdot 10^{-7}$	$1{,}4 \cdot 10^{-8}$	$1{,}4 \cdot 10^{-8}$	$1{,}4 \cdot 10^{-8}$
rms deviation from linearity $\delta L_{nl,\ rms}$ (in nm)	16	4	16	4	0,4	4
Relative rms deviation from linearity $\delta L_{nl,\ rms,\ rel}$	$5{,}6 \cdot 10^{-8}$	$1{,}4 \cdot 10^{-8}$	$5{,}6 \cdot 10^{-8}$	$1{,}4 \cdot 10^{-8}$	$1{,}4 \cdot 10^{-9}$	$1{,}4 \cdot 10^{-8}$

Example 2: 1D grating over > 1 mm (p_{nom} = 100 mm)

This example and the following one cover the characterization and use of fine 1D- and 2D-gratings as magnification standards in high resolution microscopy. Figure A.3 shows the principle of the measurement approach as well as the measurement results on a 1D grating with nominally 100 nm pitch, which extends over an area of about 1 mm on a silicon chip. This sample has been calibrated on a metrological SEM with an integrated 2D laser-controlled stage [12]. The measurement strategy was to image parts of the grating in fields of view of about 1,6 µm to determine the local phase of the grating from the image signal and then to move the sample in defined steps – controlled by the laser interferometer – to a subsequent position where again the local phase of the grating signal was analyzed from the recorded SEM image. By combination of the laser interferometer signal and the local phase information of the grating, the whole grating could be characterized over the full 1 mm square area of the sample by this hybrid measurement method, see 5.4.



NOTE Results of a calibration of a 1D grating of about 1 mm size with nominally 100 nm pitch by a metrological SEM using combined information from the laser interferometer of the sample positioning stage and the local phase information of the grating from the SEM images. Shown are the measured deviations from mean pitch (99,947 nm) as a function of the position for different horizontal measurement rows. For further details see [12].

Figure A.3 – Calibration of a 1D grating by a metrological SEM

An analysis of the data in Figure A.3 with respect to the quality parameters of the grating is given in Table A.2.

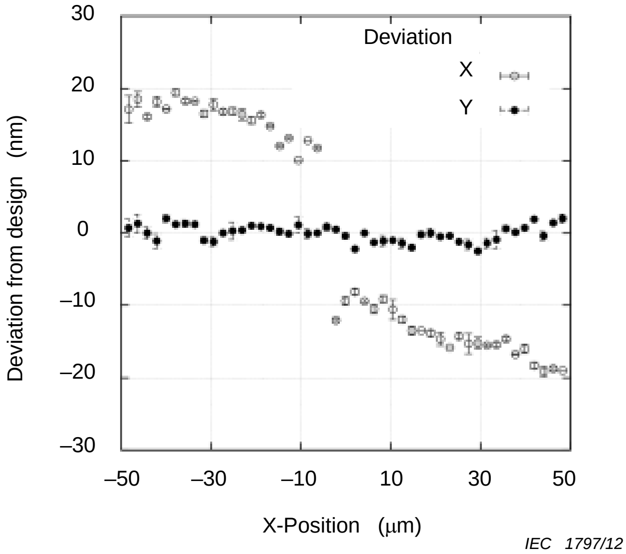
Table A.2 – Grating quality parameters of the grating in Figure A.3

Grating quality parameters: Grating from Figure A.3 (row 38) with L_{nom} = 1,16 mm and p_{nom} = 100 nm	**Measurement results (unfiltered)**	**Measurement uncer-tainties (k = 2)**
Measured mean pitch p_m (in nm)	99,947	0,001
Deviation in boundary length δL_b (in nm)	-609	10
Relative deviation in boundary length $\delta L_{b, rel}$	$5{,}25 \cdot 10^{-4}$	$8{,}6 \cdot 10^{-6}$
Deviation in characteristic length δL_c (in nm)	-612	10
Relative deviation in characteristic length $\delta L_{c, rel}$	$5{,}27 \cdot 10^{-4}$	$8{,}6 \cdot 10^{-6}$
Peak-to-valley deviation from linearity $\delta L_{nl,P-V}$ (in nm)	8	2
Relative peak-to-valley deviation from linearity $\delta L_{nl,P-V, rel}$	$6{,}9 \cdot 10^{-6}$	$1{,}7 \cdot 10^{-6}$
rms deviation from linearity $\delta L_{nl, rms}$ (in nm)	1,8	2
Relative rms deviation from linearity $\delta L_{nl, rms, rel}$	$1{,}6 \cdot 10^{-6}$	$1{,}7 \cdot 10^{-6}$

A similar approach for characterization of gratings by a combination of a laser interferometer controlled sample positioning stage and application of a high resolution SPM for local phase tracking of grating structures has been described in [4, 32]. The instrument used in this case is called large-range metrological SPM, because it offers a measurement range of 25 mm × 25 mm × 5 mm and thus also allows for the characterization of larger gratings.

Example 3: 2D grating over < 100 μm (p_{nom} = 300 mm)

Figure A.4 shows an example of a grating standard, which suffers from a so-called “phase jump” in the middle of the 100 μm wide quality area. These phase jumps can occur in sequential writing and field stitching manufacturing processes. While in some application fields, these deviations might be acceptable, they are critical in others and have to be avoided.



NOTE Results of a calibration of pitch (X) and straightness (Y) deviations on a 2D grating with nominally 300 nm pitch by a metrological SEM using combined information from the laser interferometer of the sample positioning stage and the local phase information of the grating from the SEM images For further details see [33].

Figure A.4 – Calibration of pitch and straightness deviations on a 2D grating by a metrological SEM

For example, the 2D standards shown in Figure A.4 could be used as calibration standards for image magnification in high resolution microscopes. Depending on the calibration approach, the phase jump region can be covered or missed by the calibration method, which would result in different measurement uncertainties of the mean pitch value of the standard. In the same way, the phase jump region can – by chance – be captured or left out by the calibration method of the user.

An analysis of the data shown in Figure A.4 with respect to the quality parameters of the grating for the measured deviations in x-direction (pitch) is given in Table A.3.

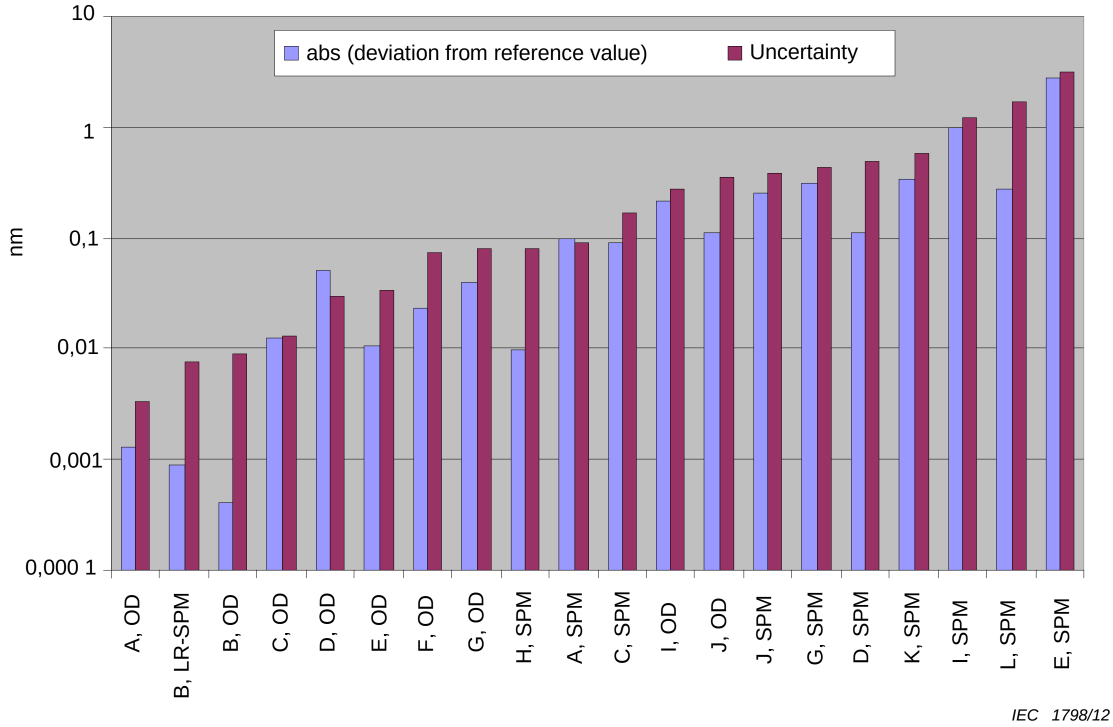
Table A.3 – Grating quality parameters of the grating in Figure A.4

Grating quality parameters: Grating from Figure A.4 (x-deviation) with L_{nom} = 99 µm and p_{nom} = 300 nm	Measurement results (unfiltered)	Measurement uncertainties (k = 2)
Measured mean pitch p_m (in nm)	299,86	0,02
Local pitch p_{loc} (-25,3 µm, 48,4 µm) = p_{loc} (12, 23) (in nm)	299,89	0,04
Local pitch p_{loc} (25,3 µm, 48,4 µm) = p_{loc} (35, 23) (in nm)	299,40	0,04
Deviation in boundary length δL_b (in nm)	-36	7
Relative deviation in boundary length $\delta L_{b, rel}$	$-3,6 \cdot 10^{-4}$	$7 \cdot 10^{-5}$
Deviation in characteristic length δL_c (in nm)	-47	7
Relative deviation in characteristic length $\delta L_{c, rel}$	$4,7 \cdot 10^{-4}$	$7 \cdot 10^{-5}$
Peak-to-valley deviation from linearity $\delta L_{nl,P-V}$ (in nm)	23	2
Relative peak-to-valley deviation from linearity $\delta L_{nl,P-V, rel}$	$2,3 \cdot 10^{-4}$	$2,0 \cdot 10^{-5}$
rms deviation from linearity $\delta L_{nl, rms}$ (in nm)	5,5	2
Relative rms deviation from linearity $\delta L_{nl, rms, rel}$	$5,6 \cdot 10^{-5}$	$2,0 \cdot 10^{-5}$

In the three examples of grating characterization discussed here, important quality parameters of gratings, like the relative total length deviation and the relative linearity deviation vary by 3-4 orders of magnitude. This should be taken into account, when discussing and choosing suitable measurement methods for grating calibration and quality characterization based on the guidance given in Clause 5. In application of the calibrated grating standards described in the 3 examples for dissemination of the length unit it has to be pointed out, that to fully benefit from the small measurement uncertainties specified in Tables A.1 to A.3 requires the users to measure the standards over exactly the same sections of the grating and in the same support conditions as during the calibration.

Example 4: International comparison on a 2D grating (p_{nom} = 1 000 nm)

Figure A.5 shows the results of a recent international comparison on 2D gratings [5]. The graph shows the deviations from the reference value as well as the estimated measurement uncertainties for the different participants and type of instruments used for the calibration of the grating with nominal 1 000 nm pitch, extending over an area of nominal 2,5 mm × 2,5 mm.



NOTE Results of an international comparison of national metrology institutes on a 2D grating with nominally 1 000 nm pitch by different participants and types of instruments: Optical Diffraction (OD), Metrological Scanning Probe Microscopes (SPM) with standard scanning range (usually below 100 µm) and a large range metrological SPM. The results presented in this figure are the deviations from the weighted mean reference value and the combined standard uncertainties u_c estimated by the participants, labeled A to L. For further details see [6].

Figure A.5 – Results of an international comparison on a 2D grating by different participants and types of instruments

The optical diffraction methods, see [7, 34], achieve the smallest uncertainties below 0,01 nm, because they are able to optically probe the whole area of the grating, while the metrological SPM with standard scanning stages are limited in determining the mean pitch with an uncertainty of about 0,1 nm. The large range metrological SPM however, can also measure the grating over the full quality area comparable to the global OD methods but in addition it is also capable to provide comparable information on the local pitch variation as the other high resolution microscopy SPM instruments. This example thus shows that hybrid measurement methods and instruments are important tools for a full quality evaluation of manufactured gratings.

A large variety of different types of calibration grating standards exists. In reference [35] an overview of existing calibration standards is given and this information will also be continuously updated. Methods for SPM based calibration of pitch standards by application of image processing algorithms are addressed in [36].

In several countries, national guidelines and standard documents exist, which cover grating standards and grating characterization methods and their use as material measures of length for different applications, mainly as image magnification standards of high-resolution microscopes. Some of these documents are listed in the Bibliography [39-45].

Annex B
(informative)

Bravais lattices

B.1 Bravais lattices

In geometry and crystallography, a Bravais lattice is an infinite array of discrete points generated by a set of discrete translation operations described by:

$$\vec{r} = k \times \vec{a} + l \times \vec{b} + m \times \vec{c}$$

where *k*, *l*, *m* are any integers and $\vec{a}$, $\vec{b}$, $\vec{c}$ are known as the primitive vectors which lie in different directions and span the lattice. For any choice of position vector $\vec{r}$, the lattice looks exactly the same. A crystal is made up of a periodic arrangement of one or more atoms (the basis) repeated at each lattice point.

In one dimension there is only one possible Bravais lattice (see Figure B.1) while in two dimensions there are five distinct Bravais lattices, and in three dimensions there are fourteen. Further details about Bravais lattices can be found in standard textbooks on crystallography or solid state physics, see e.g. [37].

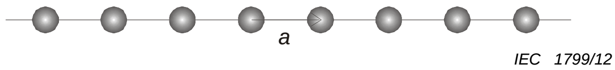
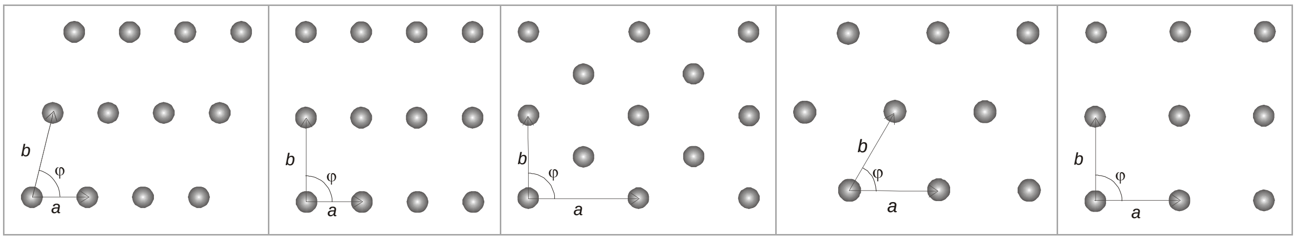


Figure B.1 – One-dimensional Bravais lattice

The absolute value of the primitive vector is also called the lattice constant of the one-dimensional lattice, see also 3.2.5.

B.2 Bravais lattices in 2D

In two dimensions, there are five Bravais lattices, see Figure B.2. They are oblique, rectangular, centered rectangular, hexagonal, and square.



Key (left to right):

oblique (φ ≠ 90°),

rectangular (φ = 90°),

centered rectangular (φ = 90°),

hexagonal (φ = 60°), and

square (φ = 90°)

Figure B.2 – The five fundamental two-dimensional Bravais lattices illustrating the primitive vectors $\vec{a}$ and $\vec{b}$ and the angle φ between them

B.3 Bravais lattices in 3D

In three dimensions there are 14 Bravais lattices, which can be grouped as follows (see Figure B.3):

- primitive centering (P): lattice points on the cell corners only;
- body centered (I): one additional lattice point at the center of the cell;
- face centered (F): one additional lattice point at center of each of the faces of the cell;
- centered on a single face (base centering): one additional lattice point at the center of one of the cell faces.

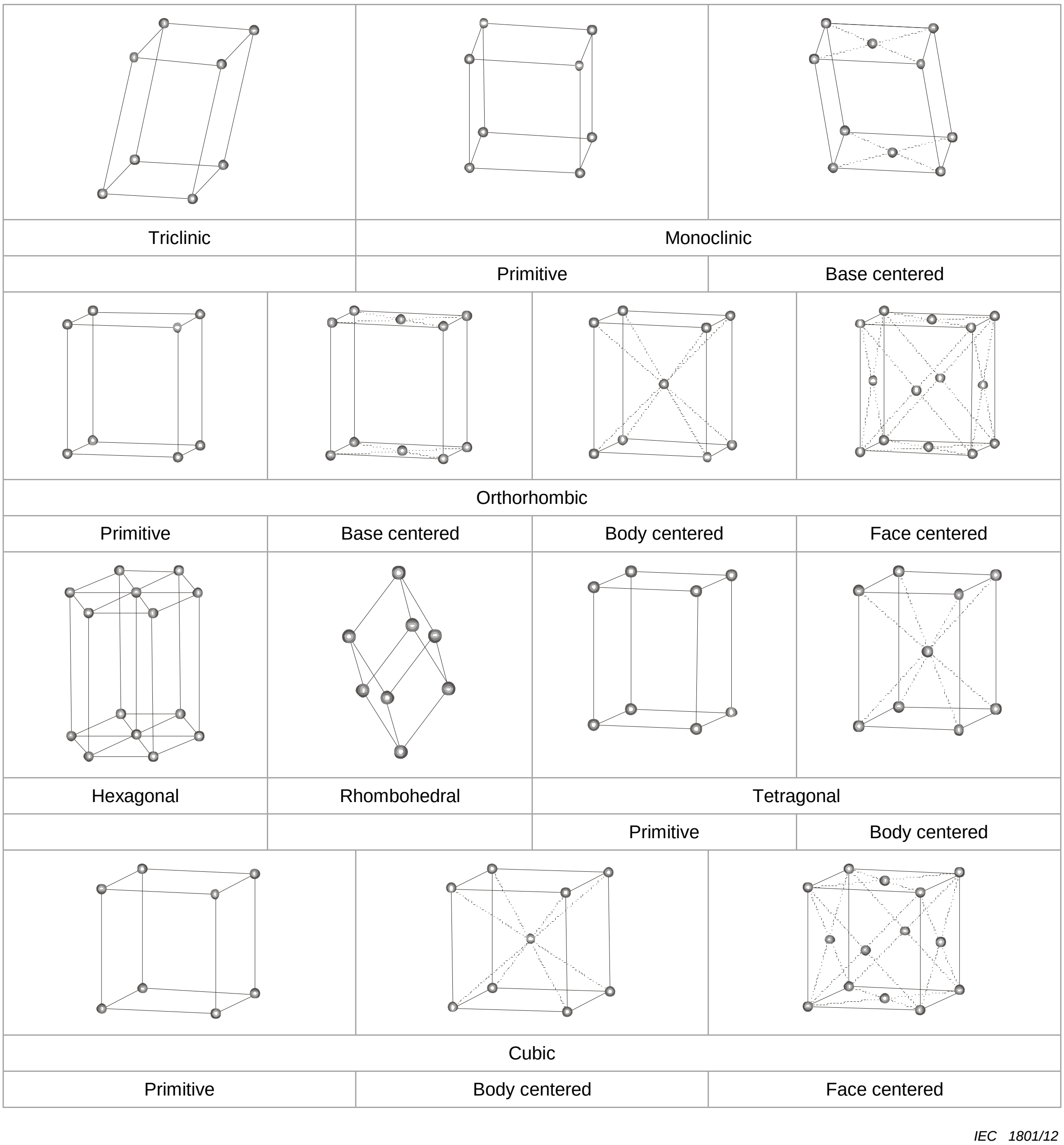


Figure B.3 – The 14 fundamental three-dimensional Bravais lattices

The volume of the unit cell can be calculated by evaluating $\vec{a}\cdot(\vec{b}\times\vec{c})$ where $\vec{a}$, $\vec{b}$ and $\vec{c}$ are the lattice vectors. The volumes of the Bravais lattices are given in Table B.1 below:

Table B.1 – Bravais lattices volumes

Crystal system	Volume
Triclinic: a ≠ b ≠ c α ≠ β ≠ γ ≠ 90°	$abc\sqrt{1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma}$
Monoclinic: a ≠ b ≠ c α = γ = 90°; β ≠ 90°	$abc\sin\alpha$
Orthorhombic: a ≠ b ≠ c α = β = γ = 90°	abc
Tetragonal: a = b ≠ c α = β = γ = 90°	a^2c
Rhombohedral: a = b = c α = β = γ ≠ 90°	$-a^3\sqrt{1-3\cos^2\alpha+2\cos^3\alpha}$
Hexagonal: a = b ≠ c α = β = 90°; γ = 120°	$\frac{3\sqrt{3}a^2c}{2}$
Cubic: a = b = c α = β = γ = 90°	a^3

B.4 Quasicrystals

It is noted here that also aperiodic, but ordered natural crystalline structures exist, which do not show full translational symmetry, like the Bravais lattices described above. These aperiodic crystalline structures are called quasiperiodic crystals or quasicrystals [38]. There are two types of known natural quasicrystals:

a) polygonal quasicrystals, which have an axis of eight, ten, or 12-fold local symmetry (they are periodic along this axis and quasiperiodic in planes normal to it), and

b) icosahedral quasicrystals, which are aperiodic in all directions.

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INTERNATIONAL
ELECTROTECHNICAL
COMMISSION

3, rue de Varembé
PO Box 131
CH-1211 Geneva 20
Switzerland

Tel: + 41 22 919 02 11
Fax: + 41 22 919 03 00
info@iec.ch
www.iec.ch