# Characterization of the Topography Fidelity of 3D Optical Microscopy

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## ABSTRACT

The topography fidelity $TF_i$ indicates the accuracy of the estimation of the real surface, describes the instrument influenced deviation of a measured topography image and depends on the interaction of the surface topography with the instrument. To understand and investigate the topography fidelity of optical surface measurement instruments, and interference microscopes in particular, an analytical model based on the fraction of the total illumination criteria and a numerical model based on Richards-Wolf theory are used to characterize the topography fidelity of 3D optical microscopy. As reference artefacts step-like micro-structures with varying spatial frequency and therefore different aspect ratios are numerically investigated with the aforementioned models. To testify the feasibility of the numerical analysis, a commercial white light interference microscope has been employed to measure these reference artefacts. The relationship between the measured heights and the spatial frequency of the samples under investigation are detailed in this paper. The aspect ratio influences on measurement results predicted by the simulation models and the agreements with the experimental results are investigated and reported in detail.

**Keywords:** 3D optical microscopy, white light interference microscopy, surface metrology, topography fidelity.

## 1. INTRODUCTION

3D Optical Microscopy such as coherence scanning interferometry and confocal microscopy has been more and more widely applied in research and industry for surface topography measurement because of their unique advantages including high speed, 3D areal and noncontact measuring [1,2,3]. Nowadays, commercially available optical surface measurement instruments equipped with objectives of high numerical aperture ($A_N$) and corrected for shorter illumination wavelengths can clearly demonstrate high lateral imaging resolution. However, their ability and capability to accurately reproduce topographical features of a surface under test is quite often questionable, since optical topography measurement results are, in essential, the convolution of the geometrical and physical properties of the surface feature and those of optical probes [4].

In the last years, many efforts have been done to investigate the instrument transfer function (*ITF*), which describes how the instrument would respond to an object surface having a specific spatial frequency [5-6]. The *ITF* is based on the well-known imaging theory (optical lateral resolution in accordance with Rayleigh or Sparrow criterion) and the imaging resolution is an influence factor in the resolving power of the instrument, together with other factors that include the measurement principle and data filtering. The *ITF* studies are performed under the assumption of rather small surface amplitudes (compared to the wavelength of light) [6].

However, in practice, surfaces and gratings often show height much higher than 100 nm. To describe the instrument response on such kinds of surfaces and structures, in the ISO standard relating to areal surface characterization (e.g. ISO25178-600:2016), a new terminology "topography fidelity" $TF_i$ is defined: the closeness of agreement between a measured surface profile or measured topography and the one whose uncertainties are insignificant by comparison [7]. The topography fidelity describes the method or instrument influenced measurement deviation of a topography related to the correct measurement of surface features, i.e. the width and the height of the feature.

Different samples for topography fidelity characterization have been under consideration, including rectangular gratings with different pitches and chirp standards having sinusoidal structures of different spatial frequencies. Batwings will occur on the edge of rectangular gratings and therefore increase the measurement uncertainty when the height is measured by 3D optical microscope.

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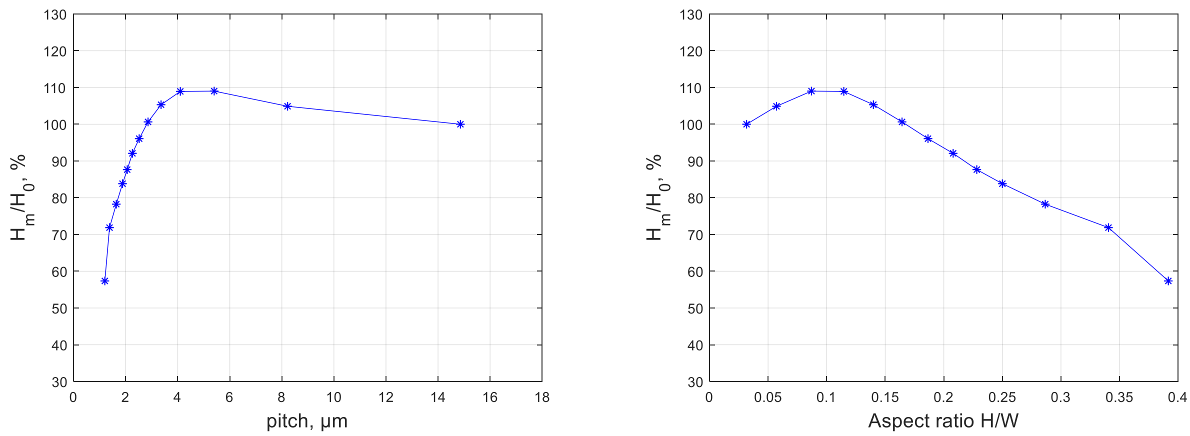
The efforts of theoretical analysis and 2D numerical simulation of the batwings in rectangular grating measurements have been made in the last years [8-10], however, analysis and simulation for the measurements of sinusoidal structures and the comparison between the measurements of different kinds of structures need to be further investigated.

In this article, two kinds of models for characterizing the topography fidelity of 3D optical microscopy are described in Section 2, measurement results will be compared with the simulated results. Section 3 shows our further investigations in this direction. The conclusions and outlook are described in section 4.

# 2. THEORETICAL INVESTIGATION OF THE TOPOGRAPHY FIDELITY OF WHITE LIGHT INTERFERENCE MICROSCOPY

## 2.1 Topography fidelity performance measured by white light interference microscope

To experimentally investigate the fidelity of typical white light interference (WLI) microscopy, a commercial WLI microscope has been employed to measure the topography of step-like gratings with different height to width ratio. In the case of the grating structure height $h$ = 240 nm and the numerical aperture of an objective $A_N$ = 0.7, typical measurement deviations are shown in Figure 1.




(a) Measured height attenuation versus pitch of the grating ($H_m$ measured height, $H_0$: nominal value)

(b) Measured height attenuation with respect to the aspect ratio of the grating structures

Figure 1. Typical topography fidelity curve obtained by a white light interference microscope.

It can clearly be seen from Fig. 1 that noticeable measurement deviation (e.g. $H_m/H_o$> 20%) will appear, even when the structural pitch (e.g. pitch > 2 µm) is actually much larger than the lateral resolution of the microscope objective in use (i.e. ~ 0.4 µm).

## 2.2 Analytical model to predict the maximum height to width ratio of a structure

An analytical model based on the fraction of the total illumination criteria [11] is applied to predict the maximum aspect ratio, with which rectangular gratings can theoretically be measured correctly by vertical scanning optical microscopy. This simplified model has only considered the reflected intensity change of the illumination spot near the edge of a grating and supposed that the surface of the grating should be flat and the optical microscope works in error-free condition.

As illustrated in Fig. 2, when the light illumination spot moves from position I to position II of the lower surface of a grating, due to the shadow effect, the energy fraction of the total illumination reflected by the measured surface decreases, and the interaction of the optical probe and the edge of the test object will influence the measurement results and thus the measurement uncertainty will be introduced. By choosing the threshold of received light energy from the test surface, the maximum height to width ratio of a test artefact can be determined.

According to the research of E. Wolff [12], the light distribution *L(u,v)* near the focus in an error-free diffraction image can be expressed as following:

$$L(u,v) = \begin{cases} \left(\frac{v}{u}\right)^2 \left[1 + \sum_{s=0}^{\infty} \frac{(-1)^s}{2s+1} \left(\frac{v}{u}\right)^{2s} Q_{2s}(v)\right] - \frac{4}{\mu}\left[Y_1(u,v)\cos\frac{1}{2}\left(u + \frac{v^2}{\mu}\right) + Y_2(u,v)\sin\frac{1}{2}\left(u + \frac{v^2}{u}\right)\right], \frac{v}{u} < 1 \\ 1 - J_0(u)\cos(u) - J_1(u)\sin(u), \frac{v}{u} = 1 \\ 1 - \sum_{s=0}^{\infty} \frac{(-1)^s}{2s+1} \left(\frac{u}{v}\right)^{2s} Q_{2s}(v), \frac{v}{u} > 1 \end{cases} \tag{1}$$

where $J_n$ stands for $n$-th order Bessel function, $Q_{2s}$ and $Y_1(u, v)$ and $Y_2(u, v)$ are given by the following equations respectively:

$$Q_{2s}(v) = \sum_{p=0}^{2s} (-1)^p \left[J_p(v) J_{2s-p}(v) + J_{p+1}(v) J_{2s+1-p}(v)\right] \tag{2}$$

$$Y_n(u,v) = \sum_{s=0}^{\infty} (-1)^s (n+2s) \left(\frac{v}{u}\right)^{n+2s} J_{n+2s}(v) \tag{3}$$

in which, $u$ and $v$ are normalized optical coordinates, and transformed from real coordinates ($x$, $z$):

$$u = \frac{2\pi R^2}{\lambda f^2} \cdot \Delta f = \frac{2\pi}{\lambda} tan^2(a) \cdot z \tag{4}$$

$$v = \frac{2\pi R}{\lambda f} \cdot x = \frac{2\pi}{\lambda} \tan\alpha \cdot x \tag{5}$$

where λ is the wavelength of the light in use; sinα is numerical aperture of the objective, $x$, $z$ are the real coordinates of the test points near focus.

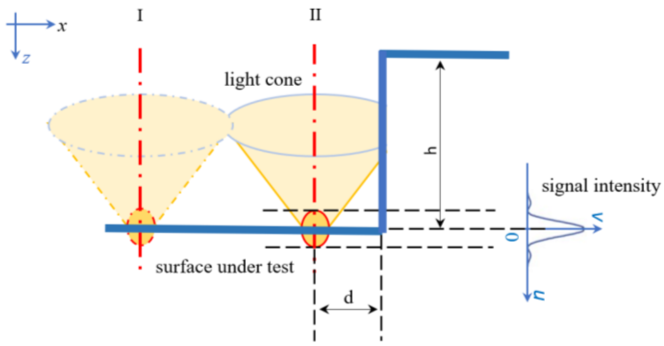



Figure 2. Schematic illustration of the light illumination on the surface and near the edge of a step height.

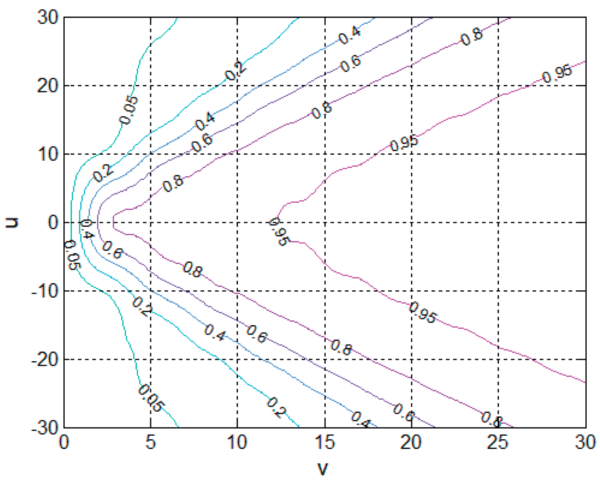



Figure 3. Contour analysis of L($u$,$v$) near focus in an error-free diffraction image

According to the light distribution Eq. (1) the contour lines of $L(u,v)$ near focus in an error-free diffraction imaging system can be deduced, as shown in Figure 3.

From some comparisons with experimental results, a criteria $L(u,v) = 0.6$ is applied in this paper. The criteria needs to be further investigated and, if necessary, optimized. In Fig. 3, one line $v = 0.773u$ can be used to fit the contour line $L(u, v) = 0.6$, by transforming the fitted line to the real coordinate system,

$$d \geq \frac{1.46 \cdot \left(1 - \sqrt{1 - A_N{}^2}\right)}{A_N} \cdot h + 0.77 \cdot \frac{\lambda}{A_N} \tag{6}$$

According to Eq.(6), it can be calculated that when the height of the rectangular grating is 240 nm, the width of the grating should be larger than 2d (see Figure 2.), i.e. 1.4 µm, which agree with the measured curve in Figure1 very well.

It can be seen that if the numerical aperture of the microscope objective and the wavelength used for illumination are given, a maximum height width aspect ratio can be preset with which the rectangular grooves can theoretically be measured correctly, however, it can only give the critical point of the grating's aspect ratio. In ISO 25178 -600 [7] a small scale fidelity limit (for instance, +/-10%) is defined: the shortest spatial wavelength for which both the height and the spatial wavelength of the measured profile or topography deviate by less than a specified amount from the values of the one to which it is being compared. A numerical model for simulating the diffraction effect on the grating surface needs to be introduced.

### 2.3 Numerical model based on Richards-Wolf theory

The Richards-Wolf model describes the electric and magnetic vectors in the image space of a linearly polarized incident field. In their research, the symmetry properties of the field with respect to the focal plane are noted and the distribution of the time-averaged intensity can be determined in the vicinity of the focus in polarized or unpolarized field. Additionally, the Richards-Wolf model is not restricted to microscopic systems of low aperture. Optical systems with high $A_N$ value can be inherently considered [13].

In [9] the Richards-Wolff model has been further extended to an interferometric configuration and simplified into a 2-Dimensional model. With this model the authors explain the batwings occurring at edges of step heights and the height-to-wavelength ratio influence on the batwings measured by scanning white light interference microscopy. Our first work in this manuscript utilized this numerical model based on the Richards-Wolf theory to investigate topography fidelity of white light interference microscopes.

Take an example of the simulated interferograms of a grating with 4 µm pitch and 240 nm height based on the Richards-Wolf modeling, three typical positions on the grating are selected, i.e. the middle position of the upper surface (position I), upper surface near or on the edge (position II) and the middle position of the lower surface (position III), as shown in Fig.4.

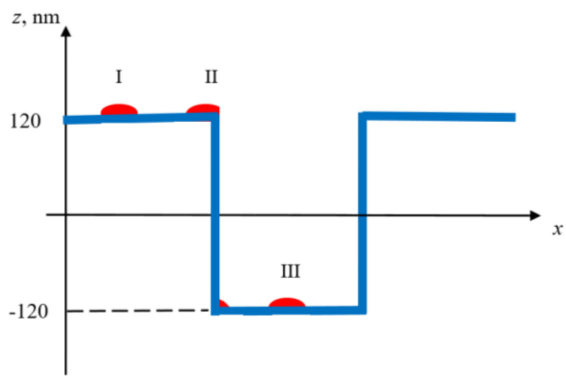
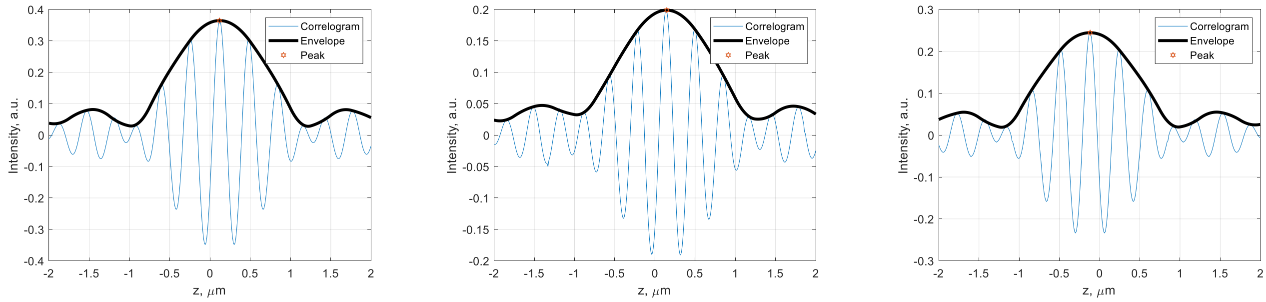



Figure 4. Three typical positions on the grating

Fig. 5(a) – (c) show the interferograms of the three different positions on the grating structure respectively ($A_N$= 0.7, λ = 630 nm). It can be seen that on the middle positions of the upper and lower surface of the grating, correct height information can be obtained, when the structural width is large enough. Close to the grating edge, overshooting (batwing) will appear.




(a) Upper surface, $z$ = 120 nm at the peak position

(b) Upper surface, near the edge, $z$ = 150 nm at the peak position, overshooting occurs

(c) Lower surface, $z$ = -120 nm at the peak position

Figure 5. Simulated interferogram of a grating with 4 µm pitch based on Richards-Wolff modeling ($A_N$= 0.7, λ = 630 nm).

When the structure width is smaller, the batwings overlapped from the neighboring two edges together, a larger height information of the structure will be obtained. When the structure width decreases further, the measured height will be smaller than the real height, as illustrated in Fig. 6.

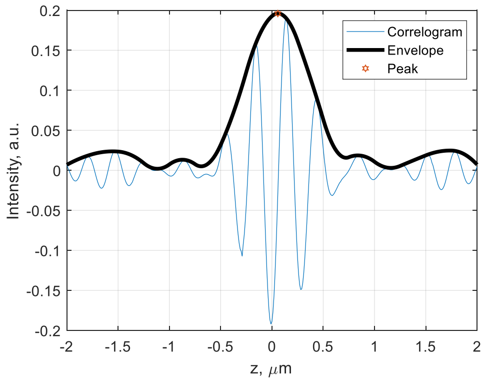



Figure 6. Simulated interferogram of a grating with 1 µm pitch based on Richards-Wolff modeling, upper surface, $z$ = 60 nm

Based on the Richards-Wolf model, simulation with different pitch parameters from 1 µm to 6 µm and a fixed structural height of 240 nm have been realized, the simulated height varying with respect to the pitch parameters of the grating is shown in Figure 7.

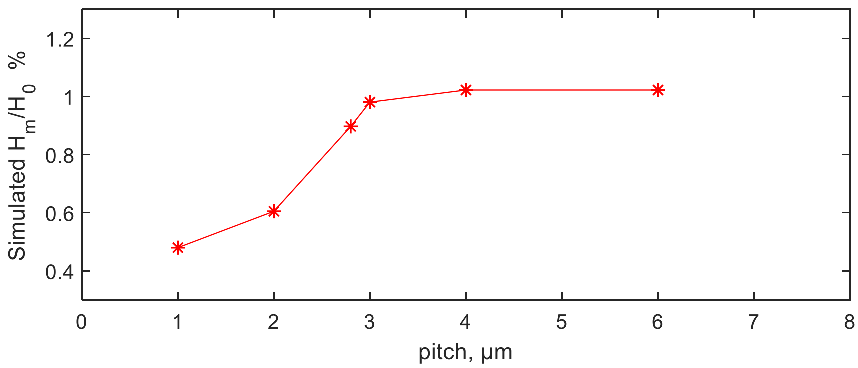



Figure 7. Simulated topography fidelity curve

Comparing Fig. 7 and Fig. 1(a), both curves show that the measured and simulated heights have good consistency with the real heights, in case that the pitch is larger than 3 µm,

It is worthwhile to mention that the numerical model applied in this paper is currently a 2D model, to simulate the microscopic measurements of step-like structures with higher accuracy, a 3D extension will be further investigated in the next step of our work.

## 3. FURTHER INVESTIGATIONS FOR THE TOPOGRAPHY FIDELITY CHARACTERIZATION

Up to now, most of test structures for simulations and experimental investigations are rectangular structures. In ISO 25178 -600, it is pointed out that ideally the ITF tells us what the measured height of a sinusoidal grating of a specified spatial frequency would be relative to the true height of the grating. For the topography fidelity investigations, sinusoidal grating should also be taken into consideration, and the measurement results for the sinusoidal and rectangular gratings should be compared.

A cosine chirp sample has been developed at PTB, Germany. It contains cosine waves with fixed amplitude and various wavelengths. The chirp standard is made of low-oxygen copper with a 100µm thick nickel-phosphorus layer and manufactured by a single diamond turning process.

Fig. 8 shows first results of the measured heights versus wavelengths measured by a white light interference microscope ($A_N = 0.55$). Numerical simulation and the comparison with rectangular structures will be further investigated.

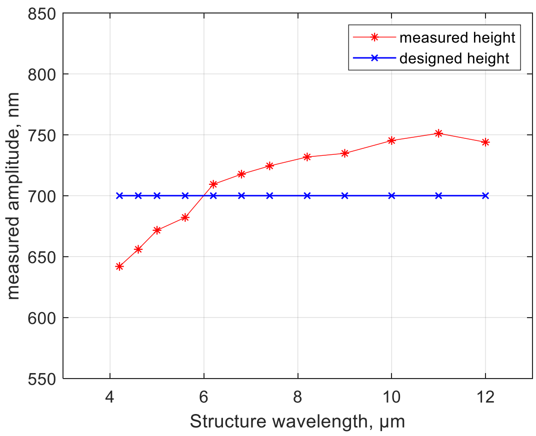



Figure 8. Measured heights of a sinusoidal grating with structure wavelength from 4.2 µm to 12 µm

## 4. CONCLUSIONS AND OUTLOOK

To understand and investigate the topography fidelity of optical surface measurement instruments, especially interference microscopes, an analytical model based on the fraction of the total illumination criteria and a numerical model based on Richards-Wolf theory are used to characterize the topography fidelity of 3D optical microscopy.

In case of grating structure height $h$ = 240 nm, when the wavelength is larger than 3 µm, a small scale fidelity limit of ±10% can be reached using a WLI microscope with an objective having $A_N = 0.70$.

The maximum height to wavelength ratio of the test artefact, which can theoretically be measured correctly, can be determined by the analytical model, and the preliminary analytical results coincide well with the experimental results.

The heights simulated by the numerical simulation and by the measurements show good consistency with the real heights, in case that the wavelength of gratings is larger than 3 µm. Topography fidelity on the sinusoidal gratings will be further investigated.

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