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Rigorous modeling of a confocal microscope

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ABSTRACT

A reliable tool for simulations of confocal microscopes shall be developed to enable improved model-based dimensional metrology. To simulate measurements on rough surfaces the boundary element method (BEM) simulation tool *SpeckleSim*, developed by the *ITO* of the University of Stuttgart, is combined with a Fourier optics based image formation. *SpeckleSim*, which calculates the light-structure interaction by solving the Maxwell equations, is compared with the well-known FEM based solver *JCMsuite* and the FDTD based solver *Ansys Lumerical*. As an example, a rectangular shaped line is used as an object. Due to different boundary conditions the results show as expected small deviations, which require further investigations. First comparison results and the general concept of the image formation method will be presented.

Keywords: confocal microscope, BEM, FEM, FDTD, image formation

1. INTRODUCTION

Confocal microscopes are often used in industry and research because the measurement is fast, contactless and has a high resolution [5]. Even though the confocal microscopes are often used there are systematic deviations between the measured and the real sample surface topography. To understand these deviations and to improve the measurement results a simulation of the complete microscope image formation process is needed. With simulations parameter studies are possible, which are difficult and expensive in the experiments. And so, the influences of individual parameters on the measurement deviations can be analyzed separately.

To develop a reliable tool for the simulation of confocal microscopes, two main parts are needed, the numerically solved Maxwell equations to simulate the interaction of the light and the object surface and the imaging process of the microscope, i.e., the propagation of the reflected and diffracted light to the image detector.

2. RIGOROUS MAXWELL SOLVER

To simulate the light-surface interaction the boundary element method (BEM) simulation tool *SpeckleSim*, provided by the *ITO* of the University of Stuttgart, is used. The simulation tool *SpeckleSim* solves the Maxwell equations numerically for large scale nonperiodic 3D surfaces with a realistic computation time and allows a physically correct modeling of more complex rough surface structures [1]. To see the differences of *SpeckleSim* to other simulation tools, a comparison between *SpeckleSim*, *JCMsuite* [2] and *Ansys Lumerical* [3] is made. Since the simulation tool *JCMsuite* is based on the finite element method (FEM) and the simulation tool *Ansys Lumerical* is based on finite difference time domain (FDTD), the comparison between the different simulation tools is also a comparison of different numerical methods. From the *Ansys Lumerical* simulation tool two boundary modes are used for the comparison. The periodic mode, which means that the structure is infinite in the x-direction, the structure has a sort of an infinite period length. The second mode is the perfectly matched layer (PML) mode, where the structure has a fixed end in the x-direction. These two modes are used to see the influence of the different boundary conditions to the reflected and diffracted light of the surface and to compare them with the other methods.

The object used for the comparison is a single rectangular shaped line. The rectangle height is 190 nm and the width is 500 nm. For the simulations with the FEM method and the FDTD method in the periodic mode, the rectangular shaped line is infinite in the x-direction. For the BEM method and the FDTD method in the PML mode the x-dimension is from - 6 µm to 6 µm. The y-direction is infinite for the FEM method and the FDTD method in both modes. Since the *SpeckleSim* needs a mesh grid from the surface with defined ends in all dimensions, the y-dimension is from - 6 µm to 6 µm for the BEM method. Figure 1 shows the meshed surface as it is used for the BEM method.

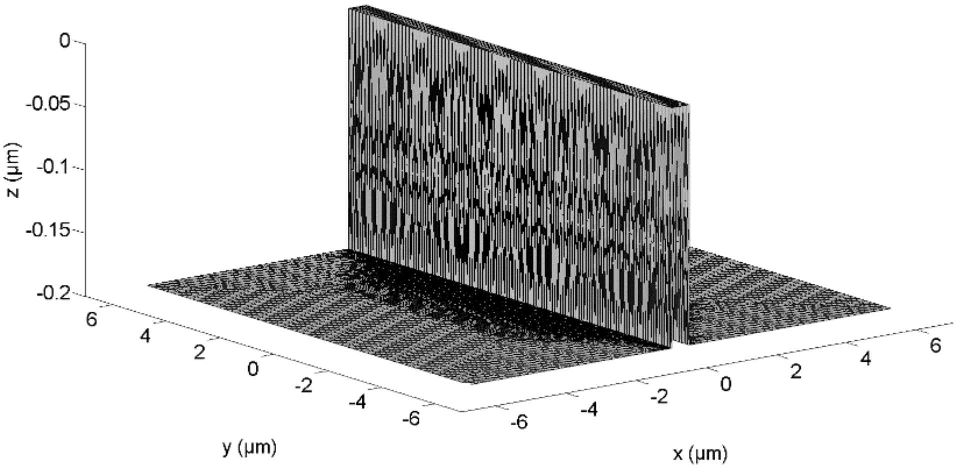

Figure 1:Meshed surface, as it is used for the BEM simulation. The surface is limited in x- and y- direction in contrast to the surface which is used for the FEM simulation and the FDTD simulation in periodic mode.

The illumination for all methods is a plane wave with a wavelength of 500 nm and an incident angle of 0 degree. Namely, the illumination is vertical to the line structure.

Figure 2 and Figure 3 show the results of the comparison for the transversal magnetic polarized light (TM-polarized) and the transversal electric polarized light (TE-polarized). To minimize the effects of the finite x-dimension of the line structure for the BEM method and the FDTD method in the PML mode, the results are only in a x-range from - 3 µm to 3 µm compared. For the BEM method the plane by y = 0 is used for the comparison.

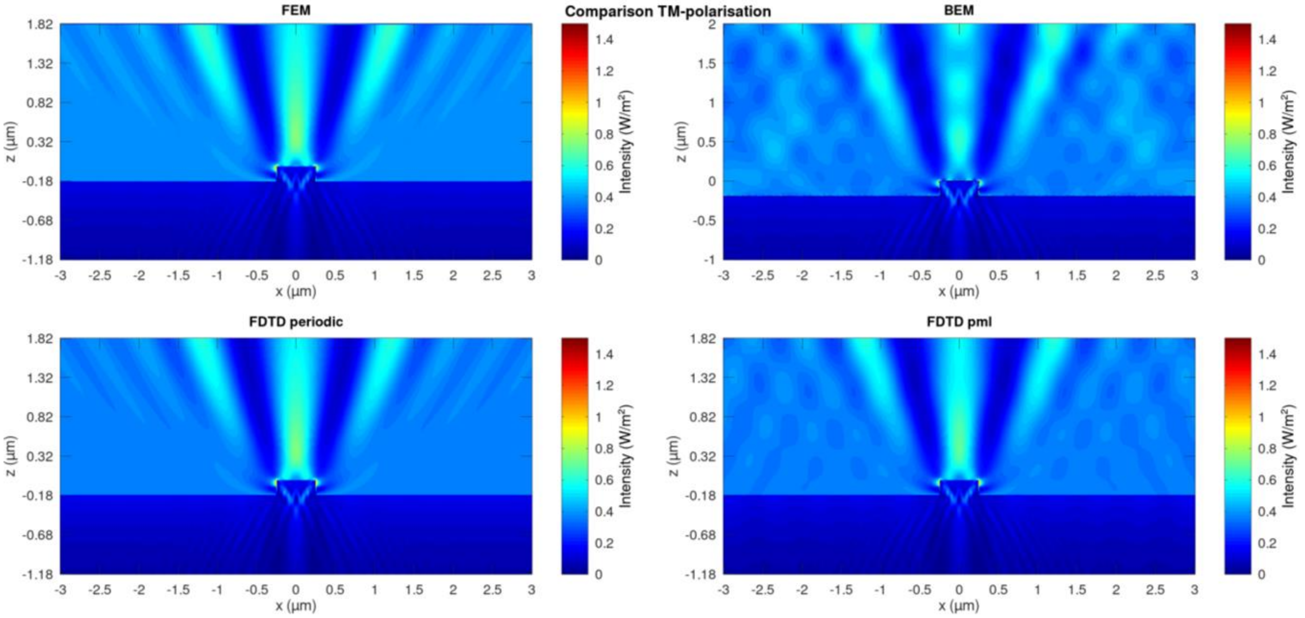

Figure 2: Comparison of the different Maxwell solvers. The rectangular line structure is illuminated with a TM-polarized plane wave.

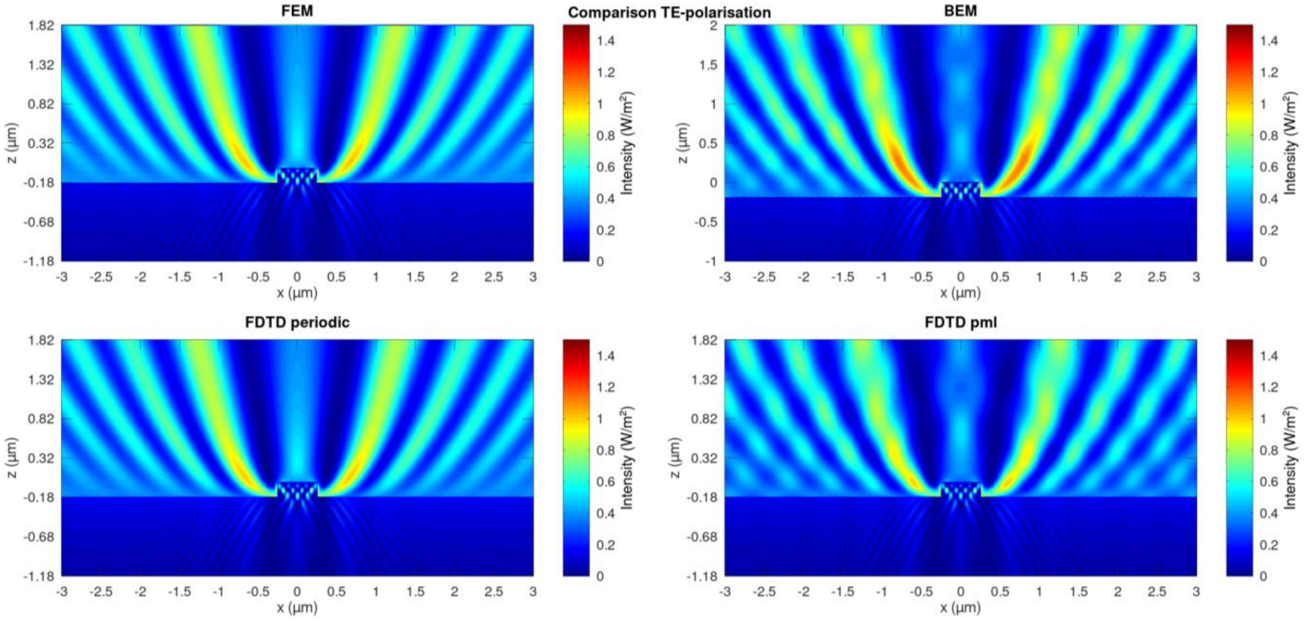

Figure 3: Comparison of the different Maxwell solvers. The rectangular line structure is illuminated with a TE-polarized plane wave.

As expected, the simulation results of the FEM and the FDTD periodic mode are similar, and correspondingly the BEM and the FDTD PML mode results are similar. In the TM-polarized results of the BEM method and the FDTD method in the PML mode, the effects due to the finite structure size in the x-direction are visible. These are the intensity variations beside the diffraction maxima's, which are not visible in the FEM and the FDTD periodic mode results. The difference in these intensity variations between the BEM and the FDTD PML mode results, are consequences of the finite structure size in y-direction for the BEM method. The finite structure size in y-direction is the difference in the boundary conditions between the BEM method and the FDTD method in the PML mode. The difference between the BEM and FDTD PML mode results are as example good to see in the diffraction maxima of 0th and 1st order, where the BEM result shows extinguished interferences. Also, in the TE-polarized comparison the effects of the finite structure size in x-direction for the BEM method and the FDTD method in the PML mode are visible through a wabble of the diffraction maxima's. The higher intensity in the diffraction maxima of 1st order in the BEM result near the line structure needs further investigations.

For a comparison in more detail, Figure 4 and Figure 5 show the intensities of the different methods at fixed z-values. Near to the top of the rectangle (z = 20 nm) the numerical effects of the tools are dominant and a useful comparison is not possible. Overall, at different z-positions the 0th and 1st orders of diffraction maxima agree well, however, there are phase shifts at the higher order diffraction. In the comparison with TM-polarized light the effects caused by the limited x-dimension for the FDTD method in the PML mode and the BEM method are clearer than for the TE-polarized light comparison.

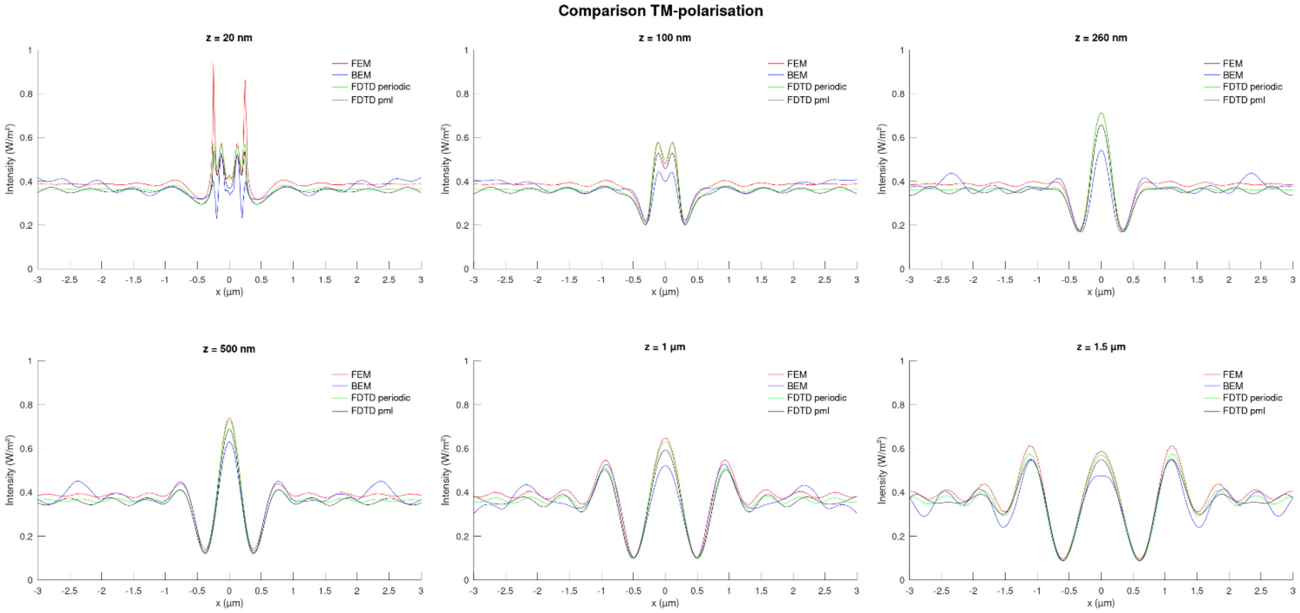

Figure 4: Comparison of the Maxwell solvers at fixed z-positions. The rectangular line structure is illuminated with a TM-polarized plane wave.

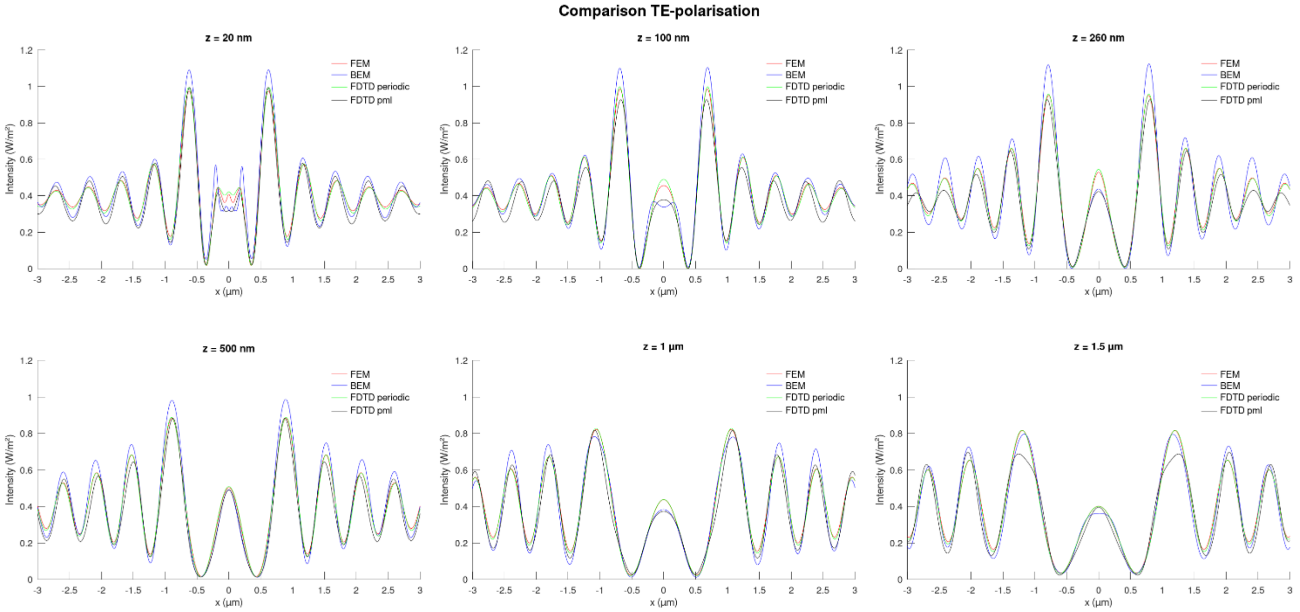

Figure 5: Comparison of the Maxwell solvers at fixed z-positions. The rectangular line structure is illuminated with a TE-polarized plane wave.

3. IMAGE FORMATION

The image formation is based on the Fourier optics and is implemented in Fortran. The main idea of the Fourier optics is, to transform the reflected and diffracted light from the surface into the Fourier space. In the Fourier space properties of the instrument, like the amplitude transfer function, are multiplied to the spectrum. After that, the spectrum is transformed back into the space. Those electromagnetic waves, which pass through the pinhole, will be detected by the detector of the instrument.

In practice, the reflected and diffracted light of the surface is collected at a constant distance to the surface. Since the *SpeckleSim* is based on the BEM method, the numerical errors are large directly on the surface. The collected light from the read-out level, some nanometers above the surface, is Fourier transformed and through a phase shift in the Fourier space it is backpropagated to the focus point of the illumination.

$$\boldsymbol{E}_{\text{prop}}(k_z, \Delta z) = \text{FFT}(\boldsymbol{E}_{\text{read-out}}(x, y, z)) \cdot e^{i \cdot k_z \cdot \Delta z} \tag{1}$$

The distance in z-direction from the read-out level to the focus point of the light is described by Δz, which indicates the phase shift. The sign of Δz depends on the read-out level which lies above or below the focus point of the light. After the propagation, the amplitude transfer function is multiplied to the spectrum. The amplitude transfer function (ATF) depends on the numerical aperture of the objective, the wave vector $\vec{k}$ and the wave number $k = \frac{2\pi}{\lambda}$. It describes which reflected and diffracted light is collected by the objective.

$$\text{ATF}(k_x, k_y) = \text{rect}\left(\frac{\sqrt{{k_x}^2 + {k_y}^2}}{2 \cdot k \cdot NA}\right) \tag{2}$$

Afterwards the evanescent waves are reduced from the spectrum, since they do not propagate This means that the frequencies, which correspond to imaginary z-components of the k-vectors are filtered out. The frequencies of the spectrum correspond to the x-part of the k-vector, k_x. Since the simulation is for the fixed y-plane at y = 0, the y-part of the k-vector is zero, $k_y = 0$. The z-part of the k-vector, k_z is determined by the length of the k-vector, $|\vec{k}|$. The length of the k-vector is given through the wavelength and corresponds to the wave number.

$$|\vec{k}| = \sqrt{{k_x}^2 + {k_y}^2 + {k_z}^2} = \frac{2\pi}{\lambda} \tag{3}$$

$$k_z = \sqrt{|\vec{k}|^2 - {k_x}^2} \tag{4}$$

$$E_{\text{evanescent}}(k_z) = \begin{cases} 0, & k_z \in \mathbb{C} \\ 1, & k_z \in \mathbb{R} \end{cases} \tag{5}$$

With an inverse Fourier transformation, the spectrum is transformed back to the space.

$$\boldsymbol{E}_{\text{out}}(x, y, z) = \text{iFFT}(\boldsymbol{E}_{\text{prop}}(k_z, \Delta z) \cdot \text{ATF}(k_x, k_y) \cdot E_{\text{evanescent}}(k_z)) \tag{6}$$

Finally, the intensities of the electromagnetic waves, which pass the pinhole are integrated. This corresponds to the intensity, which reach the detector.

$$I_{\text{pinhole}}(x, y, z) = \int_0^{r_{\text{pinhole}}} dr \int_0^{2\pi} d\varphi \, |\boldsymbol{E}_{\text{out}}(x, y, z)|^2 \tag{7}$$

This described procedure is repeated for each (x, y) point on the sample surface. For each (x, y) point on the sample surface results so an intensity curve, their maximum shows at which z-position this point was in the focus plane. The following example calculates the intensity curve only for one point of the surface.

3.1 Imaging of one point on a flat surface

As example of the image formation the intensity curve for the point $\vec{r} = (0, 0, 0)$ on a flat surface with dimensions - 2 µm x 2 µm is calculated. The illumination of the surface is realized though different plane waves, with different incident angles, which are focused into one point [4]. For the illumination no pinhole is considered. Only in front of the detector is a pinhole considered. Figure 6 shows the intensity of the diffracted and reflected light from the surface. The surface is positioned at z = - 1 µm. The read-out level is at z = - 0.9 µm and marked with the red line in Figure 6. Using equation (1 the electromagnetic field at the read-out level is propagated to the focus plane of the illumination. The focus plane of the illumination is marked with the white line in Figure 6.

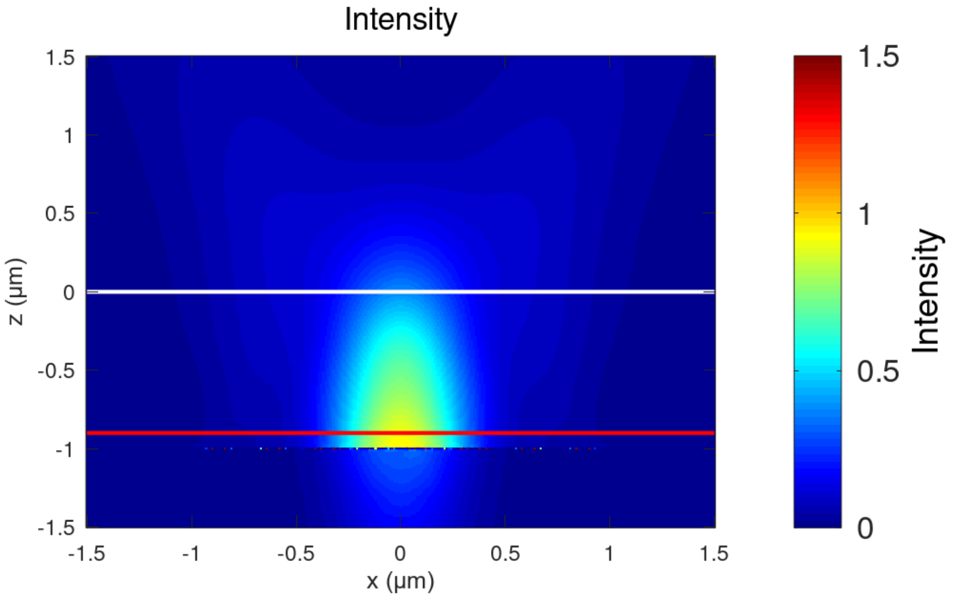

Figure 6:Intensity of the reflected and diffracted light at the surface. The intensity is normalized with the maximum intensity at z = - 0.98, which corresponds to two pixel lines above the surface. The flat surface is positioned at z = - 1 μm. The red line marks the read-out level and the white line marks the focus plane of the illumination.

Figure 7 shows the intensity of the electromagnetic wave, after taking into account the ATF and the reduction of the evanescent waves. For comparison also the intensity from the read-out level is shown in Figure 7 too. The filtering of the high frequencies results in a lower intensity around - 0.6 μm and 0.6 μm. On the other hand, the maximum intensity is a bit higher than that before the manipulations.

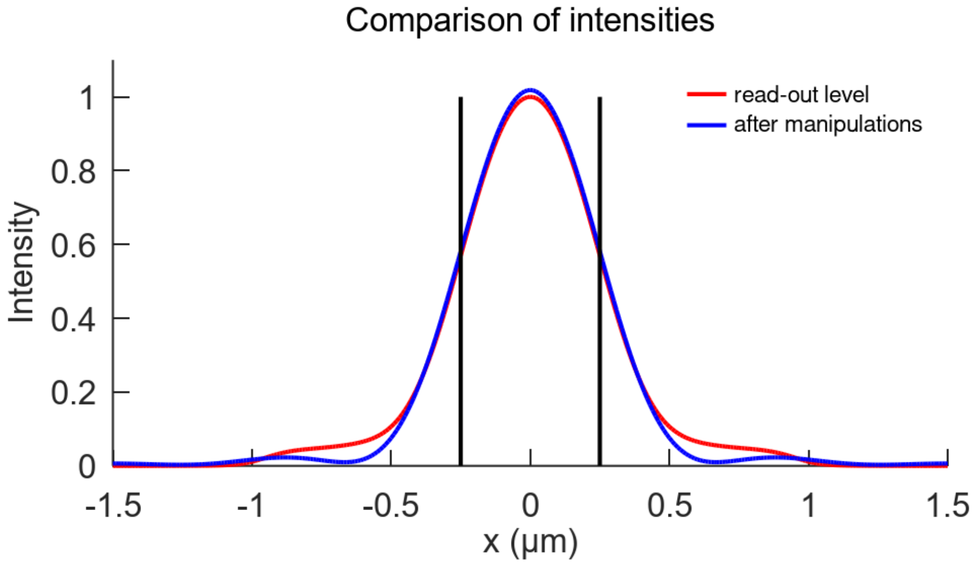

Figure 7: Comparison of the intensity curves from the read-out level and after the manipulations in the Fourier space. The black lines mark the pinhole diameter.

The intensity which reaches the detector, depends on the radius of the pinhole. For this example, a pinhole with radius 250 nm is chosen. Therefore, the intensity in the x-range from - 0.25 μm to 0.25 μm is integrated.

The flat surface is shifted to 21 z-positions between - 1 µm and 1 µm. The blue curve in Figure 8 shows the intensity curve for these 21 positions. As expected, the maximum of the curve is at z = 0. There is also the focus level of the illumination and because the flat surface has no height, the maximal intensity reaches the detector, when the surface is at z = 0. The simulation result shows that the intensity curve is not symmetric to z = 0. Since the focused illumination is symmetric in z-direction, also a symmetric intensity curve is expected. In Figure 8 the intensity curve of an analytical model is shown in orange. The analytical model is for a perfectly reflective surface and does not consider any pinhole. It depends only on the numerical aperture [5]. The comparison of these two curves shows, that the reason for the asymmetry might come from the negative z-positions of the surface. The shapes of the curves for the positive z-positions are similar, the shift between the curves can be reduced with a smaller pinhole for the imaging curve.

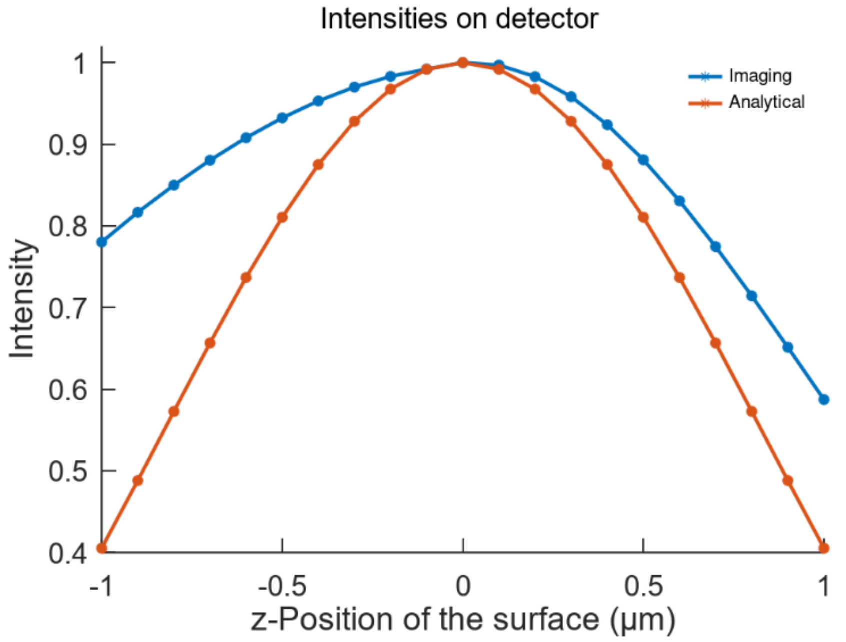

Figure 8:Intensity detected as function of z-positions of the surface. From the maximum of the curve the height of the surface can be determined. Compared are the result of the imaging, which is described in this section, in blue and the result of an analytical calculation in orange. For the imaging curve a pinhole with radius 250 nm is used. The analytical curve does not consider any pinhole.

4. CONCLUSION

The comparison of the different Maxwell solver simulation tools shows differences between the methods as expected. Since the BEM method and the FDTD method in the PML mode are not designed for periodic structures, the effects caused by the limited size in x-direction are visible. Nevertheless, the simulation tools agree well. For a focused illumination or a line structure with no x-direction expansion, e.g., a cylinder with height along to the y direction and surrounded with air, the effects of the limit in x-direction can be minimalized and can be distinguished from the effects of the limit in y-direction.

The imaging of the instrument is designed to add other characteristics of the microscope in a simple way. They can be added in the Fourier space with an additional filtering. The imaging leads to an intensity curve from which the height of the surface can be calculated. But currently the shape of the curve shown in Figure 8 in blue differs from the expected one in orange and needs further investigations. One possible reason is that there is a sign mistake in the propagation calculation or that the simulation of the illumination is not symmetric in the z-direction.

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