Numerical study of diffraction effects in light scattering by multiple cylindrical scatterers

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We compared Maxwell and radiative transfer theories for light scattering by multiple cylindrical scatterers and observed forward diffraction peaks in the Maxwell solutions. We examined diffraction by dielectric homogeneous obstacles of finite thickness and depicted differences to the scalar diffraction theory for a single slit. We show that for the interpretation of the diffraction effects in our multiple cylinder model the single slit diffraction approximation can be applied.

INTRODUCTION

The application of light has a high potential in medical diagnosis and therapy. For the development of effective methods, a theoretical investigation of the interaction of light with biological tissue is essential. Currently, in most cases, the radiative transfer equation (RTE) is used for this purpose. Nevertheless, this approach neglects effects originating from the wave nature of light, such as interference or diffraction. While general restrictions of the applicability of the RTE are known [1], the task of quantitatively examining these restrictions for special cases still remains. For these examinations it is necessary to compare the RTE results with solutions of the Maxwell equations.

In a recent publication, we examined the coupling between solutions of the RTE and Maxwell theory for the scattering by multiple cylinders arranged in a finite area [2]. Due to the finiteness of the area, diffraction effects occur in the Maxwell solutions that are not present in the RTE results. In this contribution we will further investigate these diffraction effects and highlight some ways to eliminate these effects in order to better compare the two theories.

RESULTS

Cylindrical scatterers in a finite area

In a recent publication, we presented a comparison between RTE and Maxwell theory for the solutions of the light scattering by multiple cylinders [2]. At first, similar results are shown here. The RTE has been solved using a Monte Carlo method [3], where the analytical Maxwell solution for a single cylinder has been used to specify the scattering properties in the RTE. For the Maxwell solutions an analytical multiple cylinder theory has been applied [4]. Our simulation models consisted of infinitely long parallel cylinders having a diameter of $d = 2$ µm and a refractive index of $1.33 + 0i$. The cylinders have been randomly distributed over an area $A = 10 \times 10$ µm^2 with an outer medium refractive index $n_m = 1.52$. We note that the parameters were chosen to model tubules in human dentin. The light is incident

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perpendicular to the cylinder axes, having a vacuum wavelength of $\lambda = 633$ nm. Different cylinder densities have been examined. For the Maxwell solution, results of 50 different runs of randomly oriented cylinders have been averaged for each density in order to suppress speckles.

The calculated results for both theories are shown in Fig. 1. A good agreement between Maxwell and RTE results for scattering angles higher than 20 degrees can be observed. For higher concentrations, the differences increase due to dependent scattering effects which cannot be accounted for in radiative transfer theory. Furthermore, a large deviation for small angles can be seen as shown at the right-hand side of Fig. 1. As we argued in [2], these differences are mainly caused by diffraction effects due to the finite size of our model. These effects are immanent to the Maxwell solution but cannot be observed in the RTE results.

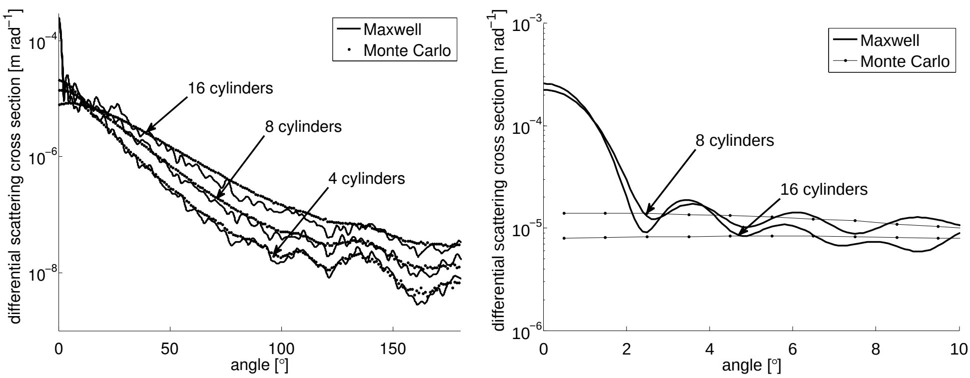

Figure 1. Left: Comparison between the Maxwell and RTE results for three different cylinder densities. Right: In the forward direction huge deviations between the Maxwell and RTE results can be observed, caused by diffraction effects of the finite scattering area.

Diffraction calculations

In this section we will discuss some fundamental issues concerning diffraction and use our Maxwell solver codes to further investigate the observed diffraction effects. For multiple cylinder problems we used the analytical method described in [4], for arbitrary structures we used a self-developed finite-difference time-domain (FDTD) [5] simulation program.

Diffraction occurs when light encounters a small obstacle or opening. The light waves that pass the object form a diffraction pattern which can be observed in the far field. Usually a scalar diffraction theory is used, where it is assumed that the obstacle is infinitely thin and perfectly absorbing. The diffraction by a single cylinder can be approximated as diffraction by an (inverse) slit where the width of the slit is given by the cylinder diameter. For slit diffraction (and also for inverse-slit diffraction as is stated by Babinet's theorem) a very simple formula exists [6]:

$$I(\theta) = I(0)\left(\frac{\sin\beta}{\beta}\right)^2, \tag{1}$$

$$\beta = \left(\frac{kb}{2}\right)\sin\theta, \tag{2}$$

where b is the width of the slit and $k = \frac{2\pi n_m}{\lambda}$ is the wavenumber in the outer medium. We also used this formula for the calculation of the diffraction by multiple cylinders, assuming that the collection of all cylinders forms a thin obstacle of the same width as the illuminated side of the finite area. We could show that the peaks of the scattering function in forward direction resemble the peaks calculated by the slit-diffraction theory (see reference [2]). The question remains if the slit-diffraction approximation is applicable for dielectric obstacles of finite thickness. On the left-hand side of Fig. 2 we compare the slit diffraction results for a 10 µm slit with the FDTD simulations output for diffraction by dielectric obstacles of finite thickness. For rectangular obstacles, a deviation from the slit diffraction results is observed even if we assume a perfectly absorbing material (perfectly electric conductor - PEC [5]). If we reduce the thickness of the rectangular obstacle, the results converge to the slit solution, also for dielectric materials. On the right-hand side of Fig. 2 the results for a broader slit of 50 µm are also depicted. In summary we can state that the slit diffraction is not applicable if we treat rectangular obstacles of finite thickness. While the period length of the minima and maxima does not change much, a location shift of the minima and maxima is observed. The location is also dependent on the (complex) refractive index of the dielectric media.

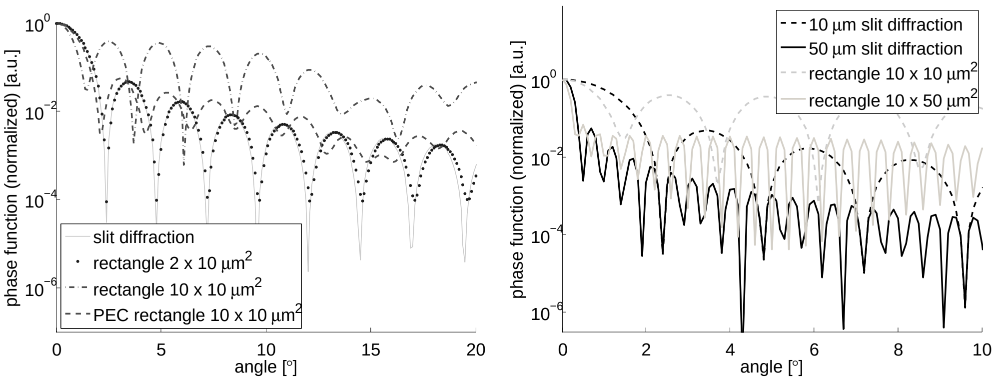

Figure 2. Left: Diffraction by a slit compared to diffraction by different rectangular obstacles. Right: Diffraction by a slit and a rectangular obstacle of various width.

Comparison of diffraction calculations with multiple cylinder scattering results

Based on the diffraction results of the previous section we would not assume that the slit diffraction theory is applicable to our multiple cylinder model, since we are dealing with dielectric cylinders arranged in a finite area. We would rather expect that the diffraction of our model resembles the diffraction pattern by a rectangular profile of the same size as the finite area. In Fig. 3 we compare the diffraction by different obstacles with sizes of $A = 10 \times 10$ µm^2 and $A = 10 \times 50$ µm^2. It can be seen that the multiple cylinder results differ from the results obtained from diffraction by the rectangular obstacle having the same size as the area occupied by the cylinders. On the other hand, the slit diffraction gives a good approximation for the location and period of the minima and maxima in the diffraction pattern of the multiple cylinder solution, especially when the cylinders are considered to be perfectly absorbing. Also, we examined an ordered structure of a grid of 4×4 and 4×20 cylinders with a grid length of 2.5 µm, respectively. For the ordered structure the slit diffraction solution fits even better.

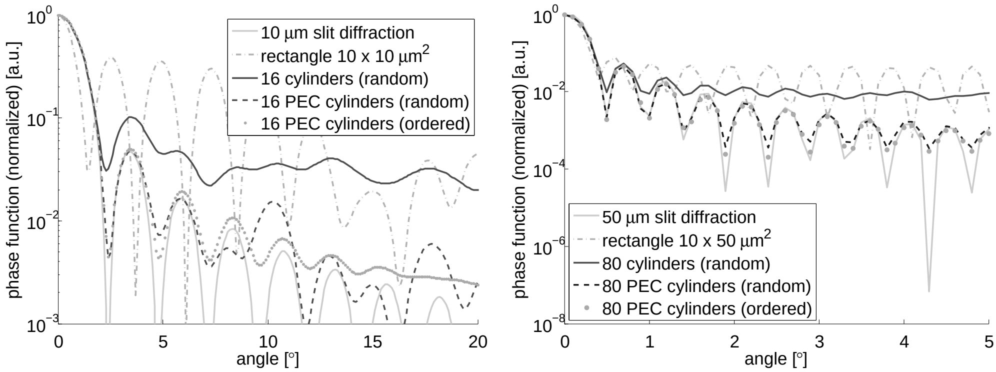

Figure 3. Left: Comparison of diffraction results for the case of $A = 10 \times 10\ \mu\text{m}^2$. Right: Comparison of diffraction results for the case of $A = 10 \times 50\ \mu\text{m}^2$. The broader side is illuminated.

CONCLUSION

We presented a comparison between Maxwell and RTE solutions and depicted the occurrence of forward diffraction peaks in the Maxwell results. We confirmed that in general it is not possible to use the single-slit diffraction approximation to explain diffraction by dielectric obstacles of finite thickness. On the other hand, we could show that this approximation indeed seems to give suitable results for the diffraction of multiple cylinders distributed in a finite area.

To do a better comparison of the Maxwell and RTE solutions, as applied to an infinite expanse of random cylinders, these diffraction effects have to be suppressed since they cannot be explained by means of radiative transfer theory. With our calculations we could qualitatively explain the cause of these effects, but we are not able to quantitatively subtract these effects from our Maxwell results. To get rid of these effects, we have to distribute the cylinders in an infinite (or very broad) slab and use a spatially limited (e.g. focused) source. The Monte Carlo solution of the RTE can easily be extended for performing these calculations. Our FDTD solution offers possibilities to perform such investigations in the Maxwell regime.

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