# Scattering of light by multiple dielectric cylinders: comparison of radiative transfer and Maxwell theory

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We have compared radiative transfer theory with analytical solutions of the Maxwell equations for light scattering by multiple infinitely long parallel cylinders at perpendicular incidence. The calculated scattering cross sections for both methods show large differences, but the angle-dependent differential scattering cross-section results are very similar for small cylinder densities, except close to the forward direction. In contrast to recently published results, it is shown that the radiative transfer equation is a useful approximation for small cylinder concentrations. © 2008 Optical Society of America

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In the field of biomedical optics the radiative transfer theory is generally used to calculate the light propagation in biological tissue. The radiative transfer theory can be derived directly from the Maxwell theory, giving general restrictions to the applicability [1]. Still, the task of quantitatively examining these restrictions for special problems remains. For example, it is not clear under what conditions radiative transfer theory can be used for the description of the light propagation in biological tissue. Since it disregards near-field scattering and other effects owing to the wave nature of light, numerical solutions of the Maxwell equations have also been applied [2]. One way of solving the radiative transfer equation is by Monte Carlo simulations [3,4]. Recently, a comparison between Monte Carlo simulations and numerical solutions of the Maxwell equations for the scattering of light by multiple spheres was presented, indicating large differences in the calculated scattering cross sections [5]. These results suggest that radiative transfer theory would not be applicable, even for small particle densities.

In this Letter we compare Monte Carlo simulations with analytical solutions of the Maxwell equations for the scattering of light by multiple cylinders. In addition to the approach presented in [5] we calculated the angle-dependent differential scattering cross sections (i.e., unnormalized phase functions). Considering these results, we show that the radiative transfer theory is indeed a useful approximation to the Maxwell equations, provided that the cylinders are randomly distributed and their concentration is small.

The analytical solution of the Maxwell equations for the scattering of obliquely incident light by multiple parallel infinitely long cylinders has been described in [6]. For the case of perpendicular incidence the nonzero elements of the amplitude scattering matrix can be calculated as

$$\begin{Bmatrix} T_1(\theta) \\ T_2(\theta) \end{Bmatrix} = \sum_{j=1}^{N} \sum_{n=-M}^{M} e^{in\theta} e^{ikR_{1j}\cos(\gamma_{1j}-\theta)} \begin{Bmatrix} b_{jn} \\ a_{jn} \end{Bmatrix}, \tag{1}$$

where $\theta$ is the scattering angle, $k$ is the wavenumber, $N$ is the number of cylinders, $\gamma_{lj}$ denotes the angle between the position vectors of the $l$th and $j$th cylinders, and their distance is represented by $R_{lj}$. In general, the second sum goes from $-\infty$ to $\infty$, but convergence of the sum is achieved at some truncation number $M$, which has been estimated using Eq. (25) in [7]. The unknown expansion coefficients $a_{jn}$ and $b_{jn}$ are related to the single-cylinder scattering coefficients $a_{jn}^0$ and $b_{jn}^0$ [8] by the following equation system:

$$\sum_{l=1}^{N} \sum_{s=-M}^{M} \left( \delta_{lj}\delta_{ns} + (1-\delta_{lj}) G_{ls}^{jn} \begin{Bmatrix} b_{jn}^0 \\ a_{jn}^0 \end{Bmatrix} \right) \begin{Bmatrix} b_{ks} \\ a_{ks} \end{Bmatrix} = \epsilon_j \begin{Bmatrix} b_{jn}^0 \\ a_{jn}^0 \end{Bmatrix}, \tag{2}$$

$$G_{ls}^{jn} = (-1)^{s-n} H_{s-n}(kR_{lj}) e^{i(s-n)\gamma_{lj}}. \tag{3}$$

Here $H$ is the Hankel function of the first kind, $\delta$ denotes the Kronecker delta, and $\epsilon_j$ comprises the phase shift of the incident wave at the $j$th cylinder relative to the reference. The differential scattering cross section, $\sigma$, the total scattering cross section, $C_{sca}$, and the anisotropy factor, $g$, for unpolarized light were calculated from the amplitude-scattering-matrix elements with [8]

$$\sigma(\theta) = \frac{1}{\pi k}(|T_1(\theta)|^2 + |T_2(\theta)|^2), \tag{4}$$

 

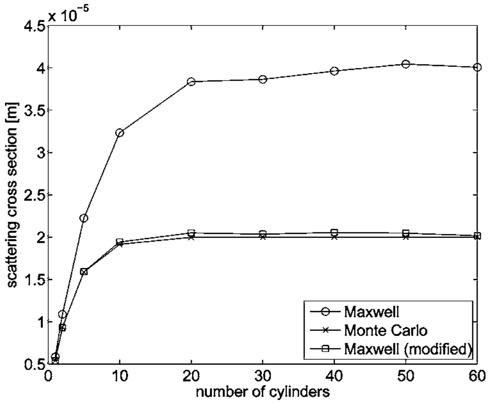


Fig. 1. Simulation results of the scattering cross section for different numbers of cylinders.

$$C_{sca} = \int_0^{2\pi} \sigma(\theta) \mathrm{d}\theta, \quad (5)$$

$$g = \frac{1}{C_{sca}} \int_0^{2\pi} \sigma(\theta)\cos(\theta) \mathrm{d}\theta. \quad (6)$$

We performed a series of simulations to compare the Maxwell solutions for the scattering of light by multiple cylinders with results of the Monte Carlo method. For our simulation model we used infinitely long parallel cylinders with a diameter of $d=2\ \mu\mathrm{m}$ and a refractive index of 1.33. The cylinders were located in an outer medium with refractive index 1.52 and placed in a region of size $A=20\times 20\ \mu\mathrm{m}^2$. We note that the parameters were chosen to model tubules in human dentin [3]. The vacuum wavelength of the incident light was set to $\lambda=633$ nm. We performed calculations for different numbers of cylinders, thus varying the cylinder density, $\rho$. One prerequisite of the applicability of the radiative transfer theory is the randomness of the particle distribution. The Maxwell solution for one certain cylinder distribution gives a scattering pattern affected by speckles. For a proper comparison we averaged our Maxwell results over multiple cylinder distributions in order to suppress the speckles. We solved the Maxwell equations for 100 different realizations for each cylinder number. For the preparation of the random distribution we used a method where we assigned randomly generated positions to the parallel cylinders, ensuring that they were located in the considered area and did not overlap.

The details of our Monte Carlo code for the calculation of the light propagation in scattering media containing cylinders were presented elsewhere [3,4]. The same geometrical and optical quantities as for the solution of the Maxwell equations were used. An area of $20\times 20\ \mu\mathrm{m}^2$ containing randomly positioned cylinders was simulated. At the border of this area matched boundary conditions were used. The quadratic area was illuminated perpendicular to a border with a line source having a length of $20\ \mu\mathrm{m}$. The applied phase function was calculated from the single-cylinder Maxwell solution using the parameters described above. The scattering coefficient was calculated using

$$\mu_s = NC_{sca}d/A. \quad (7)$$

The differential and total scattering cross sections were obtained scoring the remitted and transmitted photons versus emission angle.

In Fig. 1 the scattering cross sections versus the cylinder number for the Maxwell and the Monte Carlo solutions are depicted. One can see a large difference between the two methods. The scattering cross section for the Monte Carlo results for large $N$ converges to $20\ \mu\mathrm{m}$, which is the illuminated cross section. The deviation from the linear increase ($N<5$) is due to multiple scattering. From the Maxwell solution for single-cylinder scattering it is known that the scattering cross section may exceed the geometrical cross section considerably and is equal to twice the geometrical cross section for large particles ($d \gg \lambda$).

In Fig. 2 the differential scattering cross sections for different numbers of cylinders are shown. For angles larger than about 10° good agreement between the results of the two distinct methods can be seen. We note that in the Monte Carlo simulation for a specific cylinder number there is a distribution of the actual number of scattering events performed by each photon. For example, for the scattering by a single cylinder there is also a certain probability of the occurrence of zero, two, or more scattering events. This explains the differences between the Maxwell and the Monte Carlo results for small numbers of cylinders. We calculated a corrected differential scattering cross section for one- and five-cylinder scattering by weighting the Maxwell results according to the distribution of cylinder numbers corresponding to the Monte Carlo simulations (Fig. 2, bold curves). Owing to dependent scattering, which is not treated by the Monte Carlo simulations, the differences between the Maxwell and the Monte Carlo solutions get larger as the cylinder density increases. We note that a coherent backscattering peak is observed for the Maxwell solutions [1].

The largest disagreement between the two methods is observed close to the forward direction. Figure 3 shows the differential scattering cross sections of Fig. 2 in more detail for 0° to 20°. A strong forward-scattering peak and oscillations can be seen for the Maxwell solution that are caused mainly by two processes. The first is coherent forward scattering [1].

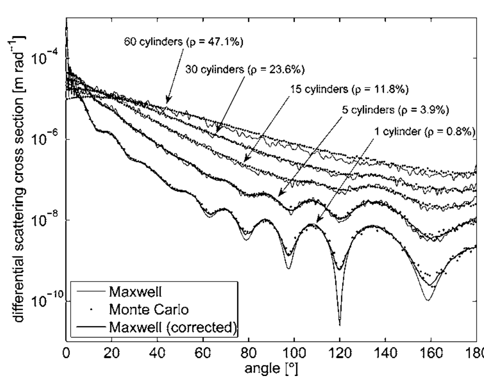


Fig. 2. Differential scattering cross section versus scattering angle for different numbers of cylinders.

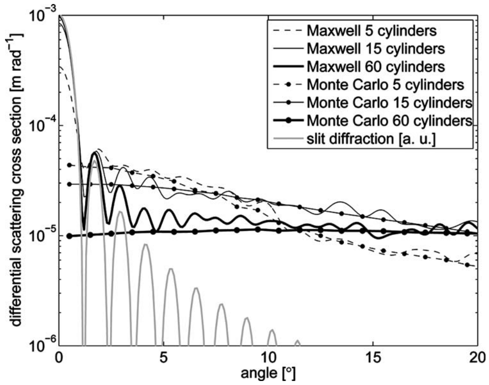


Fig. 3. Differential scattering cross section versus scattering angle for different numbers of cylinders in forward-scattering direction.

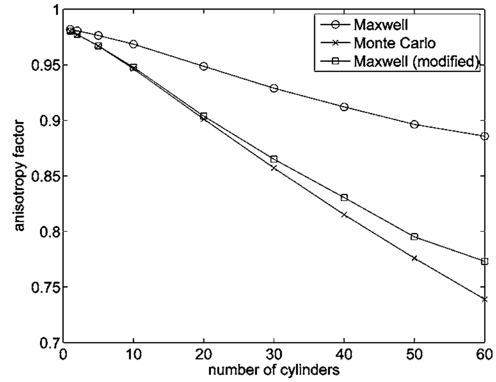


Fig. 4. Simulation results of the anisotropy factor for different numbers of cylinders.

The impact of this effect is reduced by multiple scattering. Second, since we have a finite volume that is illuminated by an infinite plane wave, diffraction effects occur. The diffraction pattern of a slit of 20 $\mu$m width is sketched in Fig. 2 (gray curve). One can see a correlation between the oscillations in the scattering patterns of the multiple cylinder and the slit solutions. These two processes, coherent forward scattering and diffraction by the finite volume, cannot be accounted for by the radiative transfer theory. However, finite volume diffraction can be neglected in a typical situation where the scattering of a light beam by an infinite slab is calculated. Additionally, since the width of the beam, $D$, is in general much larger than the wavelength, coherent forward scattering is concentrated in a narrow forward peak and is for $D \to \infty$ indistinguishable from the unscattered light in Monte Carlo simulations.

To do an adequate comparison, we investigated a simple approach to neglect the coherence and diffraction effects in the calculation of the scattering cross section for the Maxwell results. For this purpose we replaced the differential scattering cross-section values in Eq. (5) for angles smaller than 7° by the corresponding Monte Carlo results. The angle has been somewhat arbitrarily chosen, but other reasonable cutoff angles did not change the presented results significantly. With these modifications we get good agreement between the two theories for up to 60 cylinders, as can be seen in Fig. 1 (squares). In addition, we made the same modifications for the calculation of the anisotropy factor. As can be seen in Fig. 4, the raw anisotropy factor from the Maxwell solution differs largely from the Monte Carlo results. The modified data fit well with the Monte Carlo results for small numbers of cylinders but have larger differences than the modified scattering cross section, especially for high concentrations. We note that we got similar results when we used different refractive indices or different extents of the simulation area.

In summary, we showed that the main differences between radiative transfer and Maxwell solutions are due to coherent forward scattering and finite volume diffraction. By neglecting these effects we could calculate modified scattering cross section and anisotropy factor values that fit well with the Monte Carlo results for small concentrations. In conclusion, contrary to results in literature, we found that the radiative transfer theory is a good approximation to the Maxwell equations for scattering by multiple cylinders if the cylinder density is reasonably small ($\rho < 10\%$). For higher concentrations the errors get larger owing to dependent scattering. We note that for mean tubule concentrations in human dentin of $\rho \approx 12.5\%$, a small but systematic error is obtained when the radiative transfer theory is applied ($\approx 2.5\%$ for $(1-g)$, which is the relevant quantity for effective scattering).

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