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Virtual Optical Experiment: Characterizing the Coherent Effects of Light Scattering through Macroscopic Random Media

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A virtual optical experiment is established by implementing the pseudospectral time-domain technique with parallel computing resources. This numerical platform is grid-based and enables simulation of light scattering by an arbitrary geometry of macroscopic dimensions. Based upon Maxwell's equations, the proposed numerical platform simulates an idealized light scattering experiment in a practically noiseless environment with controllable variables. In this manuscript, we investigate the angular and spectral light scattering characteristics of a cluster of coated dielectric cylinders. Specific results suggest that microscopic structural details is correlated to macroscopic scattering characteristics.

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KEYWORDS: coherent light scattering, random media, Maxwell's equations

1. Introduction

Non-invasive optical imaging techniques such as optical coherence tomography[1–4] and diffuse optical tomography[5–7] are assuming greater importance in modern diagnostic technology. Without damaging live tissues, these techniques target the detection of changes in optical properties resulting from normal developmental biology, normal biologic responses to internal or external stimuli, or pathologic situations such as cancer, infections, stroke, heart attack, or jaundice. As a result, it is important to establish the connection between macroscopic scattered light (the signal that can be measured in experiments) and its microscopic origin, which will provide a firm foundation upon which optical diagnostic techniques are developed.

Recently, it has been shown that the near-field coherent effects of light may provide critical information for optical diagnostic applications,[8] yet, the underlying mechanisms of such coherent effects are not well understood. Furthermore, to date, most simulation techniques for light scattering through macroscopic, irregular geometries involve heuristic approximations which fall short to account for coherent or near-field effects. As a result, optical characteristics that may potentially play a critical role for optical diagnostic purpose may be obscured by such approximations; a rigorous simulation without heuristic approximations is desired.

Owing to the extreme complexity involved, light scattering by macroscopic random media (e.g., tissue optics) has been studied mostly involving heuristic approximations that are based upon the radiative transfer theory, including the Monte Carlo technique,[9] and diffusion approximation.[10] In order to accurately determine the optical characteristics of biological structures, a rigorous numerical method, the finite-difference time-domain (FDTD) technique, has been employed to simulate light scattering by a single cell by Drezek *et al.*[11] Nevertheless, due to the intense computations required, a simulation of a problem of macroscopic dimensions, e.g., a cluster of biological cells, was not feasible.

In this manuscript, we report employing the pseudospectral time-domain (PSTD) technique pioneered by Liu[12] to establish a numerical platform capable of accurately simulating light scattering by an irregular geometry of *macroscopic* dimensions. While achieving accuracy comparable to the rigorous FDTD algorithm, the PSTD algorithm significantly reduces computer storage requirements and run time. As a result, the PSTD technique enables simulation of a much larger system than the FDTD technique.

Similar to the FDTD technique, the PSTD technique is a grid-based simulation, enabling simulation of light scattering by an arbitrary geometry. An initial simulation study of light scattering by macroscopic random media by employing the PSTD technique was previously reported.[13] In this manuscript we report simulation of a system of complex random media — a cluster of randomly positioned coated dielectric cylinders. This is the two dimensional (2-D) analogy of a cartoonized version of a biological tissue structure. A cluster of coated cylinders bears arguable similarity to actual biological tissue; nevertheless, the virtual optical experiment reported in this manuscript represents the initial attempt to rigorously determine the optical characteristics of biological random media of macroscopic dimensions based upon fundamental electromagnetic principles — Maxwell's equations.

Our long-term goal is to analyze the optical characteristics of biological structures in a noiseless environment via the proposed virtual optical experiment while gradually increasing the complexity of structural details. By placing the simulation of light scattering within biological tissues on firm ground, the virtual optical experiment can provide essential information on near-field and coherent interference effects that may be critical for the development of medical diagnostic techniques for early detection of diseases.

2. Methods

We employ the PSTD technique to establish a numerical platform, the virtual optical experiment, to simulate light scattering by an irregular geometry of *macroscopic* dimensions. The PSTD technique is very similar to the FDTD technique, but uses fast Fourier transforms [eq. (1)] to calculate the spatial derivatives of Maxwell's equations in the frequency domain. By transforming each of the electric and magnetic fields into the frequency domain via discrete Fourier transform (DFT), multiplying them by a factor of $j\tilde{k}_x$ in the frequency domain, and inverse DFT to transform it back to the time domain, the derivatives of all fields in the entire space can be obtained accurately.

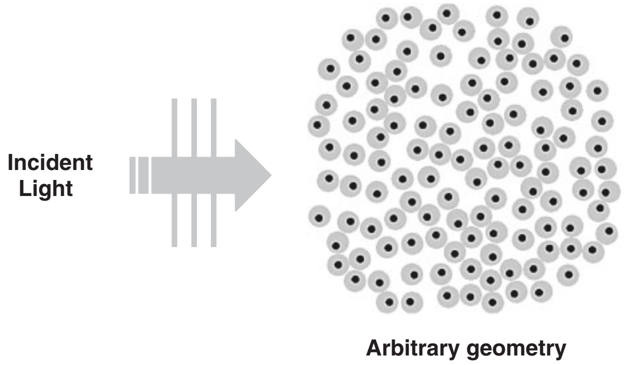

Fig. 1. Schematic of virtual optical experiment. Based upon the PSTD technique, the virtual optical experiment can simulate light scattering by *arbitrary* geometries. More importantly, it is capable of simulating a much larger problem that is infeasible using the FDTD technique. Unlike other approximation methods based upon heuristic assumptions, the error of the virtual optical experiment can be arbitrarily minimized by increasing the simulation resolution.

$$\left\{ \frac{\partial V}{\partial x}\bigg|_i \right\} = -\mathsf{F}^{-1}(j\tilde{k}_x \mathsf{F}\{V_i\}) \quad (1)$$

Here V represents the electric or magnetic fields; F and F^{-1} denote, respectively, the forward and inverse DFT, and $\tilde{k}_x$ is the DFT variable representing the x-component of the numerical wave vector. The field derivatives calculated via [eq. (1)] are spectrally accurate which permits the PSTD meshing density to approach the Nyquist limit, i.e., two samples per wavelength in each spatial dimension.

In this manuscript, we report a virtual optical experiment based upon the PSTD simulation of the transverse magnetic light scattering by a macroscopic cluster of coated dielectric cylinders in vacuum. A uniform PSTD grid with a spatial resolution of 0.3 µm is used, equivalent to $0.42\lambda_{\rm d}$ ($\lambda_{\rm d}$: wavelength in dielectric medium) at 300 THz for a refractive index (n) of 1.2. An irregular geometry of randomly positioned, coated cylinders is generated with random numbers. Two cases of study are shown: light scattering by a cluster of concentric coated cylinders (Fig. 3), and light scattering by a cluster of off-center coated cylinders (Fig. 4). Analyzing the scattering characteristics of all angles and wavelengths is too complex and infeasible; instead, we analyze the total scattering cross-section (TSCS) as a function of frequency, which can be understood as the total effective cross-sectional area that scatters light.

A schematic of the proposed virtual optical experiment is shown in Fig. 1. The cluster consists of 118 coated cylinders with diameter (d) of 10 µm; each cylinder encloses randomly positioned, 3-µm-diameter nuclei with refractive index of 1.2. With a spatial resolution of $\Delta = 0.3$ µm and temporal resolution (Δt) of 0.5×10^{-16} s, the PSTD simulation yields the frequency response from 0.5 to 300 THz ($\lambda_0 = 60$–1 µm) with a resolution of 0.5 THz. The PSTD algorithm is a grid-based simulation technique, which enables accurate simulation of light scattering by an arbitrary geometry. As a result, the proposed virtual optical experiment platform is essentially an idealized optical experiment in a practically noise less environment with controllable variables.

The virtual optical experiment yields both angular and spectral scattering characteristics, as shown in Fig. 2(a), the differential scattering cross-section (DSCS) as a function of angle, and in Fig. 2(b), the TSCS spectrum as a function of frequency, respectively. By implementing a near-to-far-field transformation,[14] the DSCS function can be calculated for a range of frequencies from the PSTD simulation with a pulse incidence of light.

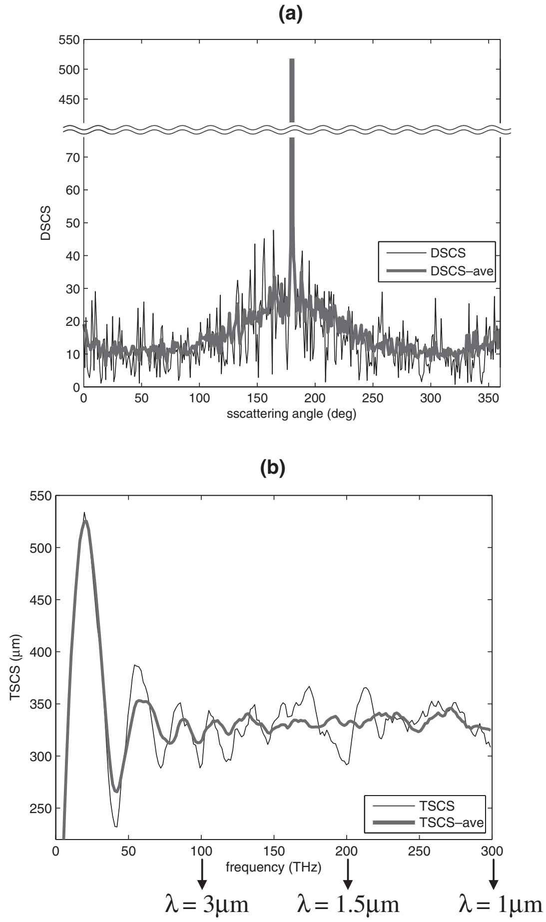

Fig. 2. Light scattering by a cluster of coated cylinders, as shown in Fig. 1, is simulated by employing a virtual optical experiment. The spatial and spectral scattering characteristics are shown in (a) and (b), respectively. (a) With an incident wavelength of $\lambda = 1$ µm, the DSCS and DSCS averaged over 12 different incident angles are shown as a function of scattering angle. (b) The TSCS and TSCS averaged over 12 different incident angles are shown as a function of frequency of the incident light.

Aside from the strong forward scattering peak, significant speckle effect is observed in Fig. 2. This was anticipated since the light source in the simulation is highly coherent, and the interference effect due to coherent scattering by random media results in speckles. By averaging over 12 DSCS functions corresponding to different illumination angles on the same cluster geometry, the speckle effect within the DSCS function is significantly reduced, as shown in Fig. 2(a) as the DSCS-ave function. Similarly, the speckle effect of the TSCS spectrum is also significantly reduced by averaging over 12 different incident angles, as shown in Fig. 2(b) as the TSCS-ave spectrum.

The motivation for calculating DSCS-ave and TSCS-ave is to average out the "randomness", while preserving the characteristics that are specific to the cluster geometry. Note that in the TSCS-ave spectrum, there are complex spectral

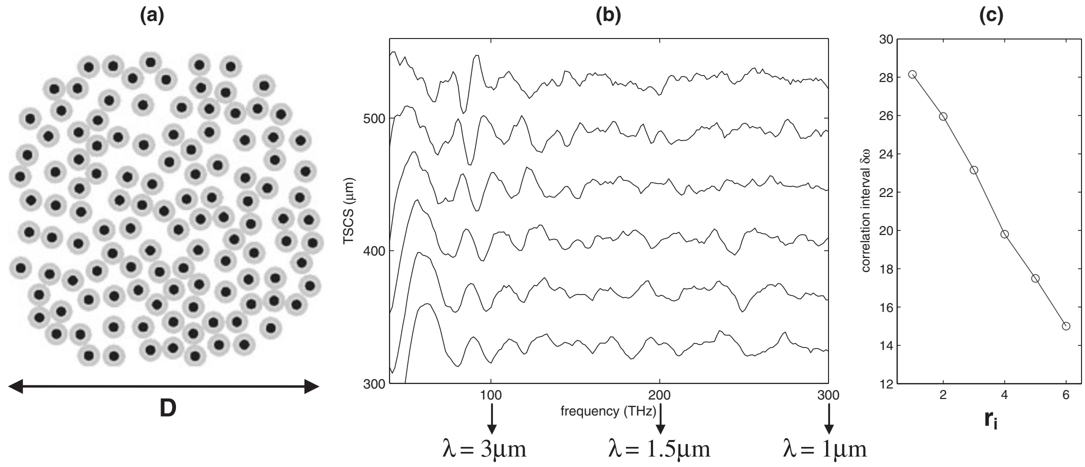

Fig. 3. TSCS-ave spectra of a cluster of concentric coated cylinders. The TSCS-ave spectra of light scattering by a cluster [cluster diameter $D = 160\,\mu$m, as shown in (a)] with an inner cylinder radii $r_{\rm i}$ are shown in (b). (Each TSCS-ave spectrum represents an average of 12 TSCS spectra corresponding to 12 different illumination angles to suppress the speckle effect; in addition, each curve is offset in the y-direction to facilitate comparison.) Note that the TSCS spectra exhibit complex structures that may be relevant to the cluster geometry. An autocorrelation analysis of the TSCS-ave spectra is performed; the $\delta\omega$ is plotted vs $r_{\rm i}$ in (c). It is shown that the $\delta\omega$ changes monotonically with $r_{\rm i}$, suggesting a direct correlation relationship between the macroscopic scattered light and $r_{\rm i}$.

characteristics even after the speckle contribution has been suppressed. This is most likely related to the specific cluster geometry. We further analyze the TSCS-ave spectrum to obtain specific information from the TSCS-ave spectrum indicative of the microscopic structure of the cluster of coated cylinders.

In order to systematically determine the effect of inner cylinder radius on the TSCS-ave spectrum, we begin by simulating the problem of light scattering by a cluster of concentric coated cylinders, in which all the coated cylinders are identical, with the inner cylinder located precisely at the center. The TSCS-ave spectra are compared, each corresponding to the same cluster geometry but with different inner cylinder radii.

3. Results

Light scattering by a 160-μm-diameter cluster consisting of 118 concentric dielectric cylinders is simulated with the virtual optical experiment and is shown in Fig. 3. Each outer cylinder is of 5-μm radius, with an $n = 1.1$, whereas each inner cylinder has an n of 1.2. Six cases are shown, each corresponding to a cluster with a different inner cylinder radius ($r_{\rm i} = 0.5$, 1.0, 1.5, 2.0, 2.5, and $3.0\,\mu$m). Minute variations in the TSCS-ave spectra are observed for different $r_{\rm i}$. In order to determine the relationship between the variations in the TSCS-ave spectra and $r_{\rm i}$, an autocorrelation analysis of the TSCS spectra was performed to obtain the correlation interval $\delta\omega$ (a small $\delta\omega$ value indicates much variations in the TSCS-ave spectrum per unit range.) As shown in Fig. 3(c), $\delta\omega$ of the TSCS-ave spectrum monotonically decreases with respect to $r_{\rm i}$, suggesting that the variations in the TSCS-ave spectra are clearly related to $r_{\rm i}$.

Although the monotonic behavior of $\delta\omega$ shows promising possibilities, we suspected that it might be the result of a special case since the inner cylinders are located precisely at the center of each coated cylinder. Therefore, in order to study a more general case, we then simulated a cluster consisting of 118 coated dielectric cylinders, but with the inner cylinder randomly positioned within each coated dielectric cylinders, as shown in Fig. 4.

Similar to Fig. 3, each outer cylinder has a 5-μm radius and an n of 1.1, whereas each inner cylinder has an n of 1.2. Five cases are shown, each corresponding to a cluster with $r_{\rm i}$ values of 0.5, 1.0, 1.5, 2.0, and $2.5\,\mu$m. Again, minute variations in the TSCS-ave spectra are observed as $r_{\rm i}$ is varied. The result of the autocorrelation analysis is shown in Fig. 4(c). Similar to Fig. 3(c), it can be easily seen that $\delta\omega$ is monotonically correlated with $r_{\rm i}$. On a broader scope, the results of Figs. 3 and 4 suggest that the microscopic structural differences in the sample is correlated to the macroscopic scattering characteristics.

4. Discussion

Although both the TSCS spectrum and DSCS function contain scattering information, it can be readily seen that the TSCS spectra contain information relevant to the structure of the sample (Figs. 3 and 4). This can be understood as different optical wavelengths yield information of different length scales; the cluster geometry exhibits different characteristics for an incident wavelength matching a specific length-scale (e.g., diameter of cylinder, diameter of nuclei, average distance between cylinders) of the cluster geometry. We consider that this is the origin of the spectral signatures of macroscopic scattered light that may be indicative of the microscopic geometry.

Temporal and spatial coherent interference effects may contain essential information indicative of the specific sample structures.[8] As shown in Figs. 2–4, the TSCS-ave spectra exhibit nontrivial structures that may provide information on the geometry. In Figs. 3(c) and 4(c), the dependence of the autocorrelation analysis is depicted. As the radius of the nuclei is increased, $\delta\omega$ decreases; this can also be attributed to the increase in the average refractive index of the coated cylinder, since the nucleus (which has a higher n) occupies a larger portion of the coated cylinder. This relationship requires further analysis for a complete

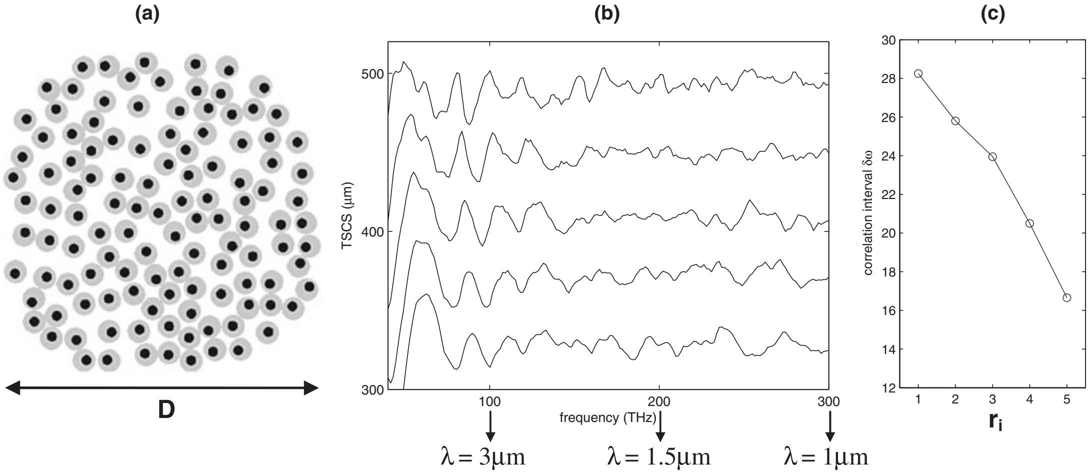

Fig. 4. TSCS-ave spectra of a cluster of coated cylinders with off-center inner cylinder location. Similar to Fig. 3, the TSCS-ave spectra of light scattering by a cluster [$D = 160\,\mu m$, as shown in (a)] of inner cylinder radii r_i are shown in (b). (Each TSCS-ave spectrum represents an average of 12 TSCS spectra corresponding to 12 different illumination angles to suppress the speckle effect; in addition, each curve is offset in the y-direction to facilitate comparison.) Unlike in Fig. 3, each coated cylinder has an off-center, randomly positioned inner cylinder. An autocorrelation analysis of the averaged TSCS spectra of (b) is performed and the results are shown in (c). Again, it is found that $\delta\omega$ changes monotonically with r_i, suggesting a direct correlation relationship between the macroscopic scattered light and the microscopic parameter—inner cylinder radius r_i.

understanding; nevertheless, the simulation results reported in this paper show that microscopic structural changes in the geometry can be detected in the macroscopic scattered light.

More importantly, the proposed optical experiment enables an idealized optical experiment in a practically noiseless environment, providing the opportunity to accurately characterize coherent optical effects. A similar idea of the proposed virtual tissue model has been applied to determine the optical characteristics of a biological cell, pioneered by Drezek *et al.*[11] using the FDTD technique. Nevertheless, due to the intense computational requirements of FDTD, it was infeasible to model a larger system containing more than a few cells. With the PSTD technique, a macroscopic light scattering problem can now be accurately simulated.

5. Conclusions

We have shown in this manuscript that the proposed virtual optical experiment is capable of accurately simulating the problem of light scattering by an irregular geometry of macroscopic dimensions, and can account for coherent interference effects. The proposed simulation is essentially a numerical realization of the analytical solution, enabling a virtual optical experiment with controllable variables in a practically noiseless environment. By employing a systematic analysis, our long-term goal is to unambiguously investigate the microscopic origin of macroscopic scattered light from irregular biological geometries.

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1) S. B. Adams, P. R. Herz, D. L. Stamper, M. J. Roberts, S. Bourquin, N. A. Patel, K. Schneider, S. D. Martin, S. Shortkroff, J. G. Fujimoto, and M. E. Brezinski: J. Orthop. Res. **24** (2006) 708.
2) G. J. Jaffe and J. Caprioli: Am. J. Ophthalmol. **137** (2004) 156.
3) J. Welzel: Skin Res. Technol. **7** (2001) 1.
4) J. G. Fujimoto, C. Pitris, S. A. Boppart, and M. E. Brezinski: Neoplasia **2** (2000) 9.
5) J. P. Culver, A. M. Siegel, J. J. Stott, and D. A. Boas: Opt. Lett. **28** (2003) 2061.
6) A. Corlu, T. Durduran, R. Choe, M. Schweiger, E. M. C. Hillman, S. R. Arridge, and A. G. Yodh: Opt. Lett. **28** (2003) 2339.
7) D. A. Boas, D. H. Brooks, E. L. Miller, C. A. DiMarzio, M. Kilmer, R. J. Gaudette, and Q. Zhang: IEEE Signal Process. Mag. **18** (2001) 57.
8) Y. L. Kim, Y. Liu, R. K. Wali, H. K. Roy, and V. Backman: Appl. Opt. **44** (2005) 366.
9) A. D. Kim, C. Hayakawa, and V. Venugopalan: Opt. Lett. **31** (2006) 1088.
10) S. H. Tseng, J. H. Greene, A. Taflove, D. Maitland, V. Backman, and J. T. Walsh: Opt. Lett. **30** (2005) 56.
11) R. Drezek, A. Dunn, and R. Richards-Kortum: Opt. Express **6** (2000) 147.
12) Q. H. Liu: IEEE Trans. Geosci. Remote Sens. **37** (1999) 917.
13) S. H. Tseng, J. H. Greene, A. Taflove, D. Maitland, V. Backman, and J. Walsh: Opt. Lett. **29** (2004) 1393.
14) A. Taflove and S. C. Hagness: *Computational Electrodynamics: The Finite-Difference Time-Domain Method* (Artech House, 2000).