行政院國家科學委員會專題研究計畫 成果報告

虛擬生物組織：精確探究巨觀生醫光訊號之微觀起源
研究成果報告(精簡版)

計 畫 類 別 ：個別型
計 畫 編 號 ：NSC 95-2112-M-002-039-
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執 行 單 位 ：國立臺灣大學光電工程學研究所

計畫主持人：曾雪峰

計畫參與人員：碩士班研究生-兼任助理：黃柏燁、翁佑菱、張維典、鐘煒竣

報 告 附 件 ：國外研究心得報告
出席國際會議研究心得報告及發表論文

處 理 方 式 ：本計畫可公開查詢

中 華 民 國 96 年 09 月 18 日

附件一

行政院國家科學委員會補助專題研究計畫 ■成果報告 □期中進度報告

虛擬生物組織：
精確探究巨觀生醫光訊號之微觀起源

計畫類別：■個別型計畫 □整合型計畫
計畫編號：NSC 95-2112-M-002-039-
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計畫主持人：曾雪峰
共同主持人：
計畫參與人員：黃柏燁，翁佑菱，張維典，鐘煒竣

成果報告類型(依經費核定清單規定繳交)：■精簡報告 □完整報告

本成果報告包括以下應繳交之附件：
□赴國外出差或研習心得報告一份
□赴大陸地區出差或研習心得報告一份
■出席國際學術會議心得報告及發表之論文各一份
□國際合作研究計畫國外研究報告書一份

處理方式：除產學合作研究計畫、提升產業技術及人才培育研究計畫、列管計畫及下列情形者外，得立即公開查詢
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執行單位：

中 華 民 國 96 年 9 月 18 日

行政院國家科學委員會專題研究計畫成果報告

虛擬生物組織：精確探究巨觀生醫光訊號之微觀起源

計畫編號： NSC 95-2112-M-002-039-

主持人：曾雪峰 國立台灣大學 光電工程研究所 助理教授

計畫參與人員： 黃柏燁, 翁佑菱, 張維典, 鐘煒竣

中文摘要

欲精確地分析出生物隨機界質的光學性質，一個根據基本電磁學理論的精確分析方法是不可或缺的。本計畫以 PSTD (Pseudospectral time-domain method) 的演算法，建構一個虛擬生物組織模型，藉以探索生物組織的光學特性。利用此虛擬實驗有系統地分析其光學特性，以精確地探索巨觀散射光與微觀細胞結構關係。本研究已完成初步分析巨觀隨機介質的光學特性。研究結果可提供生醫光電研究重要的資訊，目前已發表於 Japanese Journal of Applied Physics (*in press*) and Applied Physics Letters (2007. 91(051114), DOI: 10.1063/1.2767777)。

關鍵詞：PSTD，馬克士威方程式，隨機介質

Abstract

A virtual optical experiment is established by implementing the pseudospectral time-domain (PSTD) 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 the fundamental electromagnetic principles, the proposed numerical platform simulates an idealized light scattering experiment in a practically noise-less environment with controllable variables. In this manuscript, we investigate the angular and spectral light scattering characteristics of a cluster of dielectric coated cylinders. Specific results suggest that a spectral signature directly relating the macroscopic scattered light to its microscopic origin is identified. Research findings will provide essential information to the research of biomedical optics, and have been published in: Japanese Journal of Applied Physics (*in press*) and Applied Physics Letters (2007. **91**(051114), DOI: 10.1063/1.2767777).

***Keywords*:** Maxwell's equations, macroscopic random media, PSTD, light scattering

Introduction

We report employing the pseudospectral time-domain (PSTD) technique to establish a numerical platform capable of accurately simulating light scattering by an irregular geometry of *macroscopic* dimensions. The PSTD technique is a grid-based simulation, enabling simulation of light scattering by an arbitrary geometry. In addition, while achieving accuracy comparable to the rigorous FDTD algorithm (12), the PSTD algorithm significantly reduces computer storage and running-time, therefore enabling simulation of a much larger system than the FDTD technique (12). Combined with parallel computing resources, light scattering problems of macroscopic dimensions that were not solvable can now be accurately studied by employing the PSTD technique.

By placing the simulation of light scattering within biological tissues on firm ground, the virtual optical experiment can provide essential information regarding near-field and coherent interference effects that may be critical for the development of medical diagnostic techniques for early detection of diseases.

Method

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 $0.42\lambda_d$ (λ_d: wavelength in dielectric medium) at 300 THz for a refractive index n = 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-centered coated cylinders (Fig. 4). Analyzing the scattering characteristics of all angles and all 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. The spectral scattering characteristics, the TSCS spectrum is calculated and analyzed.

Parallel computing resource is required to simulate a light scattering problem of macroscopic dimensions. By employing a computer cluster with 4 Xeon 3.2GHz processors, each simulation with physical dimensions 200μm-by-200μm roughly takes about 4 hours. While fixing the positions of each coated cylinder and gradually varying the inner cylinder radius, the effect of the radius on the overall scattering characteristics of the irregular geometry is investigated.

The schematic of the proposed virtual optical experiment is shown in Fig. 1. The PSTD algorithm is a grid-based simulation technique, therefore enabling light scattering simulation by an arbitrary geometry. However, stair-casing error may occur as a result of coarse grid resolution. Yet, unlike other heuristic approximation methods, the stair-casing error can be arbitrarily minimized by increasing the simulation resolution. As a result, the proposed virtual optical experiment platform is essentially an idealized optical experiment in a practically noise-less environment; in addition, the virtual optical experiment allows more freedom and control over the research parameters than actual optical experiments. By means of a systematic approach, it is possible to accurately determine the effect of a certain parameter (*e.g.* radius of nuclei) without varying other parameters. The objective of this research is to rigorously determine the microscopic origin of macroscopic scattered light.

The virtual optical experiment yields both angular scattering characteristics 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 total scattering cross-section (TSCS) spectrum as a function of frequency, respectively. Aside from the strong forward scattering peak, significant speckle effect is observed in Fig. 2. This is anticipated since the light source in the simulation is highly coherent, and the interference effect due to coherent light scattered by random media results in speckles. By averaging over 12 DSCS functions corresponding to different illumination angles upon 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 is specific to the cluster geometry. Notice that in the TSCS-ave spectrum, there are complex spectral characteristics even after the speckle contribution has been suppressed. This is mostly likely relevant to the specific cluster geometry. We further analyze the TSCS-ave spectrum, our goal is 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, where each 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.

Results

Light scattering by a 160um-diameter cluster consisting of 118 concentric dielectric cylinders is simulated with the virtual optical experiment and shown in Fig. 3. Each outer cylinder is of 5-μm radius, with a refractive index of n= 1.1, whereas each inner cylinder has a refractive index of n= 1.2. Six cases are shown, each corresponding to a cluster with the inner cylinder radius

r_i= 0.5 μm, 1.0 μm, 1.5 μm, 2.0 μm, 2.5 μm, 3.0μm, respectively. Minute variations of the TSCS-ave spectra are observed for different inner cylinder radius r_i. In order to determine the relationship of the variations of the TSCS-ave spectra and r_i, an autocorrelation analysis of the TSCS spectra is performed to obtain the correlation interval $\delta\omega$ (a small $\delta\omega$ value would indicate many variations of the TSCS-ave spectrum per unit range.) As shown in Fig. 3(b), the correlation interval $\delta\omega$ of the TSCS-ave spectrum monotonically decreases with respect to r_i, suggesting that the variations of the TSCS-ave spectra is clearly related to the inner cylinder radius r_i.

Though the monotonic behavior of the correlation interval $\delta\omega$ 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 is of 5-μm radius, with a refractive index of n= 1.1, whereas each inner cylinder has a refractive index of n= 1.2. Five cases are shown, each corresponding to a cluster with a inner cylinder radius r_i = 0.5 μm, 1.0 μm, 1.5 μm, 2.0 μm, 2.5 μm, respectively. Again, minute variations of the TSCS-ave spectra are observed as the r_i is varied. The result of the autocorrelation analysis is shown in Fig. 4(b). Similar to Fig. 3(b), it is easily seen that the correlation interval $\delta\omega$ clearly exhibits a monotonic behavior with respect to r_i. On a broader scope, the results of Figs. 3 and 4 suggest that the microscopic structural differences of the sample can be related to the macroscopic scattering characteristics.

Discussion

The proposed virtual optical experiment is based upon the PSTD algorithm. Therefore, since the PSTD technique is a grid-based simulation, there will be stair-casing error due to the resolution of the grid. However, unlike other approximation methods, such error can be arbitrarily minimized with increasing resolution. In other words, the proposed virtual optical experiment is practically an idealized experiment that can be as accurate as desired.

In this manuscript we focus on exploring the spectral light scattering characteristics (TSCS spectrum). Though both the TSCS spectrum and DSCS function contain scattering information, it is suggested that the TSCS spectra may contain information relevant to the structure of the sample, as shown in Figs. 3 and 4. This can be understood as different wavelengths of light provide information of different length-scales; it is anticipated the cluster geometry will exhibit different characteristics if the incident wavelength matches a specific length-scale of the cluster geometry. We believe this is the origin of the spectral signatures of macroscopic scattered light that may be indicative of the microscopic geometry.

Significant amount of speckle effect is observed as shown in Fig. 2(a), due to the fact that the light source in the simulation is perfectly coherent, and speckles are caused by the coherent interference from the irregular geometry. In actual experiments, speckles are less pronounced for aqueous samples, due to the Brownian motion which averages out the speckle effect. In the proposed virtual optical experiment, the speckle effect in the simulations can be reduced by ensemble averaging of the DSCS function (averaging the DSCS function corresponding to a different incident angle upon the same geometry,) as shown in Fig. 2 as the DSCS-ave function. Likewise, the TSCS spectrum also consists of a significant amount of speckle effect, which can be reduced by ensemble averaging, as shown in Figs. 2, 3, and 4 as the TSCS-ave spectrum.

In addition to the speckle effect, the proposed virtual optical experiment can accurately simulate the near-field and coherent interference effects for macroscopic light scattering problems. Such effects are usually disregarded in conventional simulation methods, since the wave nature of light is often compromised by the research hypotheses. Furthermore, even in actual experiments, the coherent interference effects may be overlooked since they exhibit noise-like behavior and are indistinguishable from noise.

Temporal and spatial coherent interference effects may contain essential information indicative of the specific sample structures (8). As shown in Figs. 2, 3 and 4, the TSCS-ave spectra exhibit non-trivial structures that may provide information of the specific sample structure. More importantly, the proposed optical experiment enables an idealized optical experiment in a practically noise-less environment, providing the opportunity to accurately characterize the coherent effects; with fixing all variables and varying only one parameter at a time, it is possible to rigorously determine the origin of those coherent interference signatures.

Specifically, we report discovery of a direct relationship of the macroscopic scattered light and the microscopic structure of the sample geometry as shown in Figs. 3 and 4. It is found that there is a monotonic relationship between the correlation interval $\delta\omega$ and the inner cylinder radius r_i. In other words, the reported relationship indicates that larger inner cylinder radius would directly affect the scattering characteristics and resulting in more variations of the TSCS-ave spectrum per unit range. Indeed there should be more parameters of the geometry that may affect the TSCS-ave curve, yet, by means of a systematic analysis, one can accurately determine the effect of each parameter.

Based upon fundamental electromagnetic principles, the proposed virtual optical experiment can accurately determine the optical characteristics of an irregular geometry given the refractive index profile in space. A similar idea of the proposed virtual tissue model has been applied to determine the optical characteristics of a biological cell, pioneered by Dunn, Drezek, and Richards-Kortum (11) using the FDTD technique. However, 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 implemented on parallel computing resources, it is now possible to model the light scattering problem of macroscopic dimensions. By simulating irregular structures with increasing complexity, eventually we would like to model a virtual tissue—the forward problem of determining the optical characteristics of a biological tissue structure.

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 numerical realization of the analytical solution, enabling a virtual optical experiment with controllable variables in a practically noise-less environment. By employing a systematic analysis, it is possible to unambiguously determine the microscopic origin of macroscopic scattered light from irregular geometries.

Acknowledgements

The author is grateful to Drs. Bruce Tromberg, Vasan Venugopalan and Jerome Spanier, who have given helpful suggestions in developing the research concepts of the virtual optical experiment. Also, the author thanks the Taiwan National Science Council Grant 95-2112-M-002-039 for the support of this research, and the Computer and Information Networking Center, National Taiwan University, for the support of high-performance computing facilities. Snow H. Tseng's email address is snow@cc.ee.ntu.edu.tw.

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Figures:

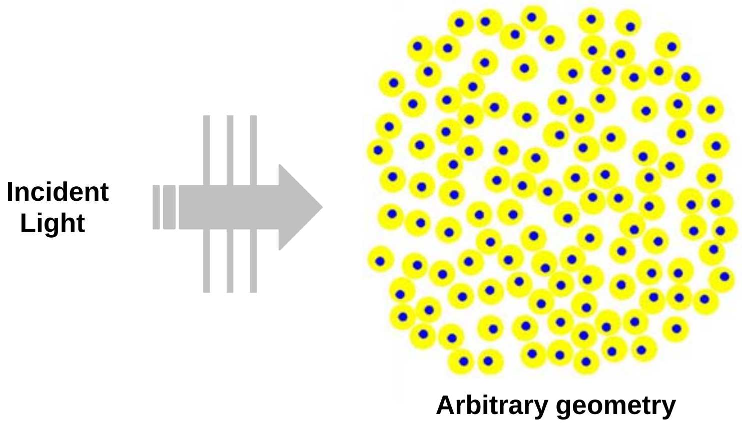

Fig. 1. Schematic of the virtual optical experiment.

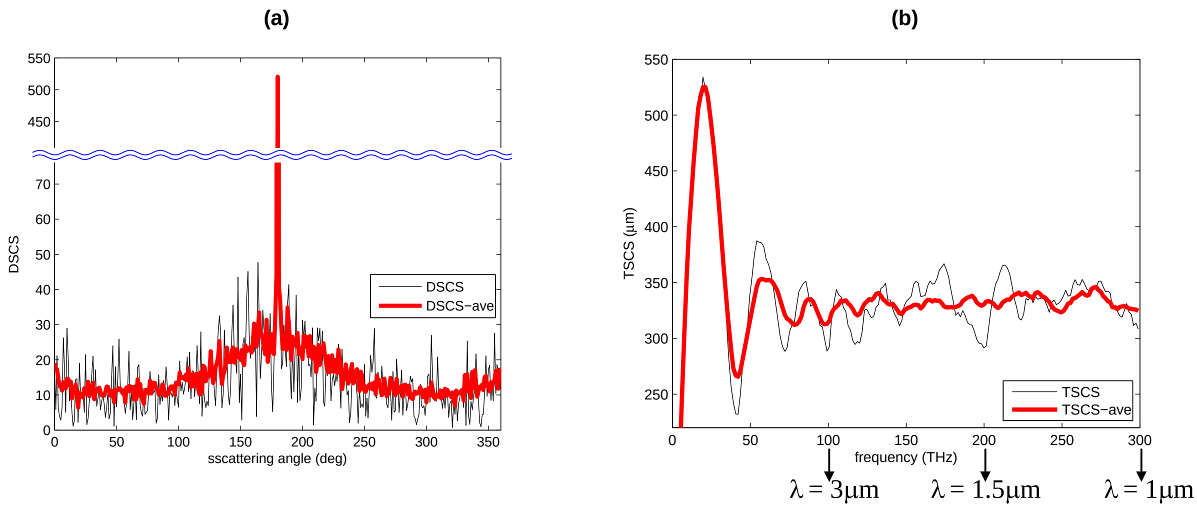

Fig. 2. Light scattering by a cluster of coated cylinders as shown in Fig. 1 is simulated by employing a virtual optical experiment. The spatial and spectral scattering characteristics are shown in (a) and (b), respectively. (a): With an incident wavelength of $\lambda = 1\mu m$, the differential scattering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

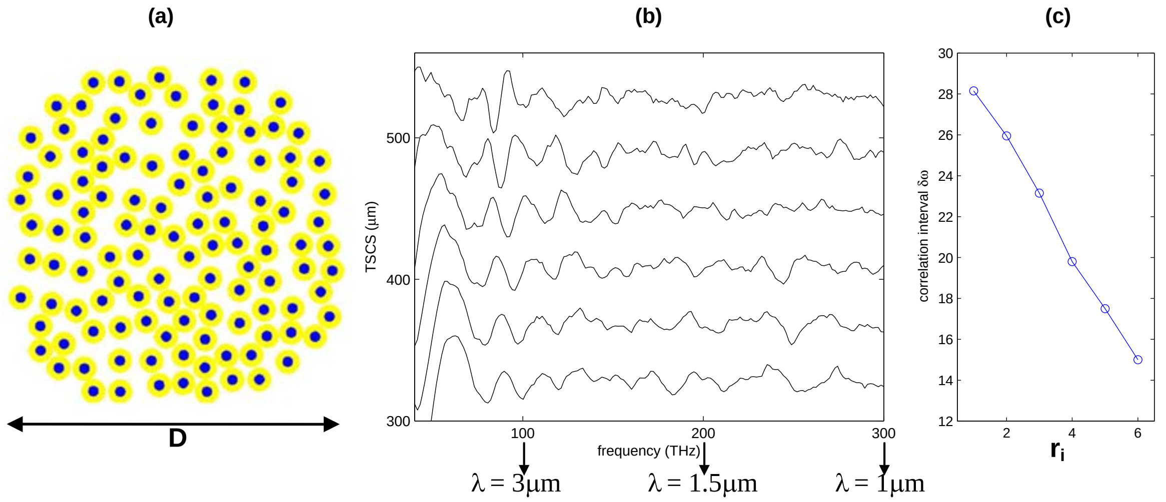

Fig. 3. TSCS-ave spectra of a cluster of concentric coated cylinders. The TSCS-ave spectra of light scattering by a cluster (cluster diameter D=160μm, as shown in (a)) of inner cylinder radii r_i are shown in (b) (Each TSCS-ave spectrum represents an average of 12 TSCS spectrum corresponding to 12 different illumination angles to suppress speckle effect; in addition, each curve is offset in the y-direction to facilitate comparison.) Notice 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 correlation interval $\delta\omega$ is plotted vs. r_i in (c). It is shown that the correlation interval $\delta\omega$ changes monotonically with r_i, suggesting a direct correlation relationship of the macroscopic scattered light and the inner cylinder radius r_i.

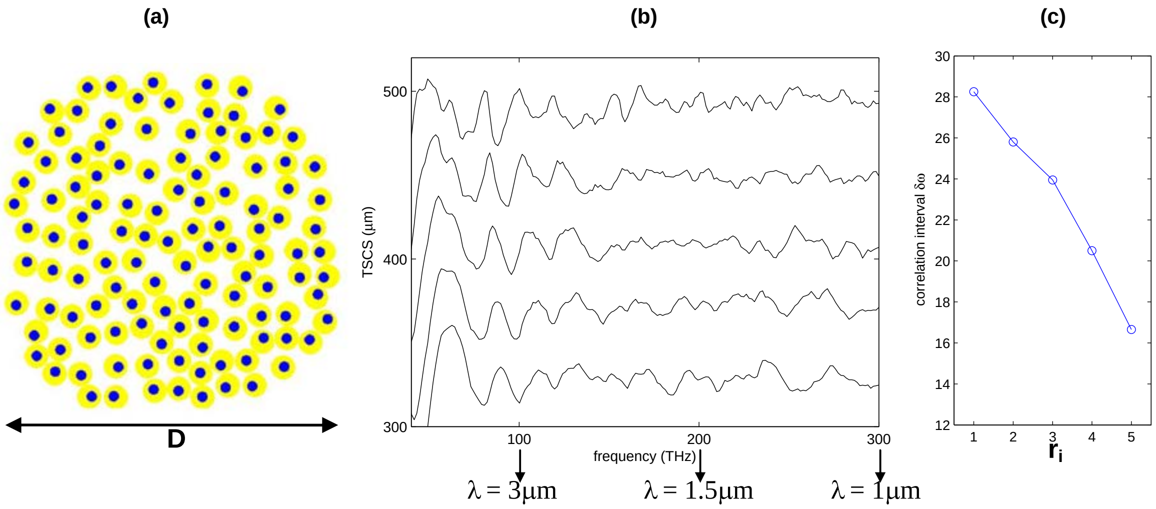

Fig. 4. TSCS-ave spectra of a cluster of coated cylinders with off-centered inner cylinder location. Similar to Fig. 3, the TSCS-ave spectra of light scattering by a cluster (cluster diameter D=160µm, as shown in (a)) of inner cylinder radii r_i are shown in (b) (Each TSCS-ave spectrum represents an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

Comparing Monte Carlo simulation and pseudospectral time-domain numerical solutions of Maxwell's equations of light scattering by a macroscopic random medium

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The Monte Carlo simulation of light scattering by a cluster of dielectric spheres is compared with numerical solutions of Maxwell's equations via the pseudospectral time-domain technique. By calculating the total scattering cross-section (TSCS) spectrum, respectively, the spectral light scattering characteristics are determined. Since the Monte Carlo simulation falls short to accurately account for coherent interference effects, it is shown that the Monte Carlo simulation yields TSCS spectra that significantly deviate from the numerical solutions of Maxwell's equations. Therefore, it is necessary to resort to Maxwell's equations in order to accurately determine the light scattering characteristics of a macroscopic geometry.
[DOI: 10.1063/1.2767777]

The problem of light scattering through macroscopic random media is commonly found in nature, including nonperiodic structures such as clouds, biological tissues, etc. However, this problem has not been rigorously studied; due to the extreme complexity involved, heuristic approximations based on the radiative transfer theory[1] are commonly employed. Among such heuristic methods, the Monte Carlo technique[2–6] is widely used for the problem of light scattering through macroscopic random media, particularly in the area of tissue optics.

However, all heuristic methods are fundamentally limited by the imposed hypotheses. For example, in the study of light scattering by random media, the Monte Carlo technique assumes *independent* scattering events between *stochastic, pointlike* scatterers; such assumptions involve modifications of the physical nature of the original problem, and fall short to accurately account for all the physics of the problem, including polarization and coherent interference. As a result, the validity and applicability of such heuristic methods remain to be determined.[7,8] In order to accurately account for the coherence effects and near-field interactions, a rigorous research method based on Maxwell's equations is preferred.

In this letter, we simulate the light scattering characteristics of closely packed dielectric spheres by employing two different approaches: the Monte Carlo technique and the numerical solutions of Maxwell's equations via the pseudospectral time-domain (PSTD) technique,[9] respectively. The Monte Carlo technique is a widely used heuristic approach based on the radiative transfer theory; by assuming light undergoes a sequence of independent scattering events, light scattering through random media is treated statistically.[10,11] On the other hand, the PSTD technique is a numerical method where the light scattering problem is simulated by solving Maxwell's equations numerically. In this letter, we report the application of both simulation techniques, where the total scattering cross-section (TSCS) spectra are calculated and compared.

Light scattering by a cluster of dielectric spheres is simulated using the Monte Carlo technique. The Monte Carlo technique has been widely used in simulating light scattering through random media.[2,6,12,13] For a specific wavelength, a total of 1 000 000 photons are injected into a cluster (cluster diameter $d=50$ μm) of N dielectric spheres; each sphere has a diameter $d=6$ μm, with a refractive index $n=1.2$. Each photon scattering angle is determined with a random number generator based on the Mie scattering phase function of a single dielectric sphere. The TSCS spectrum from 30 to 300 THz is calculated.

Alternatively, we calculate the light scattering characteristics of a cluster of dielectric spheres by employing the PSTD technique. The PSTD simulation is a grid-based technique capable of solving Maxwell's equations numerically. By assigning the spatial distribution of the refractive index, the PSTD technique can accurately determine the light scattering characteristics of macroscopic geometries, including irregular geometries. In this letter, we report the employing of the PSTD technique on a parallel computer to model *full-vector*, three-dimensional (3D) scattering of light by a cluster of dielectric spheres in free space. A standard anisotropic perfectly matched layer absorbing boundary condition[14] is implemented to absorb outgoing waves to simulate light scattering in free space. A near-to-far-field transformation[15] is employed, allowing scattered light for a broadband of wavelengths at all angles to be obtained in a single simulation. Based on Maxwell's equations, the PSTD simulation is essentially an idealized optical experiment in a *noiseless* environment, where the coherent effects can be accurately determined.

By employing the PSTD technique, light scattering by a cluster of closely packed dielectric spheres in free space is simulated, yielding the TSCS spectrum from 0.5 to 300 THz ($\lambda_0=600$ μm–1 μm) with a resolution of 0.5 THz. With a grid resolution of 0.33 μm, a PSTD simulation of light scattering by a (60 μm)^3 cluster typically takes $\sim$12 h with a parallel computer cluster of 20 2.4 GHz Pentium 4 Xeon processors.

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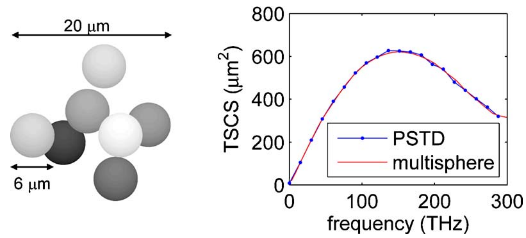

FIG. 1. (Color online) Validation of the 3D PSTD simulation. Light scattering by a cluster of seven randomly positioned, 6 μm diameter, $n=1.2$ dielectric spheres is simulated, with a grid resolution of $dx=0.33$ μm. The PSTD-computed total scattering cross-section (TSCS) as a function of frequency is compared with the multisphere expansion, which is based upon numerical expansions of Maxwell's equations.

A validation of the PSTD simulation of light scattering is shown in Fig. 1. Light scattering by seven randomly positioned, dielectric spheres is calculated using PSTD simulations and compared with the multisphere expansion.[16] The TSCS spectrum is determined. As shown in Fig. 1, the PSTD-computed TSCS spectrum shows good agreement with the analytical expansions of Maxwell's equations.

The Monte Carlo technique and the PSTD technique are employed to simulate light scattering by a cluster of dielectric spheres, respectively. Firstly, as shown in Fig. 2, the TSCS spectra of a cluster of N dielectric spheres are obtained using the Monte Carlo technique. Five cases are shown: $N=25$, 50, 75, 125, and 192. Notice that for sparse distribution of dielectric spheres (e.g., $N=25$), light impinging the cluster mostly encounters a single scattering event, and therefore the TSCS spectrum resembles the TSCS of a single dielectric sphere, showing that the Monte Carlo simulation yields results consistent with Maxwell's equations. However, as the cluster becomes closely packed with less space between adjacent spheres, the Monte Carlo assumption of "light undergoes independent scattering events" no longer holds and the

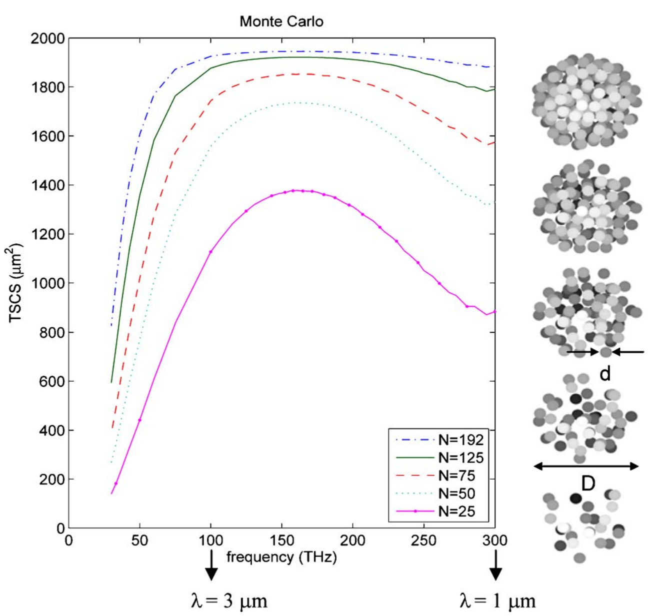

FIG. 2. (Color online) TSCS spectra obtained from the Monte Carlo simulation. By employing the Monte Carlo technique, the TSCS spectra are obtained, each corresponding to a (diameter $d=50$ μm) cluster consisting of N randomly positioned, $n=1.2$, (diameter $d=6$ μm) dielectric spheres. Five cases are shown (from bottom to top): $N=25$, 50, 75, 125, and 192.

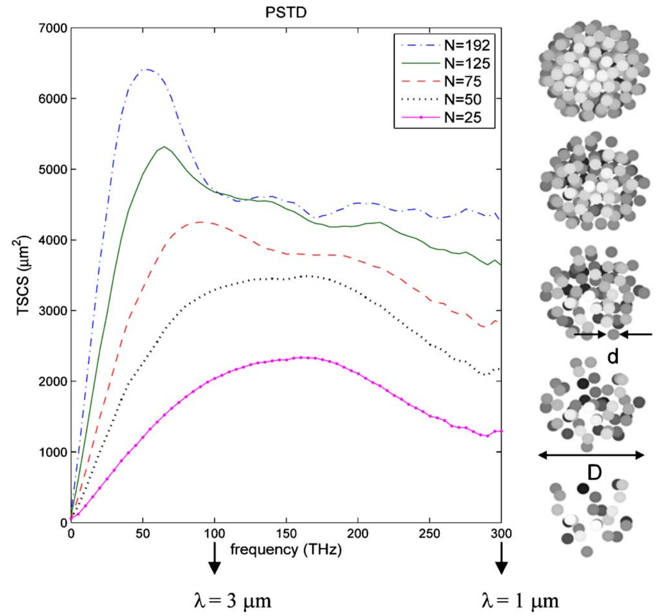

FIG. 3. (Color online) PSTD-computed TSCS spectra. Each TSCS spectra corresponds to a (overall diameter $d=50$ μm) cluster consisting of N randomly positioned, $n=1.2$, (diameter $d=6$ μm) dielectric spheres. Five cases are shown (from bottom to top): $N=25$, 50, 75, 125, and 192. Notice that as more dielectric spheres are packed together, the TSCS spectrum gradually exhibits optical characteristics due to the overall geometry which significantly differs from the TSCS spectrum obtained in the Monte Carlo simulation.

TSCS spectra obtained by the Monte Carlo simulation become less valid.

Secondly, as shown in Fig. 3, the TSCS spectra are calculated using the PSTD technique. By numerically solving Maxwell's equations, the TSCS spectrum of an arbitrary geometry is accurately determined. Notice that, due to the coherence effect, the magnitude of the TSCS spectrum based on Maxwell's equations is larger than the Monte Carlo results. Furthermore, as the cluster geometry becomes packed with more dielectric spheres, the TSCS spectra gradually exhibit optical characteristics that are significantly different from the Monte Carlo simulation (as shown in Fig. 2.)

To determine the relationship of the TSCS spectrum of a cluster of dielectric spheres and the size of the constituent spheres, we compare light scattering characteristics of two clusters, each consists of monodisperse dielectric spheres. As shown in Figs. 4(a) and 4(b), light scattering by a cluster of $d=6$ μm and $d=8$ μm dielectric spheres is simulated using the PSTD technique, respectively. Each $(60\ \mu\text{m})^3$ cluster consists of N randomly positioned, closely packed, homogeneous, dielectric ($n=1.2$) spheres of diameter d. Notice that even for an optically think cluster of closely packed dielectric spheres, the TSCS spectrum exhibits significantly different characteristics directly related to the size of the constituent spheres of each cluster.

Research findings show that the Monte Carlo simulation yields TSCS spectrum that significantly differs from the numerical solutions of Maxwell's equations, owing to the heuristic assumptions involved. Based on the radiative transfer theory, the Monte Carlo simulation of light scattering is treated as an energy transport problem by omitting the wave nature of light. Furthermore, light scattering through macroscopic random media (e.g., biological tissues) is heuristically approximated as a stochastic sum of sequences of indepen-

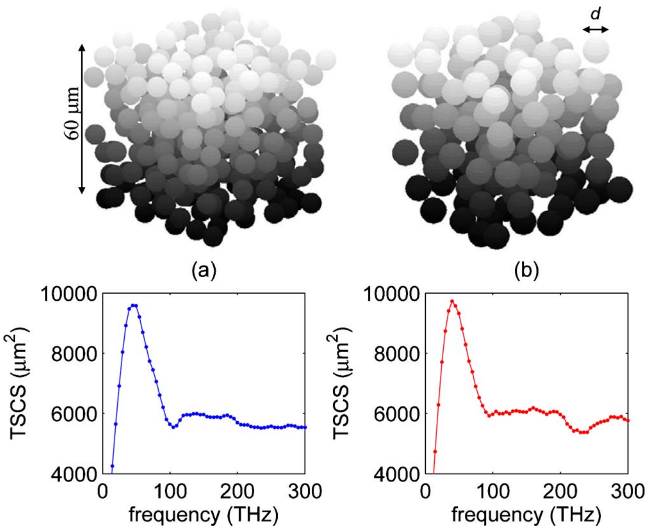

FIG. 4. (Color online) PSTD-computed TSCS spectra of a cubic cluster geometry. Each (60 μm)^3 cluster consists of N randomly positioned, closely packed, dielectric ($n=1.2$) spheres of diameter d. (a) $d=6$ μm, $N=300$; (b) $d=8$ μm, $N=140$.

dent scattering events. By omitting the wave nature of light, the complex light scattering problem is reduced to a simpler problem that is solvable but distorting the physics of the problem. As a result, such heuristic approximation in principle excludes the possibility of accurately determining the coherent effects of light using the Monte Carlo technique.

For sparse distribution of spheres (e.g., $N=25$), the Monte Carlo simulation yields a TSCS spectrum that is similar to the TSCS spectrum determined by the PSTD simulation based on Maxwell's equations, as shown in Fig. 2. This resemblance is anticipated, since with only a few dielectric spheres spaced far apart in space, the Monte Carlo assumption of independent scattering events is satisfied. However, for dielectric spheres closely packed in space, the assumption of light undergoes independent scattering events breaks down. By comparing Figs. 2 and 3, it is readily seen that the TSCS spectrum determined via the Monte Carlo simulation deviates significantly from the PSTD numerical solutions of Maxwell's equations. As the number of spheres increases and the cluster becomes closely packed, the overall TSCS spectrum is gradually dominated by the optical characteristics of the cluster as a whole and shows less of the characteristics due to individual spheres.

Specifically, (in Fig. 3) as the N increases, a TSCS peak gradually forms around 55 THz; this peak is due to the coherent interference effects of the overall cluster geometry as a whole.[17] For long wavelengths, the electromagnetic wave is insensitive to the microscopic structural details and reacts to the cluster geometry as a whole. This phenomenon is similar to the two-dimensional case, as reported in Ref. 17. In addition, notice that the amplitude of the Monte Carlo calculated TSCS spectra (Fig. 2) is significantly lesser than the PSTD calculated TSCS spectra (Fig. 3). This difference is anticipated because the Monte Carlo simulation treats each "photon" independently and does not accurately account for the coherent wave interference effects of light. As a result, the Monte Carlo simulation of light scattering falls short to determine the optical coherent effects.

Lastly, as shown in Fig. 4, the TSCS spectra exhibit optical characteristics that are related to the specific microscopic information of the cluster geometry (e.g., size of the constituent spheres). Such optical characteristics may provide essential information for innovative optical techniques. However, due to the complexity involved, a thorough analysis is required. Further analysis is currently ongoing and will be reported in future publications.

In summary, we report the comparison of the Monte Carlo simulation and PSTD numerical solutions of Maxwell's equations for the problem of light scattering by a cluster of monodisperse, dielectric spheres. Due to the heuristic assumptions, the Monte Carlo simulation falls short to account for the wave interference phenomenon. As a result, Monte Carlo simulation of light scattering yields optical characteristics that deviate from the numerical solutions of Maxwell's equations. On the other hand, based on Maxwell's equations, the PSTD technique is robust and applicable to light scattering problems of macroscopic arbitrary geometry. To accurately determine the coherent optical characteristics of macroscopic random medium, it is necessary to resort to Maxwell's equations.

The authors thank the Taiwan National Science Council under Grant No. 95-2112-M-002-039 for the support on this research. In addition, the authors would like to extend special thanks to all the computing facilities provided by the National Taiwan University Computing Center.

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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 a spectral signature of the macroscopic scattered light and its microscopic origin can be related.

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 yet 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 Dunn et al and Drezek et al[11]. Yet, 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.

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

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 $0.42\lambda_d$ (λ_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, 3μm-diameter nuclei with refractive index of 1.2. With a spatial resolution of Δ = 0.3 μm and temporal resolution (Δt) of 0.5e-16 sec, the PSTD simulation yields the frequency response from 0.5 to 300 THz (λ_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.

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 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_i = 0.5 μm, 1.0 μm, 1.5 μm, 2.0 μm, 2.5 μm, 3.0μm.) Minute variations in the TSCS-ave spectra are observed for different r_i. In order to determine the relationship between the variations in the TSCS-ave spectra and r_i, an autocorrelation analysis of the TSCS spectra was performed to obtain the correlation interval δω (a small δω value indicates much variations in the TSCS-ave spectrum per unit range.) As shown in Fig. 3(c), δω of the TSCS-ave spectrum monotonically decreases with respect to r_i, suggesting that the variations in the TSCS-ave spectra are clearly related to r_i.

Although the monotonic behavior of δω 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_i values of 0.5, 1.0, 1.5, 2.0, and 2.5 μm. Again, minute variations in the TSCS-ave spectra are observed as r_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_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 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 Dunn, Drezek, and Richards-Kortum [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.

6. Acknowledgments

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Figure Captions

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.

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 $\lambda = 1\mu m$, 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.

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 μm, as shown in (a)) with an 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.) 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_i in (c). It is shown that the $\delta\omega$ changes monotonically with r_i, suggesting a direct correlation relationship between the macroscopic scattered light and r_i.

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 μm, 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.

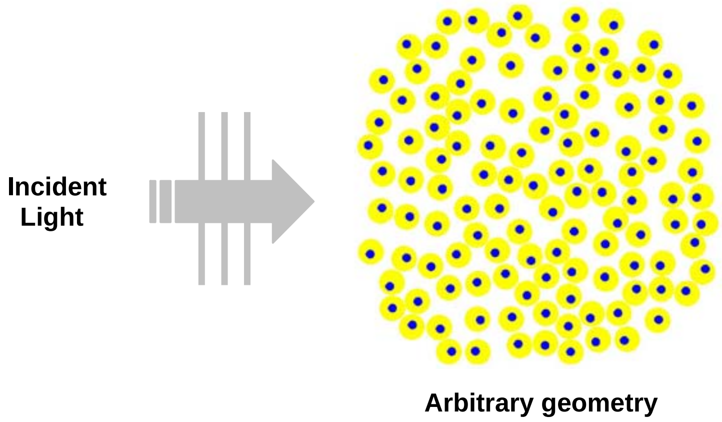
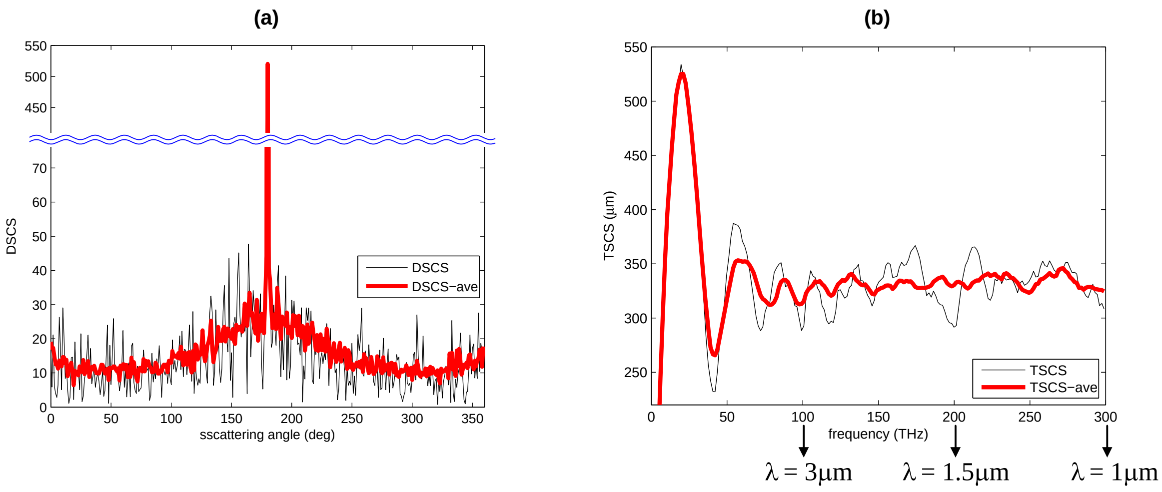


Fig. 1.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DSCS
DSCS−ave
(b)
TSCS (μm)
frequency (THz)
TSCS
TSCS−ave
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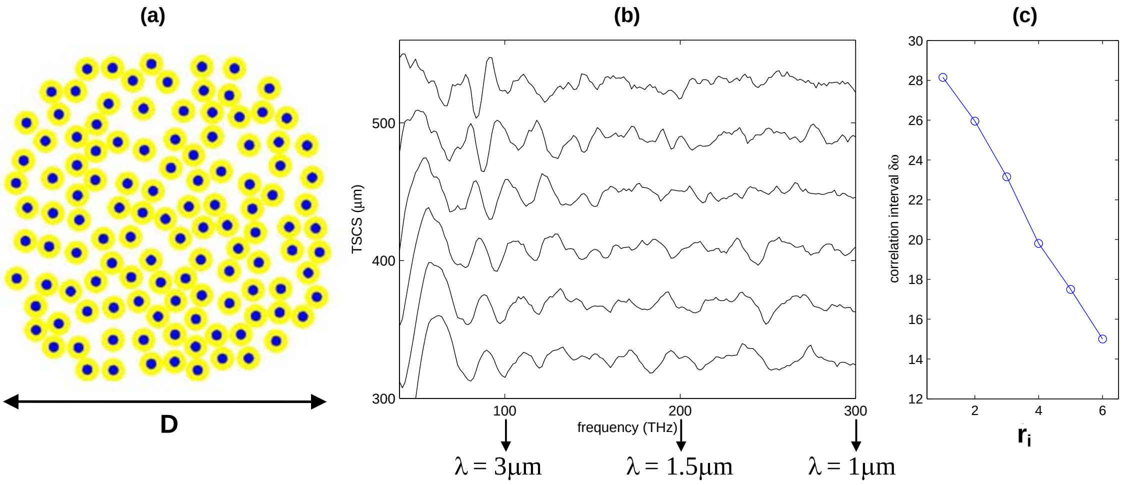
λ = 1.5μm
λ = 1μm

Fig. 2.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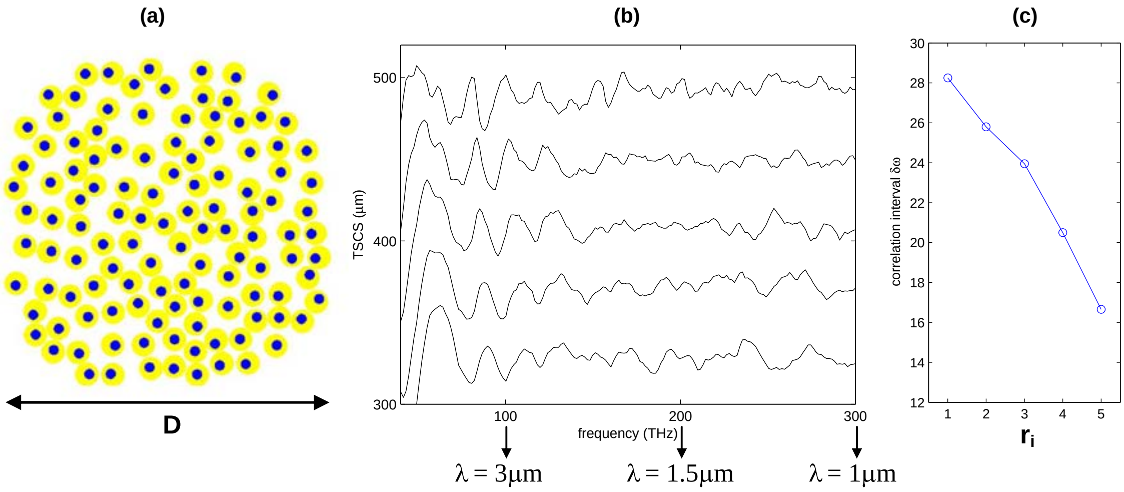
r_i

Fig. 3.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r_i

Fig. 4.

行政院國家科學委員會補助國內專家學者出席國際學術會議報告

2006 年　9 月 26 日

附件三

報告人姓名	曾雪峰　Snow H. Tseng	服務機構及職稱	台大光電所　助理教授
會議時間 會議地點	2006.07.02-2006.07.07 Plymouth, NH, USA	本會核定補助文號	95-2914-I-002-060-A1
會議名稱	（中文）高登學術年會生物醫學雷射類 （英文）Gordon Research Conference: Lasers in Medicine and Biology		
發表論文題目	（中文）探索透過隨機界質的多次散射光所隱含的光學訊息 （英文）What information can possibly be obtained from light multiply scattered through random media?		

報告內容應包括下列各項：

一、參加會議經過

The conference is organized in a way that there are plenty of chances to communicate and interact with each participant. Through various discussions, and also the presentations, I have learned a lot in many aspects.

The Board of the conference thanked me for attending the conference, and told me that I was the only participant from an Asian institute. They realized the importance and have decided to attract more participants from Asia.

After the conference, I was invited to MIT G.R. Harrison Spectroscopy Laboratory to give a presentation to introduce my research. It has been a very fruitful experience for me, and I have made many good connections for future collaboration.

二、與會心得

Participants of this conference are mostly outstanding researchers in the field of Tissue Optics. I had many discussions and brainstorming with many people, which was very helpful for my future research.

三、考察參觀活動(無是項活動者省略)

四、建議

This conference is very helpful in expanding my research scope and connections. I recommend researchers in Taiwan to attend this conference in the future.

五、攜回資料名稱及內容

“Reflections from the Frontiers”

六、其他

What Information Can Possibly Be Obtained from Light Multiply Scattered through Random Media?

Snow H. Tseng

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ABSTRACT

By numerically solving the Maxwell's equations for the problem of light propagation through closely packed random media, we report an optical signature indicative of structural information concerning the random media. On a broader perspective, our research findings may lead to a better understanding of the coherent interference effect of light scattering by closely packed random media. Specifically, based on first principles, we show that microscopic structural information of the random medium can be obtained from forward, *multiply* scattered light, even for closely packed random media, with scatterers spaced *less than a single wavelength apart*.

Activities:

In the box below, please indicate your particular activities which justify favorable consideration of you as a participant and contributor to this Conference. This information is required.

It is of unprecedented importance to understand tissue optics based upon fundamental electromagnetic theory--Maxwell's equations. Yet, very few people other than myself is taking this approach. I have some intriguing results that may be interesting. If possible, I'd like to give an oral presentation, which should be more effective for me to introduce the significances of my research findings.

行政院國家科學委員會補助國內專家學者出席國際學術會議報告

2006 年　9 月 26 日

附件三

報告人姓名	曾雪峰　Snow H. Tseng	服務機構及職稱	台大光電所　助理教授
會議時間地點	2006.07.02-2006.07.07 Plymouth, NH, USA	本會核定補助文號	95-2914-I-002-060-A1
會議名稱	（中文）高登學術年會生物醫學雷射類 （英文）Gordon Research Conference: Lasers in Medicine and Biology		
發表論文題目	（中文）探索透過隨機界質的多次散射光所隱含的光學訊息 （英文）What information can possibly be obtained from light multiply scattered through random media?		

報告內容應包括下列各項：

一、參加會議經過

The conference is organized in a way that there are plenty of chances to communicate and interact with each participant. Through various discussions, and also the presentations, I have learned a lot in many aspects.

The Board of the conference thanked me for attending the conference, and told me that I was the only participant from an Asian institute. They realized the importance and have decided to attract more participants from Asia.

After the conference, I was invited to MIT G.R. Harrison Spectroscopy Laboratory to give a presentation to introduce my research. It has been a very fruitful experience for me, and I have made many good connections for future collaboration.

二、與會心得

Participants of this conference are mostly outstanding researchers in the field of Tissue Optics. I had many discussions and brainstorming with many people, which was very helpful for my future research.

三、考察參觀活動(無是項活動者省略)

四、建議

This conference is very helpful in expanding my research scope and connections. I recommend researchers in Taiwan to attend this conference in the future.

五、攜回資料名稱及內容

“Reflections from the Frontiers”

六、其他