Extracting Geometrical Information of Closely Packed Random Media From Multiply Scattered Light via a Cross-Correlation Analysis

Snow H. Tseng, *Member, IEEE*, Allen Taflove, *Fellow, IEEE*, Duncan Maitland, Vadim Backman, and Joseph T. Walsh, Jr.

***Abstract*—We have implemented a two-dimensional (2-D) pseudospectral time-domain (PSTD) numerical solution of Maxwell's equations to calculate the total scattering cross-section (TSCS) spectrum of a macroscopic, *closely packed*, random medium consisting of dielectric cylinders. Results reported in this letter show that a TSCS spectral signature is identified, revealing structural information of the random medium. Furthermore, by means of the proposed cross-correlation analysis, the diameter of constituent cylinders within a closely packed cluster can be determined. On a broader perspective, based on first principles, our research findings may lead to a better understanding of the coherent interference effect of light scattering by closely packed random media. Specifically, we show that, microscopic structural information of the random medium can be determined from the forward, *multiply* scattered light, even for *optically thick*, closely packed random media, with scatterers spaced *less than a single wavelength apart*.**

***Index Terms*—Closely packed random media, cross-correlation, multiply scattered light, total scattering cross-section.**

I. Introduction

LIGHT propagation through random media is a very challenging problem involving an enormous number of variables. Commonly used optics techniques, including the dynamic light scattering technique and enhanced backscattering effect [1], generally utilize singly scattered light while suppressing multiply scattered light. Unlike multiply scattered light, singly scattered light is easier to analyze to provide scattering characteristics of the random media. However, for optically thick random media where most light undergo multiple scattering events, singly scattered light represents only an insignificant fraction of the total scattered light which could be difficult to detect. Therefore, it would be very valuable if useful information could be identified and harnessed from multiply scattered light.

By employing the pseudospectral time-domain (PSTD) algorithm [2], we have calculated the optical properties of closely packed random media based on first principles [3]–[5]. Specifically, it has been earlier shown in [4] that the overall total scattering cross-section spectrum (TSCS) of closely packed random media is generally determined by the global geometry and average refractive index, but is relatively insensitive to the microscopic geometrical structures. This conclusion begs the question: *Can information indicative of microscopic geometrical structures (e.g., scatterer size, spacing, refractive index, etc.) be identified and extracted from multiply scattered light?* By numerically solving Maxwell's equations, we show in this letter that multiply scattered light also contain geometrical information that can be extracted via a proposed cross-correlation analysis method.

II. PSTD Simulations and Research Findings

Initially proposed by Liu in 1997, the PSTD method has been validated [6], [7]. For electromagnetic wave interaction structures having primary geometrical or material feature sizes exceeding one-half the dielectric wavelength (λ_d), PSTD has been shown to exhibit the same computational accuracy and dynamic range as FDTD models having approximately eight-times finer resolution [6]. That is, a PSTD grid with coarse $\lambda_d/4$ resolution provides about the same accuracy as an FDTD grid with fine $\lambda_d/32$ resolution. Much experience with PSTD simulations has shown that the PSTD grids with $0.33\lambda_d$ resolution to provide sufficient accuracy to identify characteristics of light scattering by random media.

In this letter, we report application of the PSTD technique to model the problem of light scattering by a macroscopic cluster of *closely packed*, infinitely long, dielectric cylinders in free space. We use a PSTD grid with a uniform spatial resolution of 0.33 μm, yielding the total scattering cross-section (TSCS) spectra as function of frequency from 0.5–300 THz ($\lambda_0 = 600\ \mu\text{m} - 1\ \mu\text{m}$) with a resolution of 0.5 THz.

The cluster geometries were created by randomly positioning dielectric cylinders in vacuum, with a minimum (*edge-to-edge*) spacing of s between cylinders. A standard anisotropic perfectly matched layer (APML) absorbing boundary condition [9] is implemented to absorb outgoing waves, simulating an open-region light-scattering experiment. An impulsive plane wave il-

Manuscript received October 7, 2005; revised January 10, 2006. This work was supported by National Institutes of Health (NIH) National Cancer Institute Contract under Grants 5R01-CA085991 and 5R01-HD044015, by the NIH under Grant R01 EB003682, by the National Science Foundation (NSF) under Grant BES-0238903, and by the the NSF TeraGrid Grant MCB040062N. This work was performed under the auspices of the U.S. Department of Energy under Contract W-7405-ENG-48.

S. H. Tseng is with the Graduate Institute of Electro-Optical Engineering, National Taiwan University, Taipei, Taiwan (e-mail: snow@cc.ee.ntu.edu.tw).

A. Taflove are with the Department of Electrical and Computer Engineering, Northwestern University, Evanston, IL 60208 USA (e-mail: taflove@ece.northwestern.edu).

D. Maitland is with M-Division, Lawrence Livermore National Laboratory, Livermore, CA 94550 USA (e-mail: maitland1@llnl.gov).

V. Backman and J. T. Walsh, Jr. are with the Biomedical Engineering Department, Northwestern University, Evanston, IL 60208 USA (e-mail: v-backman@northwestern.edu; jwalsh@northwestern.edu).

Digital Object Identifier 10.1109/LAWP.2006.872432

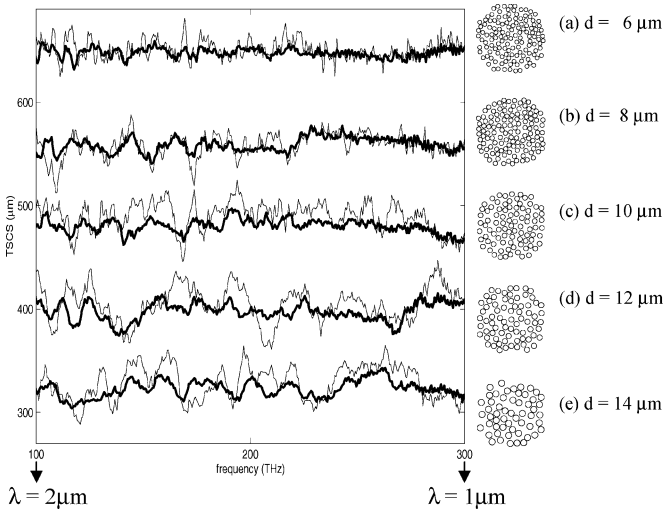

Fig. 1. PSTD-computed TSCS spectra of various cluster geometries, each consists of d-diameter, dielectric ($n = 1.2$) cylinders. Five cases are shown. (a) $d = 6\ \mu\mathrm{m}, N = 300, \mathrm{optical\ thickness} \sim 18.33$. (b) $d = 8\ \mu\mathrm{m}, N = 168$, optical thickness ~ 31.66. (c) $d = 10\ \mu\mathrm{m}, N = 126$, optical thickness ~ 15.29. (d) $d = 12\ \mu\mathrm{m}, N = 75$, optical thickness ~ 15.94. (e) $d = 14\ \mu\mathrm{m}, N = 55$, optical thickness ~ 14.89 the scattering mean free path $l_s = \sigma * \tilde{\mathrm{N}}$, whereas σ is the scattering coefficient of a single cylinder, and $\tilde{\mathrm{N}}$ is the number density of cylinders. Each thin TSCS curve represents the TSCS spectrum of a single incident angle; whereas each thick TSCS curve represents the TSCS spectrum averaged over 12 different TSCS spectra corresponding to 12 different illumination angles (upon the same geometry) spanning 0° to 360° in 30° increments.

luminates the cluster, allowing scattered light of various wavelengths at all angles to be obtained in a single run by employing a near-to-far field transformation [10].

In Fig. 1, five cases of the PSTD-computed TSCS spectra are shown, each corresponding to a *closely packed* cluster of d-μm-diameter dielectric cylinders ($d = 6, 8, 10, 12$, and $14\ \mu\mathrm{m}$, respectively.) The optical thickness of each cluster geometry for wavelength $\lambda = 1\ \mu\mathrm{m}$ is shown in Fig. 1

$$\text{optical thickness} \equiv \frac{(\text{geometrical thickness})}{(\text{scattering mean free path})}$$

the scattering mean free path $l_s = \sigma * \tilde{\mathrm{N}}$, whereas σ is the scattering coefficient of a single cylinder, and $\tilde{\mathrm{N}}$ is the number density of cylinders. Due to the coherent light source illumination and random nature of the geometry, significant speckle effect is observed [3]. In order to reduce speckle effect, the averaged TSCS spectrum is obtained by averaging over 12 TSCS spectra of the same geometry, each corresponding to a different illumination angle (spanning 0° to 360° in 30° increments.) Notice that after reduction of the temporal speckle, the averaged TSCS spectra exhibit *junk-like* spectral structures that are difficult to interpret.

In Fig. 2, we present a cross-correlation analysis that can discern the *junk-like* TSCS spectral structures shown in Fig. 1. By calculating the correlation coefficients of the averaged cluster TSCS spectra shown in Fig. 1 and various TSCS spectra of a single d-μm-diameter dielectric cylinder, it is discovered that the correlation coefficient as a function of d peaks at $d = d_p$, where d_p approximately matches the diameter of the constituent cylinders of the cluster geometry. This relationship confirms that the TSCS spectral signature is indicative of the size of the

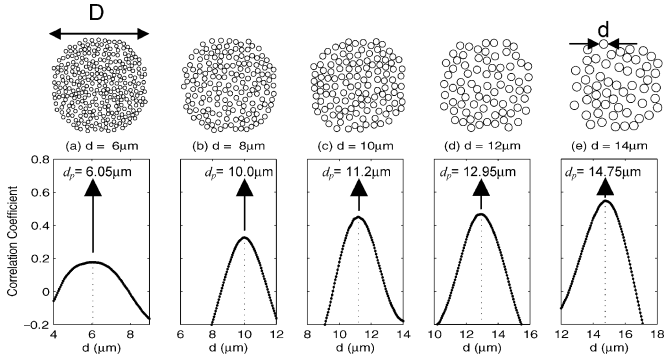

Fig. 2. TSCS spectral signature indicative of the constituent cylinder diameter is identified. By calculating the correlation coefficients of the cluster TSCS spectra shown in Fig. 1 [(a)-(e): $D = 160\ \mu\mathrm{m}$, and $d = 6, 8, 10, 12$, and $14\ \mu\mathrm{m}$], and the TSCS spectra of a single dielectric cylinder, it is found that the correlation coefficient peaks at $d = d_p$, where d_p is approximately equal to the diameter of the constituent cylinders of the cluster geometry. This relationship suggests that the TSCS spectral structure is related to the size of the constituent cylinders, even for *optically thick*, closely packed cluster of scatterers where the *edge-to-edge* spacing between adjacent scatterers is less than a single wavelength apart.

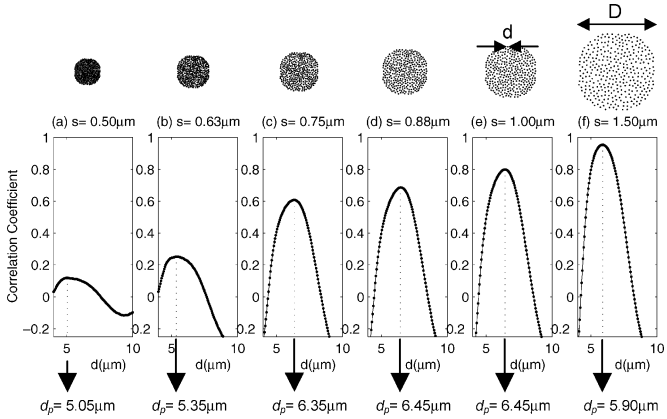

Fig. 3. Effect of spacing between cylinders on the TSCS spectral signature shown in Fig. 2. By varying D whereas fixing $N = 64$ and $d = 6\ \mu\mathrm{m}$, the effect of s (s: minimum spacing between cylinders) on the cross-correlation analysis is determined. The geometrical parameters for these cases are as follows. (a) $s = 0.5\ \mu\mathrm{m}, D = 80\ \mu\mathrm{m}$, optical thickness ~ 17.33. (b) $s = 0.63\ \mu\mathrm{m}, D = 100\ \mu\mathrm{m}$, optical thickness ~ 13.86. (c) $s = 0.75\ \mu\mathrm{m}, D = 120\ \mu\mathrm{m}$, optical thickness ~ 11.55. (d) $s = 0.88\ \mu\mathrm{m}, D = 140\ \mu\mathrm{m}$, optical thickness ~ 9.90. (e) $s = 1\ \mu\mathrm{m}, D = 160\ \mu\mathrm{m}$, optical thickness ~ 8.66. (f) $s = 1.5\ \mu\mathrm{m}, D = 240\ \mu\mathrm{m}$, optical thickness ~ 5.76. It is shown that the correlation coefficient peaks at $d = d_p$. Qualitatively, as the spacing between adjacent cylinders increases, the correlation coefficient approaches 1, whereas d_p approaches the actual cylinder diameter: $d = 6\ \mu\mathrm{m}$.

constituent cylinders, even for *optically thick*, *closely packed*, cluster of scatterers where the *edge-to-edge* spacing between adjacent scatterers is less than a single wavelength apart.

Further investigation of the TSCS spectral signature is shown in Figs. 3 and 4. By proportionally increasing the spacing s (s: minimum *edge-to-edge* spacing between cylinders) within the cluster geometry, the effect of spacing s on the TSCS spectral signature is analyzed and shown in Fig. 3. As shown in Fig. 2, the correlation coefficient as a function of d peaks at $d = d_p$, whereas d_p approximately matches the diameter of the constituent cylinders of the cluster geometry. Furthermore, as the spacing s is increased, d_p approaches the actual cylinder diameter: $d = 6\ \mu\mathrm{m}$, whereas the correlation coefficient approaches 1.

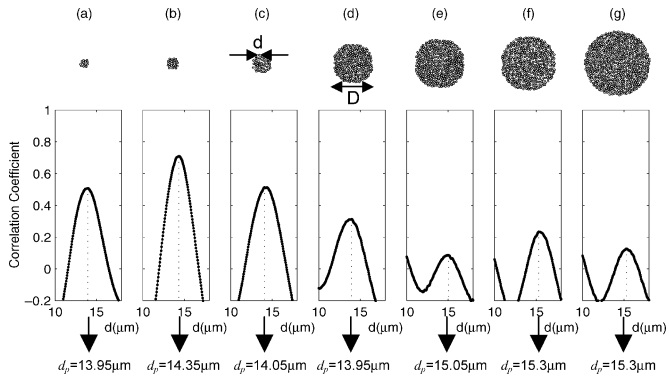

Fig. 4. Effect of optical thickness on the TSCS spectral signature shown in Fig. 2. By increasing D and N, the effect of the overall cluster size on the cross-correlation analysis is determined. Each cluster consists of N dielectric ($n = 1.2$) cylinders with diameter $d = 14\ \mu$m. (a) $N = 14$, $D = 80\ \mu$m, optical thickness ~ 7.58. (b) $N = 26$, $D = 100\ \mu$m, optical thickness ~ 11.26. (c) $N = 55$, $D = 160\ \mu$m, optical thickness ~ 14.89. (d) $N = 261$, $D = 320\ \mu$m, optical thickness ~ 35.33. (e) $N = 411$, $D = 400\ \mu$m, optical thickness ~ 44.51. (f) $N = 444$, $D = 440\ \mu$m, optical thickness ~ 43.71. (g) $N = 666$, $D = 520\ \mu$m, optical thickness ~ 55.48. Again, the correlation coefficient peaks at $d = d_p$, where d_p roughly matches the diameter of the constituent cylinder of the cluster geometry ($d = 14\ \mu$m). However, as the cluster becomes larger with increasing D and N, the correlation coefficient decreases to 0, indicating that the TSCS spectral signature becomes obscure as the optical thickness increases.

Moreover, by increasing D and N whereas fixing s, the effect of optical thickness on the TSCS spectral signature is determined and shown in Fig. 4. With $s = 0.5\ \mu$m and $d = 14\ \mu$m, seven cases are shown. (a) $D = 80\ \mu$m, optical thickness ~ 7.58. (b) $D = 100\ \mu$m, optical thickness ~ 11.26. (c) $D = 160\ \mu$m, optical thickness ~ 14.89. (d) $D = 320\ \mu$m, optical thickness ~ 35.33. (e) $D = 400\ \mu$m, optical thickness ~ 44.51. (f) $D = 440\ \mu$m, optical thickness ~ 43.71. (g) $D = 520\ \mu$m, optical thickness ~ 55.48. Again, the correlation coefficient peaks at $d = d_p$, where d_p roughly matches the diameter of the constituent cylinder of the cluster geometry ($d = 14\ \mu$m). However, as the cluster becomes larger with increasing D and N, the correlation coefficient decreases to 0, indicating that the TSCS spectral signature becomes obscure as the optical thickness increases.

Together, Figs. 1 and 2 show that, by employing the proposed cross-correlation analysis, a TSCS spectral signature is identified from the *junk-like* TSCS spectrum of a cluster geometry consisting of closely packed dielectric cylinders. Moreover, the range of applicability of the TSCS spectral signature is further investigated and shown in Figs. 3 and 4. Fig. 3 shows that as the spacing between cylinders is increased, the TSCS spectral signature becomes more and more accurate, with the correlation coefficient approaching unity. This can be understood intuitively: As the spacing between cylinders increase to infinity, light incident upon such geometry basically only encounter a single cylinder, therefore approaching the single scattering regime.

Finally, we have shown in Fig. 4 that as the overall dimension of the cluster geometry increases with more cylinders packed within, the cluster geometry becomes optically thick and the TSCS spectral signature becomes obscured. Nevertheless, even for optically thick geometry, the TSCS spectral signature can be identified, suggesting that multiply scattered light contains geometrical information and can be identified via the proposed cross-correlation analysis.

III. Summary and Discussion

We have implemented a 2-D PSTD numerical solution of Maxwell's equations to calculate the TSCS spectrum of a macroscopic, *closely packed*, random medium consisting of dielectric cylinders with an average (*edge-to-edge*) separation of less than a single wavelength. Results reported in this letter show that a TSCS spectral signature is identified, revealing structural information of the random medium. Furthermore, by means of the proposed cross-correlation analysis, the diameter of constituent cylinders within a closely packed cluster can be determined from forward, *multiply* scattered light, even for *optically thick* (optical thickness ~ 15), closely packed random media, with scatterers spaced *less than a single wavelength apart.*

Considering the applicability of the proposed cross-correlation method to more realistic systems, we have simulated geometries of a cluster consisting of *poly-disperse* dielectric cylinders, with a variation of cylinder diameter of 5% and 20%, respectively. Again, the TSCS signature also matches the average size of the constituent cylinders, suggesting that this technique may be feasible for practical systems where the diameter of scatterers varies. Furthermore, since TSCS is directly proportional to the forward scattered light intensity [11], the proposed cross-correlation analysis technique can be readily applied to forward scattered light, to yield geometrical information of the closely packed random media.

However, there are certain limitations of this cross-correlation approach. For example, for cylinders regularly packed into a lattice structure, strong peaks occur at specific wavelengths of the TSCS spectrum. This is anticipated—as the *lattice-like* cluster becomes infinitely large, the TSCS spectrum would exhibit pass bands and forbidden bands due to the coherent interference effects, which obscures the individual cylinder characteristics that the cross-correlation analysis detects. In summary, the proposed cross-correlation analysis can detect cylinder diameter for cluster consisting of *randomly-positioned* cylinders, yet, for a periodic, lattice-like cluster, the coherent constructive interference effect dominates the TSCS spectrum, and the characteristics of individual cylinder is obscured.

Together with our earlier reported results, we conclude that the TSCS spectrum of a cluster of *closely packed* dielectric scatterers is determined by the overall geometry and average refractive index, as shown in [4]. Moreover, the temporal speckle of the TSCS spectrum is related to the number of scatterers within the cluster geometry, as shown in [3]. Finally, a TSCS spectral signature indicative of the constituent cylinders has been identified in the shorter wavelength regime ($\lambda_0 < 2\ \mu$m), as shown in Figs. 1–4. Theoretically, this cross-correlation approach is general and can be readily applied to three-dimensional (3-D) problems; in fact, we have begun 3-D simulation and will report in subsequent papers.

On a broader perspective, based on first principles, our research findings provide information that may lead to a better understanding of the coherent interference effect of light scattering by closely packed random media. Even though *three-times-the-wavelength* $(3*\lambda)$ has been conventionally accepted as the minimum distance required to ensure independent scattering event, we have shown in this letter that the diameter of constituent scatterers within a closely packed cluster can be determined from the forward, *multiply* scattered light, even for closely packed random media.

ACKNOWLEDGMENT

The authors would like to thank C. Chin and Y. Kim for helpful discussions.

REFERENCES

[1] Y. L. Kim, Y. Liu, V. M. Turzhitsky, H. K. Roy, R. K. Wali, and V. Backman, "Coherent backscattering spectroscopy," *Opt. Lett.*, vol. 29, pp. 1906–1908, 2004.

[2] Q. H. Liu, "The pseudospectral time-domain (PSTD) method: A new algorithm for solutions of Maxwell's equations," in *Proc. IEEE Antennas and Propagation Society Int. Symp.*, 1997, pp. 122–125.

[3] S. H. Tseng, A. Taflove, D. Maitland, V. Backman, and J. T. Walsh, "Interpretation of noise-like temporal speckles for clusters of closely packed randomly positioned dielectric cylinders," *Opt. Express*, vol. 13, pp. 6127–6132, 2005.

[4] S. H. Tseng, J. H. Greene, A. Taflove, D. Maitland, V. Backman, and J. Walsh, "Exact solution of Maxwell's equations for optical interactions with a macroscopic random medium," *Opt. Lett.*, vol. 29, pp. 1393–1395, 2004.

[5] S. H. Tseng, A. Taflove, D. Maitland, V. Backman, and J. T. Walsh, "Simulation of enhanced backscattering of light by numerically solving Maxwell's equations without heuristic approximations," *Opt. Express*, vol. 13, pp. 3666–3672, 2005.

[6] Q. H. Liu, "Large-scale simulations of electromagnetic and acoustic measurements using the pseudospectral time-domain (PSTD) algorithm," *IEEE Trans. Geosci. Rem. Sens.*, vol. 37, no. 3, pp. 917–926, Mar. 1999.

[7] ——, "The PSTD algorithm: A time-domain method requiring only two cells per wavelength," *Microwave Optical Technol. Lett.*, vol. 15, pp. 158–165, 1997.

[8] S. H. Tseng, A. Taflove, D. Maitland, V. Backman, J. Joseph, and T. Walsh, "First exact solution of Maxwell's equations for optical interactions with a macroscopic random medium," *Opt. Lett.*, vol. 29, pp. 1393–1395, 2004.

[9] S. D. Gedney, "An anisotropic perfectly matched layer absorbing media for the truncation of FDTD lattices," *IEEE Trans. Antennas Propagat.*, vol. 44, no. 12, pp. 1630–1639, Dec. 1996.

[10] A. Taflove and S. C. Hagness, *Computational Electrodynamics: The Finite-Difference Time-Domain Method*. Norwood, MA: Artech House, 2000.

[11] C. F. Bohren and D. R. Huffman, *Absorption and Scattering of Light by Small Particles*. New York: Wiley-Interscience, 1983.