UCRL-JRNL-216488

PSTD Simulations of Multiple Light Scattering in 3-D Macrocsopic Random Media

S. H. Tseng, A. Taflove, D. Maitland, V. Backman

October 24, 2005

Radio Science

Disclaimer

PSTD Simulations of Multiple Light Scattering in 3-D Macroscopic Random Media

Snow H. Tseng, and Allen Taflove

Department of Electrical and Computer Engineering, Northwestern University, Evanston, Illinois 60208

Duncan Maitland

Medical Physics and Biophysics Division, Lawrence Livermore National Laboratory, Livermore, California 94550

Vadim Backman

Biomedical Engineering Department, Northwestern University, Evanston, Illinois 60208

Abstract

We report a *full-vector*, *three-dimensional*, numerical solution of Maxwell's equations for optical propagation within, and scattering by, a random medium of macroscopic dimensions. The total scattering cross-section is determined using the pseudospectral time-domain technique. Specific results reported in this Paper indicate that multiply scattered light also contains information that can be extracted by the proposed cross-correlation analysis. On a broader perspective, our results demonstrate the feasibility of accurately determining the optical characteristics of *arbitrary*, macroscopic random media, including geometries with *continuous variations of refractive index*. Specifically, our results point toward the new possibilities of tissue optics—by numerically solving Maxwell's equations, the optical properties of tissue structures can be determined unambiguously.

Light scattering by macroscopic random media, such as biological tissues structures, is generally a very difficult problem to study analytically, due to the enormous number of variables involved. Nevertheless, it continues to be studied in various disciplines [1-3] with a common challenge: the analysis of scattered electromagnetic waves to acquire geometrical information about the random media.

Conventionally, various degrees of heuristic approximations are involved to simplify the problem, including Monte Carlo technique [4], the effective medium theory [5], and approximation methods based on radiative transfer theory, such as Beer's Law, Kubelka-Monk approximations, the adding-doubling method, the diffusion approximation. These methods, however, generally neglect the full-vector electromagnetic wave nature of light, such as the near-field interactions and coherent interference effects, resulting in questionable accuracy and validity [6]. In order to properly characterize optical properties of closely packed scatterers, a rigorous method based on fundamental electromagnetic theory is desired.

In this Paper, we report the initial application to the tissue-optics problem of an emerging advanced variant of finite-difference time-domain (FDTD) technique: the pseudo-spectral time-domain (PSTD) technique [7]. For large electromagnetic wave interaction models in D dimensions not having geometric details or material inhomogeneities smaller than one-half wavelength, PSTD reduces computer storage and running-time by approximately $8^D:1$ relative to standard FDTD while achieving comparable accuracy [7]. This advantage is sufficient to permit rigorous numerical solution of the full-vector Maxwell's equations for optical propagation within, and scattering by, a random medium of macroscopic dimensions.

The most basic version of PSTD is implemented on an unstaggered, collocated Cartesian space grid. Let $\{V_i\}$ denote the values of field component V at all points along an x-directed cut through the grid, and let $\{(\partial V/\partial x)_i\}$ denote the x-derivatives of V at the same points needed in Maxwell's equations. Using the differentiation theorem for Fourier transforms, we can write:

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

where $\mathbf{F}$ and $\mathbf{F}^{-1}$ denote, respectively, the forward and inverse discrete Fourier transforms, and $\tilde{k}_x$ is the Fourier transform variable representing the x-component of the numerical wavevector. In this way, $\{(\partial V/\partial x)_i\}$ can be calculated in one step. In multiple dimensions, this process is repeated for each cut parallel to the major axes of the space lattice.

According to the Nyquist sampling theorem, the representation in (1) is *exact* (i.e., of "spectral accuracy") for electromagnetic field spatial modes sampled at the Nyquist rate or better. This permits the PSTD meshing density to approach two samples per wavelength in each spatial dimension. The wraparound caused by the periodicity in the discrete Fourier transform is eliminated by using the anisotropic perfectly matched layer absorbing boundary condition [8].

For electromagnetic wave interaction structures having primary geometrical or material feature sizes exceeding one-half the dielectric wavelength (l_d), PSTD has been shown to exhibit the same computational accuracy and dynamic range as FDTD models having approximately eight-times finer resolution [7]. That is, a PSTD grid with coarse $l_d/4$ resolution provides about the same accuracy as an FDTD grid with fine $l_d/32$ resolution. Much experience with FDTD modeling has shown that this level of spatial resolution yields accuracy of better than 1 dB over dynamic ranges exceeding 50 dB for the scattering intensity observed at all possible angles.

In this Paper, we report application of PSTD technique to model full-vector, three-dimensional (3-D) scattering of light by macroscopic clusters of dielectric spheres in free space. We use a PSTD grid having a uniform spatial resolution of 0.167 µm, equivalent to $0.33 l_d$ at 600 THz (l_0 = 0.5 µm) for a refractive index $n = 1.2$.

Validation of our research methodology is shown in Fig. 1, where the light scattering properties of: (a) a homogeneous dielectric sphere, (b) a cluster of $N = 19$ randomly positioned, dielectric spheres, are calculated using PSTD simulations and compared with the analytical solutio—Mie expansion [9] and multi-sphere expansion [10], respectively. Even with a coarse resolution (three grid points per wavelength), PSTD simulation yields excellent agreement with the analytical expansions. PSTD permits the electromagnetic field sampling by the space grid to approach the coarse-sampling limit allowed by the Nyquist criterion—two samples per wavelength. This is desirable for modeling electrically large regions because it minimizes the required number of field samples, and hence, computer storage. The primary drawback is that the sample geometries are resolved to only the same extent, resulting in order ($0.5 l$) stair-casing (*aliasing*) of such surfaces.

The dielectric spheres were positioned randomly with a minimum (*edge-to-edge*) spacing of 0.25 µm between spheres. A standard anisotropic perfectly matched layer (APML) absorbing boundary condition [8] is implemented to absorb outgoing waves, simulating an open-region light-scattering experiment. An impulsive plane wave illuminates 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 [11].

By employing the PSTD algorithm, light scattering by a cluster of closely packed dielectric spheres in free space is simulated, yielding the total scattering cross-section (TSCS) spectra as function of frequency from 0-600 THz (l_0 = 300 µm – 0.5 µm) with a resolution of 1.0 THz. Each cluster, with a diameter D = 25µm, consists of N randomly positioned, closely packed, noncontacting, homogeneous, dielectric (n = 1.2) d-µm-diameter spheres. The TSCS spectra corresponding to three different cluster geometries are shown in Fig. 2(a-c), respectively.

Notice that all three TSCS spectra are similar in the low frequency regime (l_0 >> 1.5 µm), suggesting that for long wavelength, the incident light cannot discern the microscopic structural difference between the three geometries [12]. However, notice that in the shorter wavelength regime (l_0 < 1.5 µm), the TSCS spectra exhibit structural differences that can potentially yield information indicative the microscopic structures [13], even for clusters consisting of closely packed scatterers as shown in Fig. 2(a-c).

We propose a cross-correlation analysis to further determine the correlation of the TSCS high-frequency spectral features (l_0 < 1.5 µm) and the corresponding cluster geometries as shown in Fig. 2. By cross-correlating the TSCS spectra shown in Fig. 2(a)-(c), and the TSCS spectra of a single dielectric sphere of diameter d (d ranging from 2µm - 10µm), it is shown that the correlation coefficient is maximized at $d = d_p$, where d_p approximately matches the actual diameter of the constituent spheres of the cluster geometry. This relationship suggests that the TSCS spectral features in the short wavelength regime (l_0 < 1.5 µm) is related to the size of the constituent spheres, even for *optically thick* (optical thickness ~ 20), closely packed cluster where the *edge-to-edge* spacing between adjacent spheres are less than a single wavelength (< 0.5 µm) apart.

Based on first principles, Figs. 2 and 3 show that the TSCS spectra contain information indicative of the geometrical details (*i.e.*, size of constituent spheres), even for closely packed random media where scatterers are spaced (*edge-to-edge*) less than a single wavelength apart. Furthermore, by employing the proposed cross-correlation analysis, information concerning the constituent scatterer size of closely packed random media can be identified and obtained from multiply scattered light. Conventionally, singly scattered light has been utilized in sizing applications while discarding multiply scattered light [14]; the results reported in this Paper suggest that multiply scattered light also contains information that can be utilized by the proposed cross-correlation analysis.

The largest dimensions of random media shown in this Paper is ~ (30 μm)^3 for wavelength l_0 = 0.5 μm, with a grid resolution of dx = 0.167 μm. Each PSTD simulation of such a system typically takes ~12 hours with 20 processors. Nevertheless, larger systems can be simulated, but would require more computer resource. The computation required is typically proportional to ~ $(Lx*Ly*Lz) / (l_0)^3$, where *Lx, Ly,* and *Lz* are the dimensions of the system, and l_0 is the shortest wavelength simulated; therefore, for wavelength l_0 = 1.0 μm, a system of (60 μm)^3 with a grid resolution of dx = 0.33 μm can be simulated using the same amount of computational power.

On a broader perspective, the results reported in this Paper demonstrate the feasibility of *first-principle, full-vector,* 3-D simulation of light scattering by macroscopic, arbitrary random media, including media consisting of continuous variations of refractive index. More importantly, our results point toward the new possibilities of tissue optics—by numerically solving Maxwell's equations, the optical properties of tissue structures can be determined without heuristic approximations.

Acknowledgments

The authors thank Prof. Q. H. Liu for his valuable comments and suggestions on overcoming technical challenges of implementing the PSTD algorithm. Also, the authors thank the National Institutes of Health National Cancer Institute Contract Grants 5R01-CA085991 and 5R01-HD044015, NIH grant R01 EB003682, NSF Grant BES-0238903, and the NSF TeraGrid Grant No. MCB040062N for their support of this research. This study was performed under the auspices of the U.S. Department of Energy under Contract No. W-7405-ENG-48(UC,LLNL)
Snow H. Tseng's email address is snow@ece.northwestern.edu.

Reference list

1. Barrowes, B. E., Ao, C. O., Teixeira, F. L., Kong, J. A., Tsang, L. (2000), Monte Carlo simulation of electromagnetic wave propagation in dense random media with dielectric spheroids, *IEICE Transactions on Electronics*, E83C, 1797-1802.
2. Jaruwatanadilok, S., Ishimaru, A., Kuga, Y. (2003), Optical imaging through clouds and fog, *IEEE Transactions on Geoscience and Remote Sensing*, 41, 1834-1843.
3. Mishchenko, M. I., Videen, G., Babenko, V. A., Khlebtsov, N. G., Wriedt, T. (2004), T-matrix theory of electromagnetic scattering by particles and its applications: a comprehensive reference database, *Journal of Quantitative Spectroscopy & Radiative Transfer*, 88, 357-406.
4. Welch, A. J., van Gemert, M. J. C. (1995) Optical-Thermal Response of Laser-Irradiated Tissue (Lasers, Photonics and Electro-Optics). Plenum Publishing Corporation
5. Busch, K., Soukoulis, C. M. (1995), Transport Properties of Random Media: A New Effective Medium Theory, *Physical Review Letters*, 75, 3442-3445.
6. Marti-Lopez, L., Bouza-Dominguez, J., Hebden, J. C., Arridge, S. R., Martinez-Celorio, R. A. (2003), Validity conditions for the radiative transfer equation, *JOSA A*, 20, 2046-2056.
7. Liu, Q. H. (1999), Large-scale simulations of electromagnetic and acoustic measurements using the pseudospectral time-domain (PSTD) algorithm, *IEEE Transactions on Geoscience and Remote Sensing*, 37, 917-926.
8. Gedney, S. D. (1996), An anisotropic perfectly matched layer absorbing media for the truncation of FDTD lattices, *IEEE transactions on Antennas and Propagation*, 44, 1630-1639.
9. Mie, G. (1908), *Ann. Phys.*, 25, 377.
10. Xu, Y.-L., Wang, R. T. (1998), Electromagnetic scattering by an aggregate of spheres: Theoretical and experimental study of the amplitude scattering matrix, *Physical Review E*, 58, 3931-3948.
11. Taflove, A., Hagness, S. C. (2000) Computational Electrodynamics: the finite-difference time-domain method. Artech House
12. Tseng, S. H., Greene, J. H., Taflove, A., Maitland, D., Backman, V., Walsh, J. (2004; 2005), Exact solution of Maxwell's equations for optical interactions with a macroscopic random medium, *Optics Letters*, 29, 1393-1395; 30, 56-57.
13. Tseng, S. H., Taflove, A., Maitland, D., Backman, V., Walsh, J. T. (2005), Interpretation of Noise-like Temporal Speckles for Clusters of Closely Packed Randomly Positioned Dielectric Cylinders, *Optics Express*, 13, 6127-6132.
14. Wax, A. (2005), Low-coherence light-scattering calculations for polydisperse size distributions, *Journal of the Optical Society of America A-Optics Image Science and Vision*, 22, 256-261.

Figure Captions

1. Validation of the 3-D PSTD simulations. (a): PSTD-computed differential scattering cross-section (DSCS) as a function of angle is compared with the analytical solution (Mie expansion). Light scattering (wavelength l_0 = 0.75 μm), by a single 8μm-diameter, dielectric (n = 1.2) sphere is simulated using the PSTD technique, with a grid resolution of dx = 0.0833 μm; and, (b): PSTD-computed TSCS as a function of frequency is compared with the multi-sphere expansion. Light scattering (wavelength l_0 = 1 μm) by a 20μm-diameter cluster consisting of 19 randomly positioned, 6μm-diameter, dielectric spheres is simulated using the PSTD technique, with a grid resolution of dx = 0.167 μm. Notice that the PSTD simulations yield excellent results compared to the analytical solutions: the Mie solution and the multi-sphere expansion, even with a coarse PSTD grid with noticeable stair-casing error of the geometry.

2. PSTD-computed TSCS spectra of 25μm-diameter clusters consisting of N randomly positioned, closely packed, homogeneous, dielectric (n = 1.2) spheres of diameter d. (a): d = 3μm, N = 192, with an optical thickness ~ 26; (b): d = 5μm, N = 56, with an optical thickness ~ 21; (c): d = 7μm, N = 14, with an optical thickness ~ 10 [optical thickness = (geometrical thickness) / (scattering mean free path)].

3. Cross-correlation analysis of the TSCS spectra shown in Fig. 2. By calculating the cross-correlation coefficients of the cluster TSCS (as shown in Fig. 2(a)-(c)), and the TSCS spectra of a single dielectric sphere, it is shown that the correlation coefficient peaks at d = d_p, where d_p is approximately equal to the diameter of the constituent spheres of the cluster geometry. This relationship suggests that the TSCS spectral features is related to the size of

the constituent spheres, even for *optically thick*, closely packed cluster of scatterers where the *edge-to-edge* spacing between adjacent spheres is less than a single wavelength (< 0.5 μm) apart.

Figures:

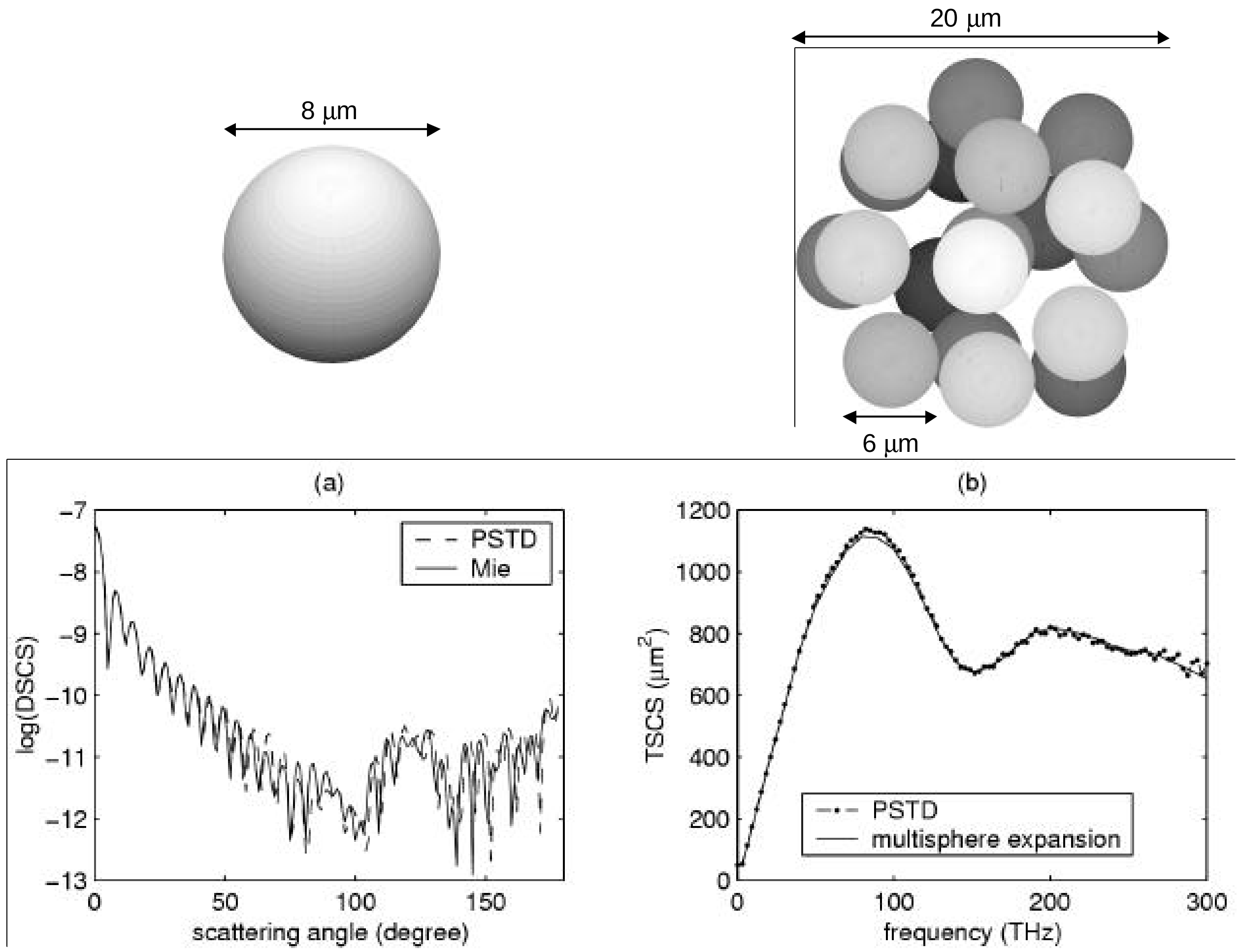

Fig. 1. Validation of the 3-D PSTD simulations. (a): PSTD-computed differential scattering cross-section (DSCS) as a function of angle is compared with the analytical solution (Mie expansion). Light scattering (wavelength l_0 = 0.75 μm), by a single 8μm-diameter, dielectric (*n* = 1.2) sphere is simulated using the PSTD technique, with a grid resolution of *dx* = 0.0833 μm. (b): PSTD-computed TSCS as a function of frequency is compared with the multi-sphere expansion. Light scattering (wavelength l_0 = 1 μm) by a 20μm-diameter cluster consisting of 19 randomly positioned, 6μm-diameter, dielectric spheres is simulated using the PSTD technique, with a grid resolution of *dx* = 0.167 μm. Notice that the PSTD simulations yield excellent results

compared to the analytical solutions: the Mie solution and the multi-sphere expansion, even with a coarse PSTD grid with noticeable stair-casing error of the geometry.

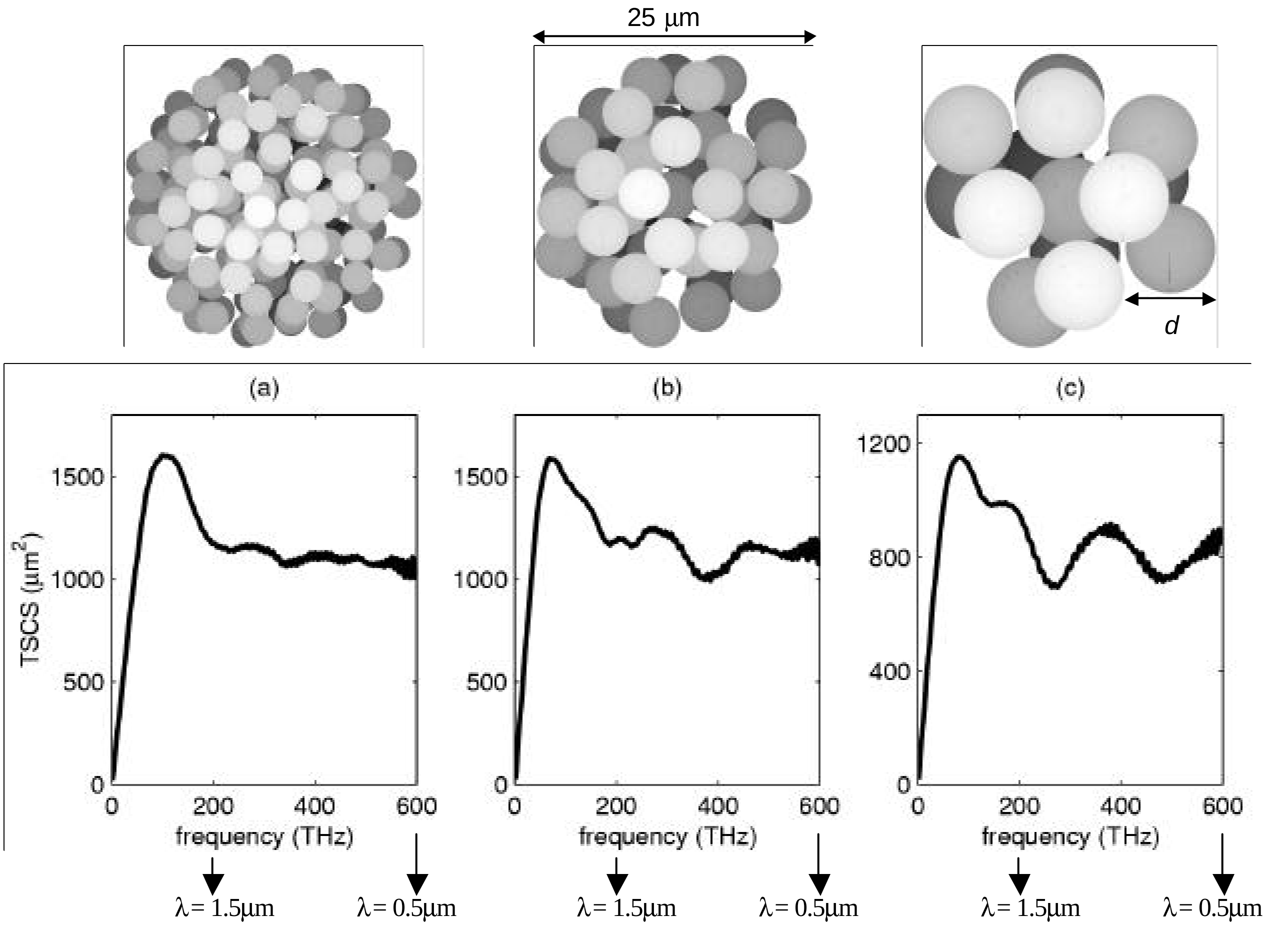

Fig. 2. PSTD-computed TSCS spectra of 25μm-diameter clusters consisting of N randomly positioned, closely packed, homogeneous, dielectric (n = 1.2) spheres of diameter d. (a): d = 3μm, N = 192, with an optical thickness ~ 26; (b): d = 5μm, N = 56, with an optical thickness ~ 21; (c): d = 7μm, N = 14, with an optical thickness ~ 10 [optical thickness = (geometrical thickness) / (scattering mean free path)].

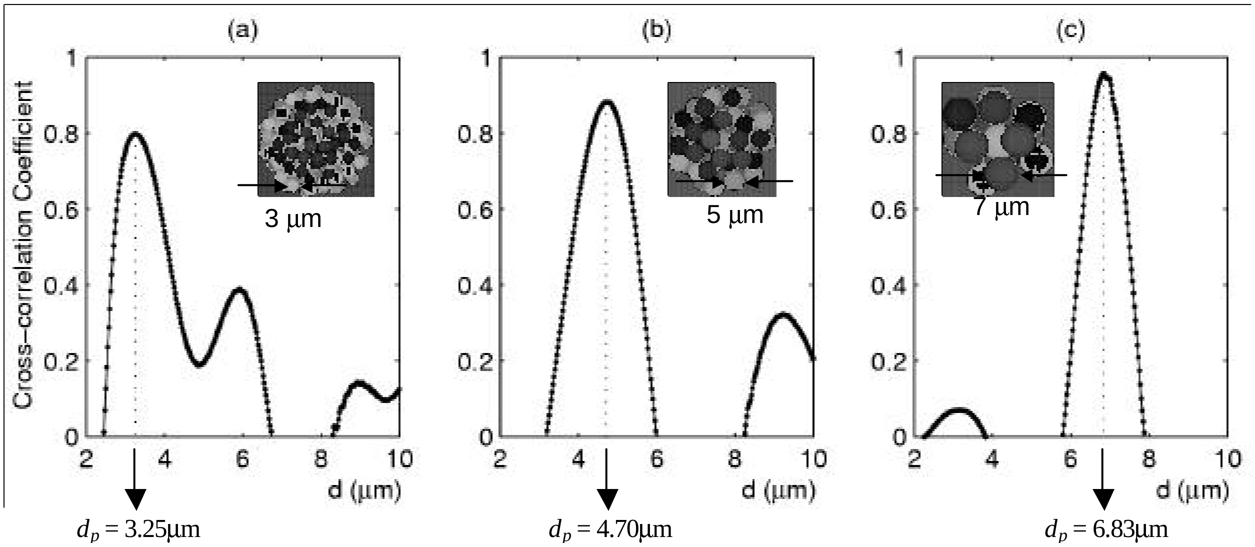

Fig. 3. Cross-correlation analysis of the TSCS spectra shown in Fig. 2. By calculating the cross-correlation coefficients of the cluster TSCS (as shown in Fig. 2(a)-(c)), and the TSCS spectra of a single dielectric sphere, it is shown that the correlation coefficient peaks at $d = d_p$, where d_p is approximately equal to the diameter of the constituent spheres of the cluster geometry. This relationship suggests that the TSCS spectral structure is related to the size of the constituent spheres, even for *optically thick*, closely packed cluster of scatterers where the *edge-to-edge* spacing between adjacent spheres is less than a single wavelength (< 0.5 µm) apart.