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Multiple scattering in turbid media containing chiral components: A Monte Carlo simulation

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ABSTRACT

A Monte Carlo simulation was performed for an infinite plane medium containing spherical particles as well as a chiral component. The optical activity shifts patterns in the two-dimensional map of the effective scattering Mueller matrix in the azimuthal direction. The reduced effective matrix obtained by the simulation approximately satisfies reciprocity in spite of the theoretical prediction. The pattern shifts are explained by the mixing of elements of the reduced effective Mueller matrix owing to multiplication of two rotation matrices. The reduced effective matrix was factorized using the Lu-Chipman polar decomposition affording the polarization components as a function of the distance. The functions as a retarding linear diattenuator of the medium decreases, whereas the optical rotation increases, as the distance increases. The estimated specific rotation on the medium surface is 1.6 times larger than the specific rotation in the medium used in the simulation.

1. Introduction

Noninvasive glucose monitoring is one of the most important issues in medicine for intensive treatment of diabetes and its related complications. Considerable efforts have been made to realize such monitoring devices especially utilizing optical techniques [1]. However, these techniques are designed to measure glucose concentrations in body liquids with a low scattering coefficient including aqueous humor. Optical approaches to detect chiral components in turbid media like tissue have generated interest because of their noninvasive monitoring capability [2]. The potential for measuring small optical rotations due to the presence of glucose has been shown in spite of difficulties in scattering media such as large depolarization and simultaneous occurrence of several polarization effects [3–6]. Since the sensitivity is still low, further improvement is strongly required. Wang et al. have reported that chiral components alter the Mueller matrix of backscattered and forward-scattered light from turbid slab media in such a way that the patterns of the matrix elements are rotated around the illumination point [7].

In this paper, the backscattering from an infinite plane medium containing a chiral component is examined by the use of the Monte Carlo simulation. We explain why the optical activity shifts patterns of the two-dimensional distribution of the effective scattering Mueller matrix in the azimuthal direction. The polarization characteristics of the medium are evaluated by factorizing the reduced effective matrix using the Lu-Chipman polar decomposition. We estimated the specific optical rotation on the surface of the infinite plane medium for the first time to our knowledge.

2. Theory

As Raković et al. have shown [8], the effective backscattering Mueller matrix $\tilde{\mathbf{M}}$ is represented in two-dimension by

$$\tilde{\mathbf{M}}(r,\Phi)=\mathbf{R}(\Phi)\tilde{\mathbf{M}}^{r}(r)\mathbf{R}(\Phi), \tag{1}$$

where r and Φ are the polar coordinate of each point on the surface of the medium, $\tilde{\mathbf{M}}^{r}(r)$ is the reduced effective scattering Mueller matrix, and $\mathbf{R}(\Phi)$ is the rotation Mueller matrix as represented by

$$\mathbf{R}(\Phi)=\begin{bmatrix}1 & 0 & 0 & 0\\ 0 & \cos 2\Phi & \sin 2\Phi & 0\\ 0 & -\sin 2\Phi & \cos 2\Phi & 0\\ 0 & 0 & 0 & 1\end{bmatrix}, \tag{2}$$

The reduced effective matrix $\tilde{\mathbf{M}}^{r}$ is expressed as a summation over all orders of the multiple-scattered light

$$\tilde{\mathbf{M}}^{r}=\sum_{n=1}^{\infty}\tilde{\mathbf{M}}_{n}, \tag{3}$$

where $\tilde{\mathbf{M}}_{\mathrm{n}}$ stands for the contribution of the light that has been scattered exactly n times by particles and actually includes

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contributions from all possible trajectories of the light. In isotropic media, a contribution from one of such trajectories is described as a matrix multiplication $\tilde{\mathbf{M}}_n$ as

$$\tilde{\mathbf{M}}_n = \tilde{\mathbf{M}}(\theta_n)\ldots\ \tilde{\mathbf{M}}(\theta_2)\tilde{\mathbf{M}}(\theta_1), \quad (4)$$

where $\tilde{\mathbf{M}}(\theta_i)$ is the effective Mueller matrix for the i-th single scattering represented using the meridian plane [9,10]. Meanwhile, the Mueller matrix for single scattering by homogeneous spheres satisfies reciprocity and mirror symmetry. If the spherical particles are randomly oriented in the medium, the reduced effective matrix $\tilde{\mathbf{M}}^r$ also satisfies these symmetry relations, as proved previously [8].

Optical activity brings about a rotation of the plane of linearly polarized light. This rotation results from the difference in the refractive indices for left- and right-handed circularly polarized light due to the molecular asymmetry. Hence, the Mueller matrix for the optical activity takes a form of the rotation matrix in Eq. (2), $\mathbf{R}(-\alpha)$, where α is the rotation angle due to the optical activity [7]. Thus, for media containing chiral components, the matrix multiplication becomes

$$\tilde{\mathbf{M}}_n = \mathbf{R}(-\alpha_n)\tilde{\mathbf{M}}(\theta_n)\mathbf{R}(-\alpha_{n-1})\ldots\ \mathbf{R}(-\alpha_1)\tilde{\mathbf{M}}(\theta_1)\mathbf{R}(-\alpha_0) \quad (5)$$

While reciprocity is represented for Mueller matrices as $\mathbf{M}^t = \mathbf{PMP}$, where $\mathbf{P} = \mathrm{diag}(1, 1, -1, 1)$ and t indicates the matrix transpose, mirror symmetry is represented as $\mathbf{M} = \mathbf{QMQ}$, where $\mathbf{Q} = \mathrm{diag}(1, 1, -1, -1)$ [9]. Both matrix operations convert the rotation matrix $\mathbf{R}(-\alpha)$ to $\mathbf{R}(\alpha)$, where the rotation angle with an opposite sign brings the optical rotation in a reverse sign. Then both matrix operations do not transform the matrix multiplication $\tilde{\mathbf{M}}_n$ to either itself or its transpose. Thus, both reciprocity and mirror symmetry do not hold for the reduced effective scattering Mueller matrix $\tilde{\mathbf{M}}^r$. Because the matrix $\tilde{\mathbf{M}}^r$ takes the most general form, the effective scattering Mueller matrix $\tilde{\mathbf{M}}$, derived from Eqs. (1) and (2), is expressed as

$$\tilde{\mathbf{M}} = \begin{bmatrix} m_{00} & m_{01}\cos 2\phi - m_{02}\sin 2\phi & m_{01}\sin 2\phi + m_{02}\cos 2\phi & m_{03} \\ m_{10}\cos 2\phi + m_{20}\sin 2\phi & \frac{1}{2}(m_{11}-m_{22}) + \frac{1}{2}(m_{11}+m_{22})\cos 4\phi - \frac{1}{2}(m_{12}-m_{21})\sin 4\phi & \frac{1}{2}(m_{12}+m_{21}) + \frac{1}{2}(m_{11}+m_{22})\sin 4\phi + \frac{1}{2}(m_{12}-m_{21})\cos 4\phi & m_{23}\sin 2\phi + m_{13}\cos 2\phi \\ -m_{10}\sin 2\phi + m_{20}\cos 2\phi & \frac{1}{2}(m_{12}+m_{21}) - \frac{1}{2}(m_{11}+m_{22})\sin 4\phi - \frac{1}{2}(m_{12}-m_{21})\cos 4\phi & -\frac{1}{2}(m_{11}-m_{22}) + \frac{1}{2}(m_{11}+m_{22})\cos 4\phi - \frac{1}{2}(m_{12}-m_{21})\sin 4\phi & m_{23}\cos 2\phi - m_{13}\sin 2\phi \\ m_{30} & -m_{32}\sin 2\phi + m_{31}\cos 2\phi & m_{32}\cos 2\phi + m_{31}\sin 2\phi & m_{33} \end{bmatrix}. \quad (6)$$

3. Results

The Monte Carlo simulation in this paper is an extension of one reported elsewhere [11]. The rotation angle α induced by the optical activity is given [7] as

$$\alpha = [\alpha]_\lambda^T LC, \quad (7)$$

where $[\alpha]_\lambda^T$ is the specific rotation of a chiral molecule given in deg ml $g^{-1}dm^{-1}$ and dependent on the temperature T and wavelength λ of the light, L is the photon path length through the medium, and C is the concentration of the chiral molecule. The present simulation used the optical rotation for the medium of 15.8°cm^{-1}, which is much higher than that for the physiological glucose level in blood, 0.046°cm^{-1} at the wavelength of 632.8 nm [3].

The other simulation parameters were as follows. The scattering medium has a refractive index of 1.334, the scattering coefficient of 11.88 cm^{-1}, and a negligible absorption. Spherical particles with 0.7 μm radius and 1.59 refractive index were used. The photon wavelength was 632.8 nm. The asymmetry parameter was estimated to be 0.932. The photon was incident on the sample surface in the positive z direction at the same point (0, 0, 0), implying a zero beam diameter. The photon exit acceptance angle was 10°. The calculation was repeated until 10^9 photons were simulated.

The elements of the calculated effective scattering matrix $\tilde{\mathbf{M}}$ are presented as surface maps. in Fig. 1. The matrix elements except $\tilde{m}_{00}$ are normalized by $\tilde{m}_{00}$ and their unit is dimensionless. Infinite plane media without chiral component show intensity patterns of the matrix elements that have rotational and radial symmetry about the incident point, which is at the center of each map [11]. In contrast, for the present medium containing chiral components, the patterns become spiral with only rotational symmetry; the patterns shift in the azimuthal direction with increasing distance.

According to Eqs. (1) and (2), the reduced effective scattering Mueller matrix $\tilde{\mathbf{M}}^r$ is calculated as

$$\hat{\mathbf{M}}^r(r) = \mathbf{R}(-\Phi)\tilde{\mathbf{M}}(r, \Phi)\mathbf{R}(-\Phi) \quad (8)$$

Apparent non-zero values are observed for m_{12} and m_{21} as well as 2×2 diagonal elements, as shown in Fig. 2; m_{00} and m_{33} are not affected by the matrix multiplication. In contrast, the reduced effective matrix is virtually 2×2 diagonal for the medium containing no chiral component [11]. All elements display radial dependences but little azimuth dependence, as predicted from Eq. (8).

Each element of the reduced effective matrix was azimuthally averaged at varying distance from the center (d). The dependence of the elements on the distance is shown in Fig. 3. Appreciable values are observed over the whole distance for the 2×2 diagonal elements as well as m_{12} and m_{21}. Four elements m_{02}, m_{13}, m_{20}, and m_{31} have slight but considerable values. On the other hand, m_{03} and m_{30} fluctuate between plus and minus values around 0, and can be considered to be zero over the whole distance. The simulation results show that the relationships, $m_{10} \cong m_{01}$ and $m_{32} \cong -m_{23}$, hold over the whole distance. Moreover, the relationships, $m_{20} \cong -m_{02}$, $m_{21} \cong -m_{12}$, and $m_{31} \cong m_{13}$, are satisfied in the range of $d \geq 7$ mm. These results show that the reduced effective matrix fulfills reciprocity in the middle and large distance range in spite of the theoretical consideration.

The rotational symmetry and the shift of pattern of the effective matrix $\tilde{\mathbf{M}}$ agree well with the prediction in Eq. (8). The appreciable values of m_{12} and m_{21} are responsible for the pattern