Monte Carlo modelling of Raman scattering in a multi-layered tissue

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Abstract. The report is concerned to Monte Carlo modelling of Raman scattering. A model of Raman scattering in multi-layered tissues has been built. A number and optical properties of tissue layers, number of photons, geometric size of the model and parameters of the light source may be varied by users. Some of computational results have been compared with other investigators.

1. Introduction

Recent technical advances in Raman spectrometer hardware have paved the way for exploiting the Raman effects in clinical applications. Raman spectroscopy has shown great potential in noninvasive cancer screening. It is essential to have an accurate model for illustrating the properties of Raman excitation and Raman photon escape process in order to facilitate the quantitative analysis of *in vivo* Raman spectra.

2. Skin model

A two-layer skin optical model has been built with optical transport parameters and Raman active components extracted from skin *in situ*. As the most important model components collagen, elastin, keratin, cell nucleus, triolein, ceramide, melanin and water are chosen (table 1).

The basis spectra of those skin constitutes have been used to simulate human skin spectra. We used the spectra and key biophysical changes of skin components with different tissue types by Xu Feng et al. [1]

The medium is defined as a cube with cube-shaped voxels (figure 1). Each voxel is assigned an integer value which identifies a particular type of tissue with unique optical properties of an absorption coefficient, scattering coefficient, anisotropy factor, and concentration of skin components.

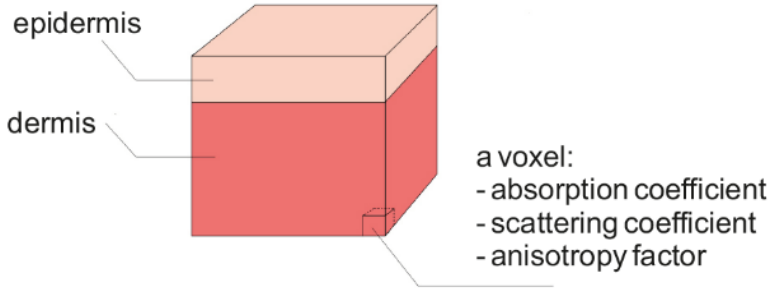

Figure 1. Skin model.

Table 1. Skin components in percentage for different tissue types (the arrow indicates the most characteristic changes for each lesion type).

	Normal skin	Malignant Melanoma	Basal Cell Carcinoma
Collagen	18%	18%	15%↓
Elastin	12%	14%	23%↑
Triolein	41%	11%↓	28%↓
Nucleus	9%	6%	20%↑
Keratin	1%	2%	1%
Ceramide	9%	17%↑	4%
Melanin	5%	29%↑	3%
Water	5%	3%	6%

3. Methodology

3.1. Raman scattering

Raman scattering is the inelastic scattering of a photon by molecules (figure 2). The scattered photons have a frequency and energy different from those of the incident photons. The difference in energy for each inelastically scattered photon corresponds to a molecular vibration of a particular component of the specimen. Therefore, the molecular vibrations of each substance produce a characteristic Raman fingerprint spectrum that can be used to determine the chemical and structural composition of the sample.

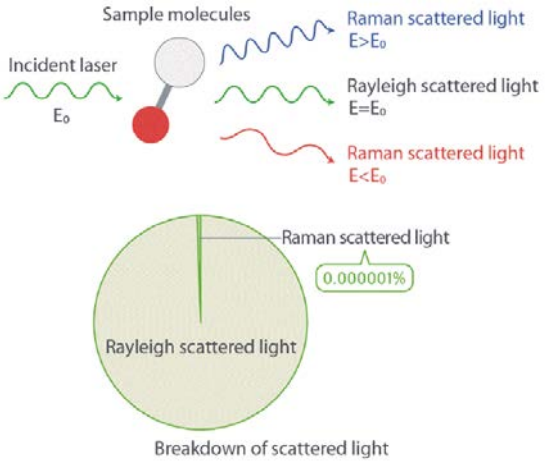

Figure 2. Raman scattering.

3.2. Monte Carlo method

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A two-step model of Raman scattering in multi-layered tissues has been built. Calculation of excitation light distribution inside the model tissue is performed with Monte Carlo code from Wang and Jacques (figure 3) [2].

In the first step, the program simulates the propagation of the incident photons through the sample, which results in a distribution of the excitation photons, *Fex (x; y; z)* within the sample. In the second

step, Raman scattered photons are launched from each point where parent photons were absorbed in isotropically distributed directions and with a weight of:

$$wRaman = Fex\ (x; y; z) \cdot \mu Raman \cdot (sRaman1 \cdot C1 + \ldots + sRamanN \cdot CN),$$

where *Fex (x; y; z)* represents results in a distribution of the excitation photons, *μRaman* is comparable with the Raman probability and depends on the frequency of the emission photons, *sRaman1…sRamanN* are given by Raman spectra of skin components, *C1…CN* are concentrations of components.

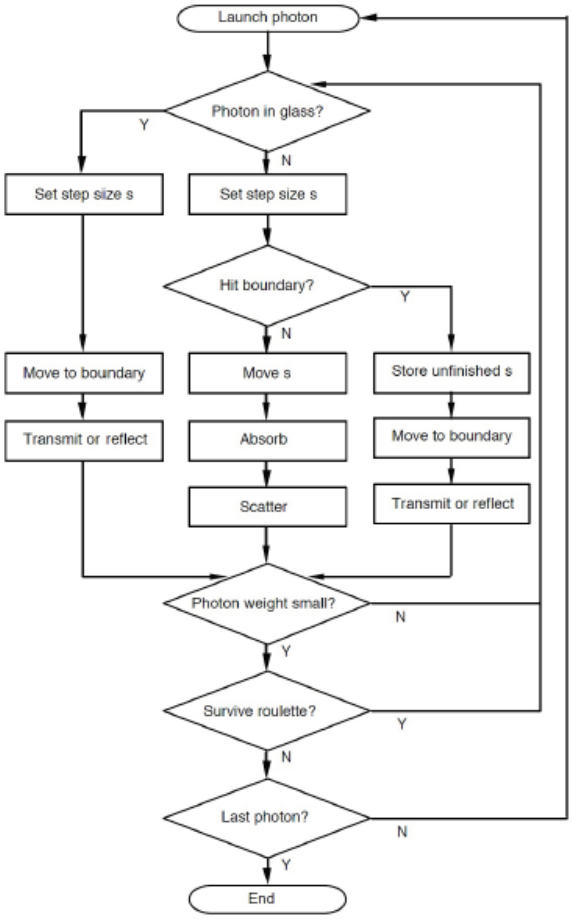

Figure 3. Flowchart for Monte Carlo simulation of multi-layered tissue.

During the second step, the program is executed sequentially at each wavelength and the sum of all the photons captured by the detector is calculated. The normalized sums represent the Raman spectrum.

4. Results & Discussion

In this study, we established a Raman "biophysical model", a program for modelling Raman spectra. Monte Carlo simulation were performed to record Raman spectra of skin for 785 nm excitation light and for different emission wavelengths at am interval of 1 nm from 840 nm to 910 nm. In each simulation, 1,000,000 photons were launched.

We obtained Raman spectra spanning normal skin, Malignant Melanoma (MM), and Basal Cell Carcinoma (BCC). We use eight of the most relevant skin constitutes contributing to the spectral differences among different skin malignancies. Figure 4 shows mean Raman in vivo spectra (black solid lines), model fits by Xu Feng et al. (dotted lines) and reconstructed Raman spectra (blue solid lines). The Raman spectra were normalized to their respective area under curve.

In general, the reconstructed Raman spectra match reasonably well with the *in vivo* Raman spectra. In particular, the major Raman peaks of normal skin Raman spectra reconstructed by this Monte Carlo simulation match very well with the *in vivo* spectra. There are also differences between the reconstructed and the *in vivo* Raman spectra in the case of MM and BCC. These differences may be

due to the fact that the composition of diseased skin varies depending on the stage of the disease and individual characteristics of patients.

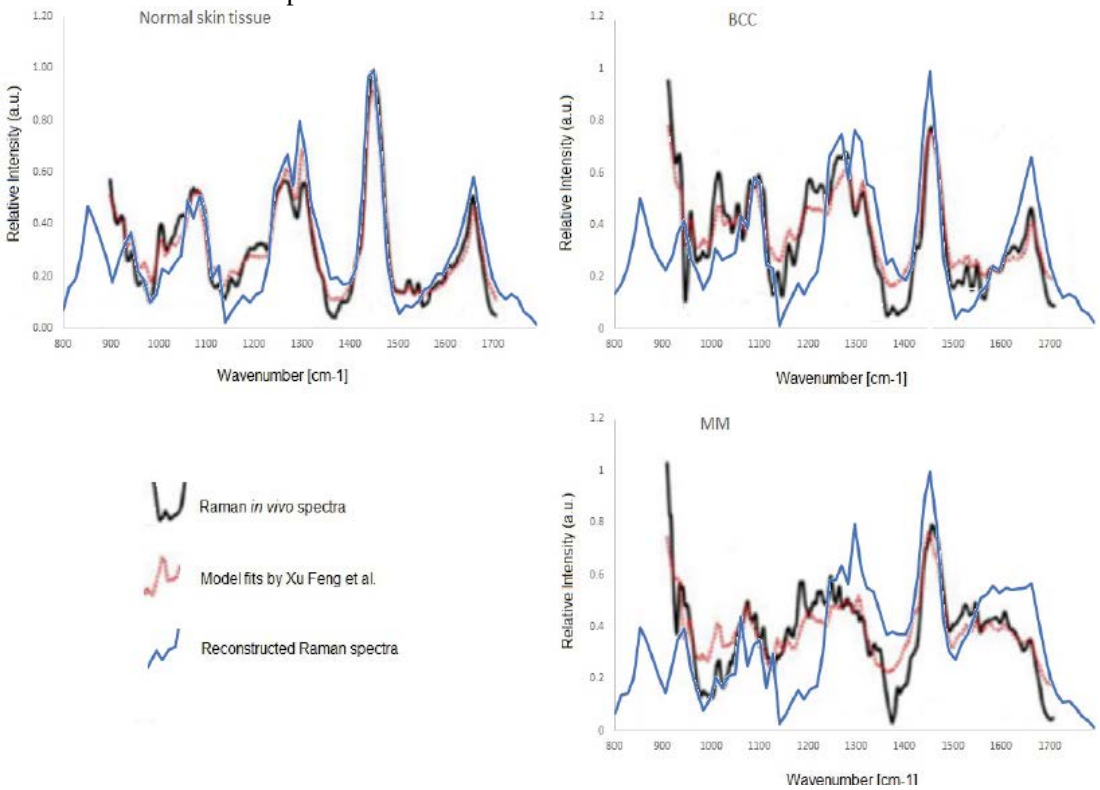

Figure 4. Normalized Raman spectra of normal skin tissue, Malignant Melanoma (MM), and Basal Cell Carcinoma (BCC).

In summary, spectra modelled were found to be consistent with previous studies. Monte Carlo simulations of photon propagation offer a flexible yet rigorous approach toward Raman scattering in turbid tissues.

5. References

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[2] Wang, L. MCML – Monte Carlo modeling of light transport in multi-layered tissues / L. Wang, S.L. Jacques, L. Zheng // Computer Methods and Programs in Biomedicine. – 1995. – Vol. 47(2). – P. 131-146.

Acknowledgments

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