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Time-Domain Raman Forward Solver in a Two-layer Diffusive Medium

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Abstract: An analytical model to describe the time-domain reflectance Raman signal in a two-layer diffusive medium was developed. The accuracy of the model is verified by comparison with the results of Monte Carlo simulations.

1. Introduction

Time-Domain Diffuse Raman spectroscopy [1–5] is a newborn technique that merges Time-Domain Diffuse Optics with Raman Spectroscopy offering the advantages of both techniques, [3] that is the possibility to extract information deeply from the medium and to reconstruct hidden information on its chemical composition. The development of time-domain diffuse Raman spectroscopy depends critically on the availability of a forward model capable of describing photon migration in the media of interest. To date, time-domain spontaneous Raman scattering in diffusive media involves three approaches: stochastic forward solvers based on Monte Carlo simulations [6–8], analytical heuristic solutions of the Raman interactions [5, 7, 8] and analytical rigorous solutions of diffusion equation (DE) [5, 7, 8]. Although Monte Carlo (MC) simulations can be carried out for any geometry, they are computationally expensive and their use for the inverse problem may be very limited. Conversely, exact analytical forward solvers are much faster, however they are available only for some homogeneous geometries [6–8]. In this work, the photon migration of the Raman signal through a two-layer medium is calculated with both MC simulations and an analytical heuristic forward solver which offers significant advantages compared to the existing ones [5]. The MC results are used as a reference for the verification of the analytical model.

2. Theory

The usual approach used to obtain solutions for the Raman signal in diffusive media across any geometry involve two coupled DEs, one at the excitation wavelength (λ), and one at the emission wavelength (λ_e) [6–8]. From now on, the quantities without suffix are related to the excitation wavelength, and the quantities with the suffix e refer to the emission wavelength. It is considered a two-layer cylinder of radius L and with s_1 and s_2 the thicknesses for the first and second layer, respectively. At λ, we denote by μ_{a1} and μ_{a2} the absorption coefficients of first and second layer, by μ'_{s1} and μ'_{s2} the reduced scattering coefficients of first and second layer, by μ_{sR1} and μ_{sR2} the Raman scattering coefficients of first and second layer, and by n_1 and n_2 the refractive indices in first and second layer. In a similar way, the symbols μ_{a1e}, μ_{a2e}, μ'_{s1e}, μ'_{s2e}, n_{1e} and n_{2e} are referred to the optical properties at λ_e.

We started from a previous heuristic approach proposed by Šušnjar et al. [5] according to which the time-domain Raman fluence signal at λ_e, Φ_e, in a two-layer cylinder can be written, under the hypothesis that the optical properties of the medium were the same at λ and λ_e, as:

$$\Phi_e(\vec{r},\mu_{a1e},\mu'_{s1e},\mu_{a2e},\mu'_{s2e},t,\lambda_e) \approx \Phi(\vec{r},\mu_{a1},\mu'_{s1},\mu_{a2},\mu'_{s2},t,\lambda) \times [\mu_{sR1} v_1 \langle t_1\rangle(t) + \mu_{sR2} v_2 \langle t_2\rangle(t)], \tag{1}$$

with Φ fluence of the two-layer medium at λ, $\langle t_1\rangle$ and $\langle t_2\rangle$ the average times spent by detected light in the first and second layer, respectively and v_1 and v_2 the speed of light in the layers. It is worth to note that $\langle t_1\rangle$ and $\langle t_2\rangle$, according to the Radiative Transfer Equation properties, can be expressed as [7–9]:

$$\langle t_1\rangle(t) = -\frac{1}{v_1 \Phi(\vec{r},\mu_{a1},\mu'_{s1},\mu_{a2},\mu'_{s2},t,\lambda)} \frac{\partial \Phi(\vec{r},\mu_{a1},\mu'_{s1},\mu_{a2},\mu'_{s2},t,\lambda)}{\partial \mu_{a1}}, \tag{2}$$

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$$\langle t_2\rangle(t) = -\frac{1}{v_2\Phi(\vec{r},\mu_{a1},\mu'_{s1},\mu_{a2},\mu'_{s2},t,\lambda)}\frac{\partial\Phi(\vec{r},\mu_{a1},\mu'_{s1},\mu_{a2},\mu'_{s2},t,\lambda)}{\partial\mu_{a2}}. \tag{3}$$

In this previous model the solution suffers irremediably in accuracy by the fact that it is not correctly represented the dependence of the solution from the optical properties at λ_e that in reality affects the Raman signal emerging from the medium. We denote this model as “Model 0”.

We propose to improve this model by first heuristically replacing in Eq. (1) the term Φ by the average of the fluence in the two-layer medium at λ and λ_e. We denote this improved model as “Model I”.

The time-domain Raman signal received in reflectance configuration from the two-layer medium illuminated by a pulse source can be obtained as

$$R_e(\rho,t) = \frac{\Phi_e(\rho, z=0, t)}{2A}, \tag{4}$$

with A a coefficient related to Fresnel reflection coefficient [7–9].

3. Results

The results of the heuristic solution Model I for the reflectance are calculated and compared to MC results together with the prediction of the previous Model 0. The results presented in the below figure pertain to a two layer medium with optical properties typical of a tissue constituted by a fat layer and an underlying muscle tissue. It is considered a two-layer cylinder where a pencil light beam is impinging at the center of the entrance surface. In the analytical heuristic model the pencil beam is modeled by inserting an isotropic unitary pulse $\varepsilon(\vec{r},t) = \delta(\vec{r}-\vec{r}_s)\delta(t)$ at a transport mean free path, i.e., $\vec{r}_s = (0,\, 0,\, z_0 = 1/\mu'_{s1})$ [7–9]. It is considered a two-layer cylinder having at λ, $\mu_{a1} = 4\cdot 10^{-3}$ mm^{-1} and $\mu_{a2} = 10^{-2}$ mm^{-1}, $\mu'_{s1} = 1$ mm^{-1} and $\mu'_{s2} = 0.5$ mm^{-1}, $\mu_{sR1} = 10^{-5}$ mm^{-1} and $\mu_{sR2} = 2\cdot 10^{-5}$ mm^{-1}, $n_1 = n_2 = 1.4$ and an external medium with unitary refractive index. While at λ_e we have $\mu_{a1e} = 5.2\cdot 10^{-3}$ mm^{-1} and $\mu_{a2e} = 1.3\cdot 10^{-2}$ mm^{-1}, $\mu'_{s1e} = 0.9$ mm^{-1} and $\mu'_{s2e} = 0.45$ mm^{-1}, and $n_{1e} = n_{2e} = 1.4$. The cylinder considered had first and second layer thickness $s_1 = 15$ mm and $s_2 = 80$ mm, respectively, and a radius $L = 80$ mm. Figure 1 shows two examples of results for source-detector distances $\rho \in \{5, 10\}$ mm. The figure compares the results for the Raman time-resolved reflectance signal obtained with Model 0 and I to the MC simulations. The comparisons show, despite the heuristic nature of the model, an excellent agreement between Model I and MC simulations; while it highlights appreciable deficiencies of the previous Model 0. Similar results to those shown in the figures for $s_1 = 15$ mm, were obtained for the thickness of the first layer $s_1 = 8$ mm and for larger source-detector distances.

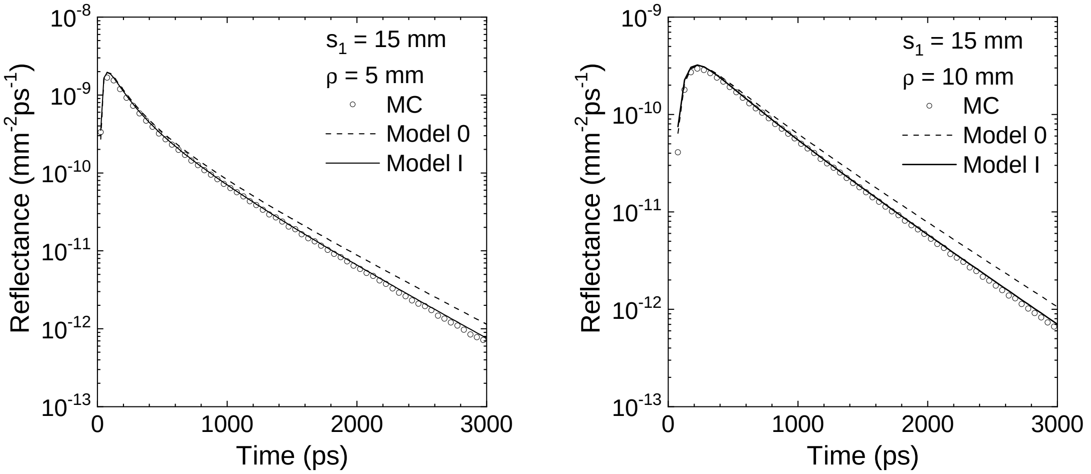

Fig. 1. Comparison between models and MC results. We have a two-layer cylinder with $s_1 = 15$ mm, $s_2 = 80$ mm, and having at λ, $\mu_{a1} = 4\cdot 10^{-3}$ mm^{-1} and $\mu_{a2} = 10^{-2}$ mm^{-1}, $\mu'_{s1} = 1$ mm^{-1} and $\mu'_{s2} = 0.5$ mm^{-1}, $\mu_{sR1} = 10^{-5}$ mm^{-1} and $\mu_{sR2} = 2\cdot 10^{-5}$ mm^{-1}, $n_1 = n_2 = 1.4$ and external medium with unitary refractive index. While at λ_e we have $\mu_{a1e} = 5.2\cdot 10^{-3}$ mm^{-1} and $\mu_{a2e} = 1.3\cdot 10^{-2}$ mm^{-1}, $\mu'_{s1e} = 0.9$ mm^{-1} and $\mu'_{s2e} = 0.45$ mm^{-1}, and $n_{1e} = n_{2e} = 1.4$.

4. Conclusions

We have presented the basic performance of the developed heuristic model for describing the time-domain Raman signal from a two-layer medium that can account the full dependence of the signal from the optical properties of the layers at excitation and emission wavelength. This model, compared to previous works [5], is capable of accounting for the dependence of the Raman signal on the optical properties of the layers at the emission wavelength, which had been omitted in the previous contributions. The overall characteristic of the model, despite its approximate structure, show to be excellent in predicting the time-resolved Raman signal.

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