

Monte-Carlo Modeling of Light Propagation in Hard Dental Tissues

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Abstract

In the present work, it is described the propagation of visible light in human tooth based on a Monte-Carlo computer simulation. In the model, tooth is treated as a turbid medium formed by two distinct layers: one of enamel and another of dentine. Consequently, differences in optical properties data (absorption and scattering coefficients) of these two hard tissues must be taken into account. These data are not completely established in the literature, particularly in the visible range of the electromagnetic spectrum. Hence, some extrapolations were done and the results of light distribution from the model are compared with experimental data of Cu-HyBrID laser light propagation in human molar teeth, in order to evaluate the scattering coefficient. The Cu-HyBrID laser has very peculiar characteristics: it emits green (510 nm) and yellow (578 nm) radiation with high output peak power (20 kW) at high repetition rates (13.7 kHz) and practically there is no report of applications of this laser in Dentistry. The purpose of this numerical modeling is to correlate the Cu-HyBrID laser energy deposition with the tooth thermal response. Hence, this model was also used to simulate the temperature distribution, which reflects the energy deposited in the tooth by the laser. According to the simulation, the tooth thermal response is strongly affected by the value of the absorption coefficient, which is not yet precisely known.

Introduction

The propagation of visible light in human tooth can be calculated by solving analytically the equations of the transport theory, but the complexities involved frequently restrict its applicability. Numerical calculations based on Monte-Carlo method, on the other hand, have been extensively used with satisfactory predictions in many cases [1, 2]. Hence, in the present work, it will be described a numerical model for the visible light propagation where the tooth is treated as a turbid medium constituted by two distinct layers (one of enamel and another of dentine), with distinct optical properties (absorption and scattering coefficients). The approach is similar to the one used by Fried et al. [3], except for the lasers. Fried studied three wavelengths: 543 nm (HeNe laser), 632 nm (HeNe laser) and 1053 nm (Nd:YAG laser), all of them from CW lasers that were chopped at 1.6 kHz. Here, it will be simulated the green emission (510 nm) from a Cu-HyBrID laser [4]. This laser operates in pulsed regime with very peculiar characteristics: in addition to the green radiation, it also emits yellow (578 nm) radiation, both of them with high output peak power (20 kW) at high repetition rates (13.7 kHz) and practically there is no report of applications of this laser in Dentistry. The purpose of this numerical modeling is to correlate the Cu-HyBrID laser energy deposition with the tooth thermal response and hence the temperature distribution is also simulated. The results of light distribution from the model are compared with experimental data of Cu-HyBrID laser light propagation in human molar teeth.

The Monte-Carlo Model

The basic idea of the Monte-Carlo model used in this work is to follow the optical path of a photon through a turbid medium. The first step is to generate the photons in a thin artificial surface layer 60 μm thick, with the same refraction index as enamel, but higher scattering coefficient ($\mu_s = 650 \text{ cm}^{-1}$), coefficient of anisotropy $g = 0.94$ and no absorption ($\mu_a = 0 \text{ cm}^{-1}$), similar to the one proposed by Seka et al. [5]. The second step is to account for absorption and scattering. The absorbing and the scattering sites are supposed to be randomly distributed through the medium and, to account for scattering, a mean free path L between two collisions must be evaluated. The value of L is equal to $1/\rho_s\sigma_s$, where ρ_s is the density of scattering sites, σ_s is the respective scattering cross-section and $\rho_s\sigma_s = \mu_s$ is the scattering coefficient. A random number z is generated by the computer so as the distance $L(z)$ follows a statistical distribution whose average value corresponds to $1/\mu_s$. For absorption, a weight is attributed to each photon in such a way that, during propagation, this weight is reduced by $\exp[-\mu_a L(z)]$, where μ_a is the absorption coefficient. Hence, when the weight is lesser than a given cutoff value, the photon is considered completely absorbed. If the projection of $L(z)$ on the z -axis is greater than the

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enamel thickness, the optical properties of enamel are replaced by dentine in the model. Reflections from the air/tissue boundaries are taken into account in accordance with the Fresnel equations.

Obviously, the numerical model requires accurate values of absorption and scattering coefficients. As these values are not completely established in the literature, particularly in the visible range of the electromagnetic spectrum, some extrapolations from the data published by Fried [3] were done. The values adopted in this work were $\mu_a \leq 1 \text{ cm}^{-1}$ (this coefficient was not estimated in [3]) and $\mu_s = 127 \text{ cm}^{-1}$ for enamel and $\mu_a = 4 \text{ cm}^{-1}$ and $\mu_s = 280 \text{ cm}^{-1}$ for dentine. The angular distribution of the scattered photons is described by a combination of anisotropic and isotropic phase functions, as it was done in [3] by using the same anisotropy coefficients.

The total energy δE deposited in the tissue per unit of volume can be calculated by simply counting the number of photons that was absorbed in an element of volume δV . This energy is then correlated with the temperature variation by the equation:

$$\frac{\partial E}{\partial V} = \rho \cdot c_p \cdot \Delta T \quad (1)$$

where ρ is the enamel or the dentine mass density, c_p is the specific heat and ΔT is the temperature variation. A curve of temperature distribution can be easily obtained from the equation (1) above. In this work, we developed the Monte Carlo code based on MathCAD® language (*MathSoft Engineering & Education, Inc., USA*).

Results and Discussions

Figure 1 illustrates comparatively the lateral maps of (a) theoretical and (b) experimental scattering intensities. The theoretical map was calculated from the Monte-Carlo model for a laser beam with 0.1 mm circular spot size, whose center is 1.0 mm far from the cross-section visualized. The experimental map was recorded by a CCD camera, for a human third molar irradiated by the green emission (510 nm) of a Cu-HyBrID laser with 106 μm spot size, tangentially to the cross-section analyzed [6]. Both maps had the intensities normalized to the highest value of the pixel intensity. Except for discrepancies due to differences in beam diameter, it can be seen that the general behavior is quite similar: both seem to have isotropic attenuation.

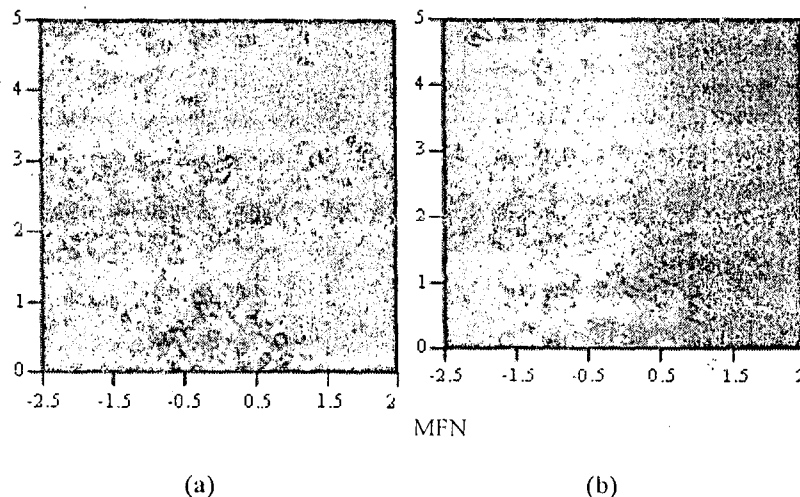


Figure 1: (a) theoretical intensity distribution map calculated for a laser beam with 0.1 mm circular spot size whose center is 1.0 mm far from the sample boundary and (b) experimental intensity distribution map for a human third molar irradiated with Cu-HyBrID laser.

In order to make a quantitative comparison of the light attenuation in the figures above, the curve of pixel intensity in a line passing the center of each map was drawn in Figure 2. Both theoretical and experimental curves showed good agreement.

The simulated thermal distribution in space for a single laser pulse is shown in Figure 3. The dimensions are set in millimeters and the color map represents the temperature amplitude in logarithmic scale. The scattering and absorption coefficients are the same as mentioned above except for $\mu_a = 0.1 \text{ cm}^{-1}$ for enamel. The tooth model considers a 1-mm-thick enamel layer on the top of a 5-mm-thick dentin layer. Figure 3 (b) shows the temperature profile along the laser central line. As it was expected, due to the low absorption coefficient of enamel, the temperature is higher on enamel-dentin junction.

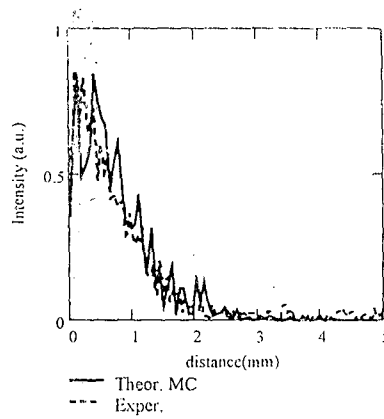


Figure 2: theoretical and experimental intensity attenuations in a line passing the center of the maps shown in Figure 1 above.

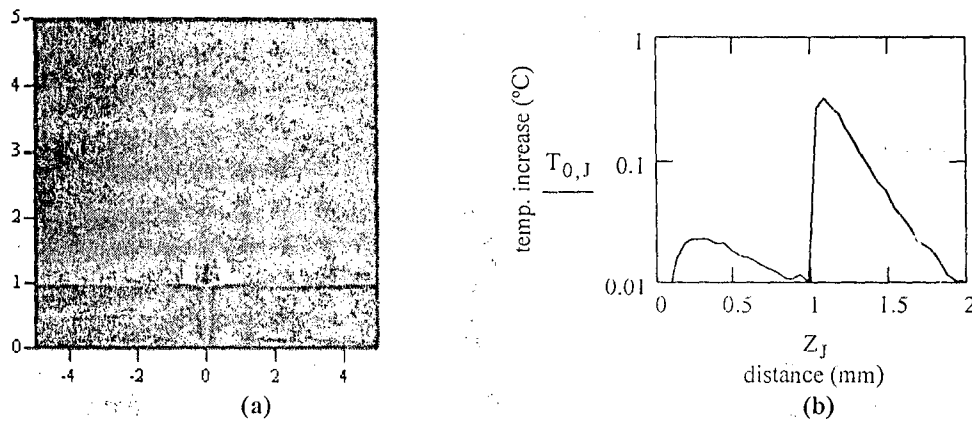


Figure 3: (a) Topographic map of the temperature (in logarithmic scale) with $\mu_a = 0.1 \text{ cm}^{-1}$ for enamel where the horizontal axis corresponds to the radial coordinate in mm and the vertical axis, to the distance in mm from the top of the tooth and; (b) Temperature profile along the central line.

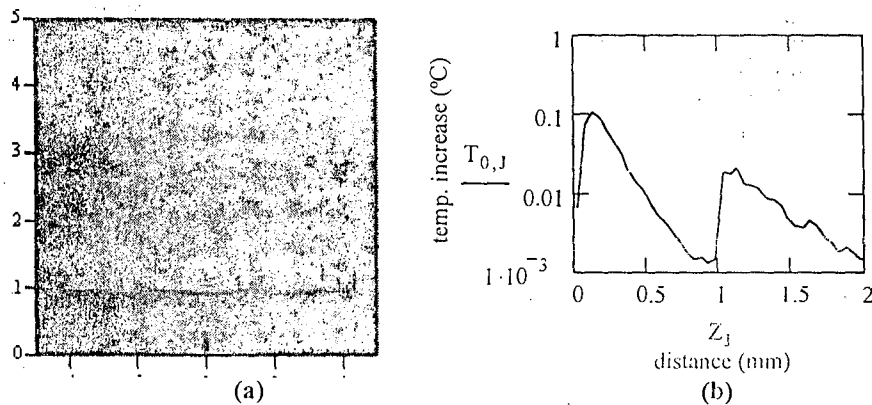


Figure 4: (a) Topographic map of the temperature (in log scale) with $\mu_a = 1 \text{ cm}^{-1}$ for enamel where the horizontal axis corresponds to the radial coordinate in mm and the vertical axis, to the distance in mm from the top of the tooth and; (b) Temperature profile along the central line.

Figure 4 (a) and (b) are simulated thermal distributions obtained using a higher value for the enamel absorption coefficient ($\mu_a = 1 \text{ cm}^{-1}$). Observe that, in this case, the temperature is higher near the tooth surface.

The above results indicate a strong variation of the temperature profile as a function of the absorption coefficient of the enamel. In their study, Fried et al. [3] presented some experimental results with a Nd-YAG laser indicating that there is a higher temperature on enamel-dentin junction and this fact could corroborate the smaller absorption coefficient for enamel. However, it was recently observed in ablation experiments on the tooth

surface by applying several pulses of the Cu-HyBrID laser that there was no apparent changes on dentin, which could indicate that absorption coefficient on enamel should be higher than those estimated in [3], at least for this laser wavelength. We are in process of calculating the temperature distribution after applying several laser pulses on tooth surface in order to explain the our experimental results of tooth laser ablation using the Cu-HyBrID laser. We expect thus determine a more actual value for the dental tissues absorption and scattering coefficients.

Conclusions

A numerical model based on the Monte-Carlo method was developed to simulate the Cu-HyBrID laser light propagation and correlated energy deposition on dental tissues. According to the model, the tooth thermal response is strongly affected by the value of the absorption coefficient, which is not yet precisely known.

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