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Modeling the penetration of laser radiation in enamel-dentin tissue

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A model for numerical calculation of laser radiation penetration in enamel-dental tissue has been developed. For these numerical computations a phase function suitable for the specific case is used and statistical methods for modeling the behavior of photons in the turbid media are implemented. By means of this model, we can get an idea of the proportion of radiation that passes and that is dissipated inside the tissue. Similar calculations are convenient to guide us in the use of certain techniques for laser impact on the dental tissues.

Keywords: Penetration laser radiation, enamel-dental tissue, Monte-Carlo simulation

INTRODUCTION

The penetration of laser radiation in dental tissues is a very important process related with the interaction of this radiation with tissues and respectively its impact on their structure and properties. Understanding the light propagation in teeth is important for therapeutic laser applications [1, 2] or diagnostics. For the treatment of hard tooth tissue, the parameters of laser radiation should be precisely controlled. The exposure of the pulp to laser radiation depends on the penetration of this radiation through the enamel and dentin. Upon irradiation with laser radiation a fraction of the energy is absorbed in the enamel and dentin, which in turn leads to increase in their temperature. The evaluation of this thermal effect is an important procedure.

In this article we consider a model of passing series of photons with the same parameters in enamel-dentin structure. The estimates based on this model are made of the portion of photons absorbed into the enamel and dentin respectively (in percentage).By varying the parameters such as wavelength, anisotropic factor and thickness of the layers enamel and dentin we can estimate the absorption in the respective layers in these set parameters.

MODELING

The enamel is the hardest substance of the human body [3]. It is made ofapproximately 95% (by weight) hydroxyapatite, 4% water, and 1% organic matter. Hydroxyapatite is a mineralized compound with the chemical formula $Ca_{10}(PO_4)6(OH)_2$. Its substructure consists of tiny crystallites which form so called enamel prisms with diameters ranging from 4 μm to 6μm. This forms the inorganic apatite-like tooth surface [4]. The crystallattice itself is intruded by several impurities, especially Cl^-, F^-, Na^+, $K^+$and Mg^{2+}. The crystals are approximately 15 to 40 nm in the diameter and can be as long as 20 μm. Prisms are surrounded by a protein/lipid/water matrix.

The dentin, on the other hand, is much softer. Dentin can be described as a conglomerate of several compartments. Only 70% of its volumeconsists of hydroxyapatite, whereas 20% is organic matter – mainly collagen fibers – and 10% is water. The internal structure of dentin is characterizedby small tubuli which measure up to a few millimeters in length, and between100nm and 3 μm in diameter. These tubuli are essential for the growth of the tooth. It contains long tubules surrounded by the peritubular dentin. Between the tubules with their peritubular dentin lays intertubular dentin.

Intertubular dentin, in its turn, is divided into collagen fibrils and interfibrillar compartments. Except for the tubules all compartments contain mineral crystals of hydroxyapatite, which are needle shaped with an ~ 5 nm thickness and an ~ 20 nm length. The tubules have the diameter of 1 to 5 μm, and its density is 15 000–75 000 tubules per mm^2 [4]. They are uniformly oriented from the

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enamel-dentin junction to the pulp, and so in a small sample they lay more or less parallel (Fig. 1).

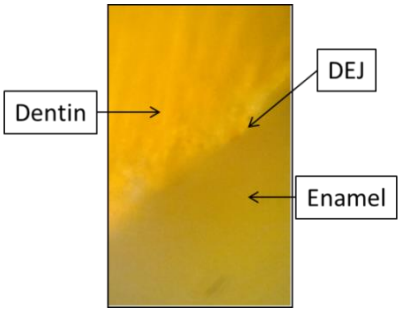


Fig. 1. Optical microscope picture of tooth structure - enamel, dentin and DEJ (dentin-enamel junction).

In stochastic models of photon transport through tissue, individual photon paths are simulated by considering the probability of absorption and scattering interactions. One of the most commonly used stochastic models is the Monte Carlo method.

The term Monte Carlo (MC) method (stochastic) refers to numerical simulations based on random sampling from appropriate probability distributions. Light is considered as a stream of particles (photons) that are injected into the medium, and move in straight lines through tissue between successive interactions. The advantages of the Monte Carlo method include simple implementation, the ability to handle any complex geometry and inhomogeneity, as well as the possibility to incorporate time-dependency. It is even possible to model wave phenomena such as polarization and interference. The main disadvantage is the inherently high computational cost.

Fig. 2 presents a simple model of enamel-dentin structure. There are denoted three layers of enamel, DEJ (dentin-enamel junction) [5, 6] and dentin through which passes the laser radiation.

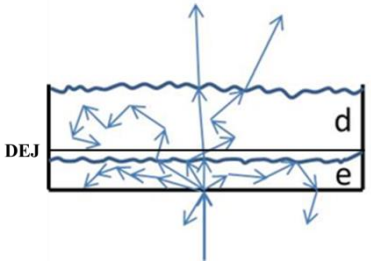


Fig. 2. Model of enamel-dentin structure representing the three successive layers – enamel, DEJ and dentin.

This radiation is represented as series of photons which sequentially enter perpendicularly to the surface of the enamel (the first layer) after which each of these photons undergoes reflection or multiple scattering in the structure with the result that the photon is reflected, absorbed or passes. We model these processes with Monte Carlo [7, 8, 9] simulation and Henyey-Greenstein (HG) phase function [10], since this phase function is a good approximation of the light scattering in the turbid tissue.In our model, we consider the penetration of the laser radiation with a wavelength of 1,064μm in dental tissue. This laser radiation is directed along the normal to the surface of the tooth sample, and has the shape of a Gaussian pulse. For the intensity of this impulse we can write:

$$I = I_{max}.e^{-2\frac{r^2}{\omega^2}} \quad (1)$$

where $r = \sqrt{x^2 + y^2}$, and ω is the width of the laser beam. In our case we have chosen r=0.1 mm and ω=1 mm.

The first assumption in our model is that for each particular step the number of photons in the pulse is proportional to the intensity. Thus at some initial value for the number of photons, the intensity value is close to the maximum and we can get values for the number of photons at other levels of intensity, using approximation for a given distribution. So with every step we take certain volume of the spatial distribution of energy in the pulse, which corresponds to the number of photons, entering through the surface of the tissue. It is clear that in this case, at each step the area through which the photons enter increases. In the model, this is done using Monte-Carlo simulation for each step.

Next assumption in our model is that the anisotropy factor ***g*** of DEJ is not a constant, but is a function of the coordinate ***z***, i.e. it is a function of the depth of penetration of laser radiation. In this way we consider it appropriate to introduce a function in the form:

$$g(z) = (Ag_1 + Bg_2 \frac{1}{e^{\beta(z-z_0)}}) \quad (2)$$

where g_1 and g_2 are anisotropic factors for enamel and dentin respectively and ***g(z)*** is the anisotropy factor in junction. Coefficients A and B show which anisotropy dominates from the respective border. Here ***z*** denotes the current coordinate and z_0 corresponds to the coordinate at DEJ depth. Coefficient β indicates how deep the change of anisotropy in DEJ is.

If we assume also that the A=B=1/2 and coefficient β≈1 (in order to ensure almost complete anisotropy of DEJ in close proximity to the dentin), we can write:

$$g(z) = \frac{1}{2}\left(g_1 + \frac{g_2}{e^{(z-z_0)}}\right) \quad (3)$$

Also the coefficients of the scattering are a function of the wavelength [11]. These functions are introduced by their polynomial approximations. The parameters which are required to trace a

photon path through some arbitrary random medium are the local absorption coefficient μ_a, scattering coefficient μ_s, and scattering phase function. Scattering in tissue is characterized by the Henyey-Greenstein phase function:

$$p(\theta) = \frac{1}{4\pi}\frac{1-g_{1,2}^2}{(1+g_{1,2}^2-2g\cos\theta)^{3/2}} \quad (4)$$

where $\boldsymbol{g}$ is the mean cosine of the scattering anisotropy angle $\boldsymbol{\theta}$. This coefficient $\boldsymbol{g}$ is called factor of anisotropy and is expressed as follows:

$$g = \int_0^\pi p(\theta)\cos\theta\, 2\pi\sin\theta d\theta \quad (5)$$

The assumption of random distribution of scatters in a medium, leads to normalization

$$\int_0^\pi p(\theta)\, 2\pi\sin\theta d\theta = 1 \quad (6)$$

Photons are emitted by a source and travel in straight lines until theyare scattered. The probability for a photon to be scattered after a distance $d\tau$ is defined by

$$p(\tau)d\tau = e^{-\mu_s\tau}d\tau \quad (7)$$

Hence the cumulative probability of being scattered after travelling a distance τ is

$$\int_0^\tau e^{-\mu_s\tau'}d\tau' = 1 - e^{-\mu_s\tau} = \rho_1 \quad (8)$$

where $\rho_1 \in [0...1]$ is a random number. Thus the distance between scattering events is given by

$$\tau = -\frac{1}{\mu_s}ln(\rho_1) \quad (9)$$

The azimuthally and polar scattering angles, θ and ψ, relative to the previous direction of motion are given by

$$\psi = 2\pi\rho_2 \quad (10)$$

$$\int_0^\theta p(\theta')\, d\theta' = \rho_3 \quad (11)$$

where ρ_2 and $\rho_3 \in [0...1]$ are uniformly distributed random numbers.

Absorption can be taken into account either by terminating an absorbed photon's path or by introducing a weighting scheme. Thereby the photon's weight $W \in [0...1]$ is reducedbetween successive scattering events according to

$$W = W'e^{-\mu_a\tau}, \quad (12)$$

where W is the weight before the interaction, and τ is the distance travelled since the lastscattering event. Photon paths are terminated when either the weight becomes negligible (by a predetermined value) the photon leaves the boundary or region of interest, or hits the detector. In the latter event the detection count rate is increased by the remaining photon weight W.

The possibility of internal reflection occurs when the photon is propagated across the boundary into the region with a different index of refraction. The probability that the photon will be internally reflected is determined by the Fresnel reflection coefficient $R(\theta_i)$

$$R(\theta_i) = \frac{1}{2}\left[\frac{sin^2(\theta_i-\theta_t)}{sin^2(\theta_i+\theta_t)} + \frac{tan^2(\theta_i-\theta_t)}{tan^2(\theta_i+\theta_t)}\right] \quad (13)$$

Where $\boldsymbol{\theta_i = cos^{-1}\,\mu_z}$ is the angle of incidence on the boundary and the angle of transmission $\boldsymbol{\theta_t}$ is given by Snell's law

$$n_i\sin\theta_i = n_t\sin\theta_t \quad (14)$$

where $\boldsymbol{n_i}$ and $\boldsymbol{n_t}$ are the indices of refraction of the medium from which the photon incident and transmits, respectively. The random number ρ_2 uniformly distributed between zero and unit is used to decide whether the photon is reflected or transmitted. If $\rho_2 < R(\theta_i)$ the photon is internally reflected, otherwise the photon exits the tissue and the event is recorded as backscattered light or transmitted light (when it exits the bottom). If the photon is internally reflected, then the position and direction of the photon is adjusted accordingly. For a slab geometry, infinite in the x and y directions with a thickness τ in the z-direction, the internally reflected photon position (x'',y'', z'') is obtained by changing only the z-component of the photon coordinates

$$\begin{aligned}&(x'', y'', z'') = (x, y, -z) \text{ if } z < 0\\ &(x'', y'', z'') = (x, y, 2\tau - z) \text{ if } z < \tau\end{aligned} \quad (15)$$

The new photon direction (μ_x',μ_y', μ_z') is

$$(\mu_x', \mu_y', \mu_z') = (\mu_x', \mu_y', -\mu_z') \quad (16)$$

and both μ_x and μ_y remain unchanged.

A normalized phase function describes the probability for density function for the azimuth and longitudinal angles for a photon when it is scattered. If the phase function has no azimuth dependence, then the azimuth angle $\psi$is uniformly distributed between 0 and 2π, and may be generated by multiplying a pseudo-random number ρ_2 uniformly distributed over the interval zero to one by 2π ($\psi = 2\pi\rho_2$). The deflection angle θ for an isotropic distribution is given by

$$\cos\theta = 2\rho_2 - 1 \quad (17)$$

If a photon is scattered at an angle (θ, ψ) from the direction (μ_x, μ_y, μ_z) in which it is travelling, then the new direction (μ_x',μ_y', μ_z') is specified by

$$\mu_x' = \frac{\sin\theta}{\sqrt{1-\mu_z^2}}(\mu_x\mu_z\cos\psi - \mu_y\sin\psi) + \mu_x\cos\theta \quad (18)$$

$$\mu_y' = \frac{\sin\theta}{\sqrt{1-\mu_z^2}}(\mu_y\mu_z\cos\psi + \mu_x\sin\psi) + \mu_y\cos\theta \quad (19)$$

$$\mu_z' = -\sin\theta\cos\psi\sqrt{1-\mu_z^2} + \mu_z\cos\theta. \quad (20)$$

RESULTS AND DISCUSSIONS

We performed numerical method Monte Carlo using a computer program designed for the specific case. Into the computer program we used the following coefficients, as shown in Table 1 [4,5]. The results of numerical calculation are presented in Table 2.

Table 1. Specific coefficients of enamel and dentin tissues

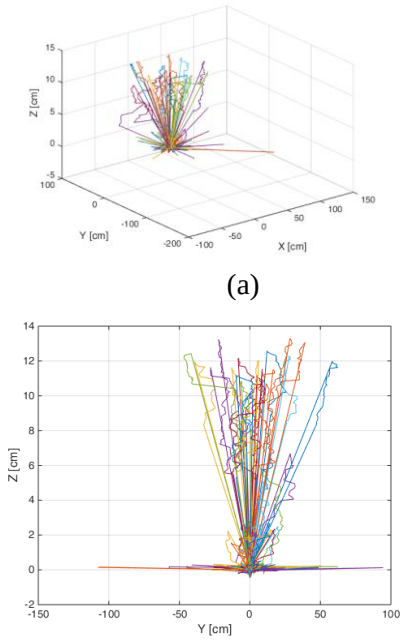
Coefficients	Enamel	Dentin
μ_a	<1,cm^{-1}	4, cm^{-1}
$\mu_s(\lambda)$	18, cm^{-1}	205, cm^{-1}
$g_{1,2}$	0,93	0,96
Thickness	1, mm	3, mm
$n_{e,d}$	1,63	1,54
Weight	10^{-4}	
λ	1064nm	

In Table 2 are presented coefficients for absorption in enamel (Abs1) and dentin (Abs2) respectively as well as reflectance (Ref) and transition (Tr) coefficients for this biological structure. These results were obtained by computer simulation program created by us in Matlab software package by implementation thirty numbers of calculations with a total number of 10^6 photons.

Table 2. Results of numerical calculation

Abs1	Abs 2	Ref	Tr
23%	66%	24%	0,34%

Computer calculations are shown graphically in Figs 3 - 4 for one case of photons penetrating in tooth tissue.



(a)

(b)

Fig. 3. (a) 3D view and (b) 2D (Y, Z axis) view of path of the penetrating photons.

Our calculations show that the assumptions made in the model are selected appropriately and the obtained results come close to the experimental results [12, 13]. For the transition of radiation through the dentine at [12] we have obtained experimentally 4% with a wavelength of 1064 nm, laser beam diameter 1 mm and incident energy of 10mJ. The thickness of the test slice is 1 mm. For this case we have a thickness of 3 mm, i.e. if is valid the Beer-Bouguer-Lambert law then we must have approximately 20 times greater attenuation of radiation. This means that in this case the photons will have a transition to the amount of 0.2 %. Computer calculations show value of 0.34 %.

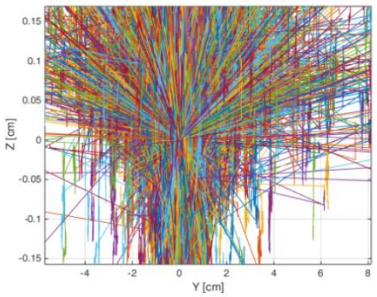


Fig. 4. Enlarged view of the photons path (Y, Zaxis).

CONCLUSIONS

Use and development of numerical methods, in particular methods based on Monte Carlo simulations are an essential part of the whole scientific study of penetration of laser radiation in turbid tissues. Monte Carlo modeling has been used for applying the technique to light dosimetry in tissue by receiving quantitative estimates of absorbed and transited radiation through various components of the tissue, which is very complex and difficult experimental process.

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Моделиране на проникването на лазерно лъчение в емайл-дентинна тъкан

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(Резюме)

В настоящата работа е развит модел за числено пресмятане на проникването на лазерно лъчение в емайл-дентин биологична тъкан. За числеността пресмятане е използвана фазова функция, подходяща за дадения случай, както и статистически методи за моделиране на поведението на фотоните в мътна тъкан. От получените чрез този модел резултати можем да добием представа за преминалото лъчение и за лъчението, погълнато от тъканта. Подобни пресмятания ни помагат за подбора на определени техники за лазерно въздействие върху зъбна тъкан.