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Dental biothermophotonics: A quantitative photothermal analysis of early dental demineralization

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Abstract. Photothermal Radiometry (PTR) is applied as a safe, non-destructive, and highly sensitive tool for the detection of early enamel demineralization. Teeth were treated sequentially with artificial demineralization to simulate controlled mineral loss. PTR frequency scans were performed at the same surface spot before and after each treatment. After 4 days of demineralization, the signal changed significantly compared to sound enamel scans. A coupled diffuse-photon-density-wave and thermal-wave theoretical model was developed to describe the biothermophotonic phenomena in the turbid medium consisting of a demineralised layer, sound enamel, and dentin. As a result of the fittings, thermal and optical properties of the layers were obtained.

1 Introduction

Early dental enamel demineralization is very difficult to detect or monitor with either x-rays or visual examination. High-resolution techniques, such as Scanning Electron Microscopy (SEM) or Transverse Microradiography (TMR) are ex-situ and require destruction of the tooth. In this study, Photothermal Radiometry (PTR) is applied as a safe, non-destructive, and highly sensitive tool for the detection of early enamel demineralization.

In the experiments, teeth were treated sequentially with artificial demineralization gel (0.1M lactic acid, 0.1M NaOH to raise the pH to 4.5, and 6% w/v hydroxyethylcellulose) to simulate controlled mineral loss on the enamel surface. The experimental setup (Fig. 1) included a semiconductor laser (659 nm, 80mW) as a source of the PTR signal. During the experiments, frequency scans were performed at the treatment location. Here, the width of the laser beam was a key issue in order to achieve one-dimensionality of the thermal-wave field, so the adoption of one-dimensional theory for the analysis of the process would be justified. The preliminary tests showed that 3 mm was the minimal beam width assuring one-dimensional thermal-wave profile.

Modulated laser light generated infrared blackbody radiation from teeth upon absorption and nonradiative energy conversion. The infrared flux emitted by the treated region of the tooth surface was focused by two off-axis paraboloidal mirrors and monitored with a mercury-cadmium-telluride (MCT) infrared detector three times: before and after 2 and 4 days of treatment. Due to the change in the optical and thermal properties of the enamel in the etched region, the emitted flux changed after each treatment. The developed theoretical model was aimed at fitting the properties of the layers, as well as the thickness of the demineralized layer.

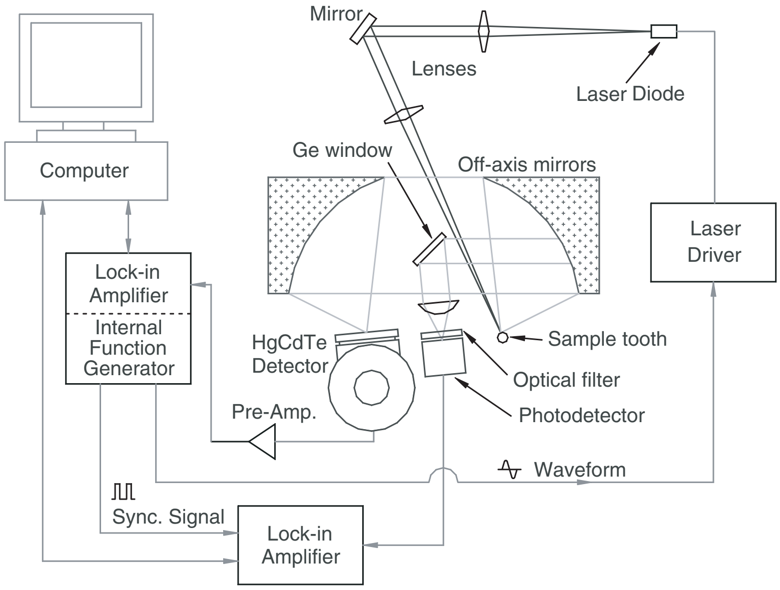


Fig. 1. Experimental setup.

2 Theoretical model

As a result of the incident laser radiation, the one-dimensional total photon field arises inside the turbid medium. It can be divided into two components [1], namely coherent and diffuse:

$$\Psi_{t_i}(z;\omega) = \Psi_{c_i}(z;\omega) + \Psi_{d_i}(z;\omega). \tag{1}$$

Here and further in the text, the subscript i denotes 1 – demineralized layer, 2 – intact enamel, 3 – dentin (Fig. 2).

Taking into account boundary conditions for the three-layer field, the resulting diffuse-photon-density solution depends on the absorption, μ_a, and scattering μ_s, coefficients of the layers, as well as the mean cosine of the scattering angle, laser intensity, and the medium reflectivity [2].

The total diffuse photon field Ψ_t is a source of thermal-wave field, T_i, given by:

$$\frac{d^2}{dz^2}T_i(z;\omega) - \sigma_i^2 T_i(z;\omega) = -\eta_{NR}\frac{\mu_{a_i}}{\kappa_i}\Psi_{t_i}(z;\omega) \tag{2}$$

where $\sigma = \sqrt{i\omega/\alpha_i}$ is the thermal-wave number, [m^{-1}], of i-th layer, η_{NR} is the nonradiative quantum yield, μ_a is the absorption coefficient of the medium, and κ is the thermal conductivity of the medium. The resulting theoretical PTR signal is a function of the effective mean infrared

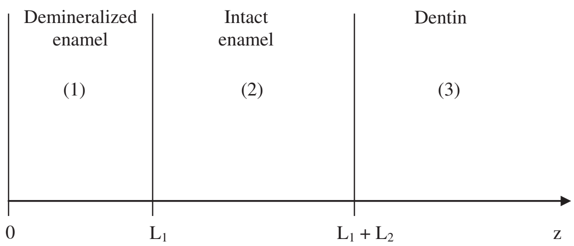


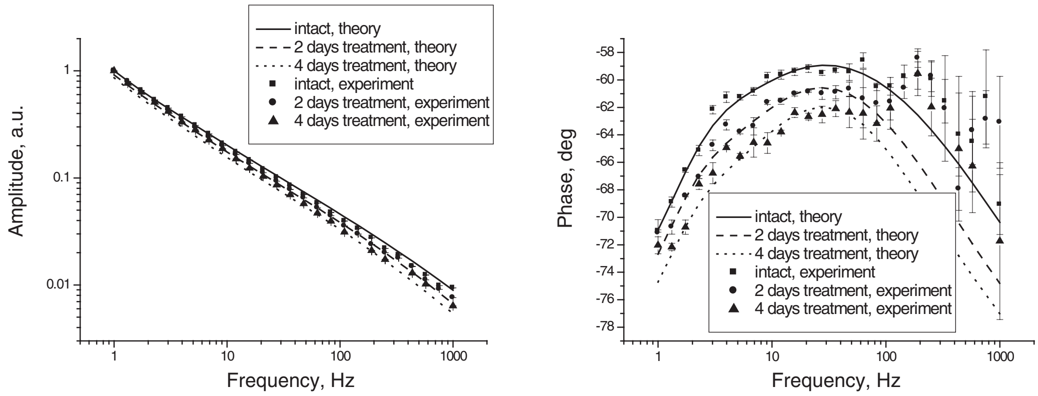
Fig. 2. Three-layer scheme of a tooth section.

absorption coefficient of the medium μ_{IR} and the thermal-wave field obtained as a solution of Eq. (2) [2]:

$$S = c\mu_{IR}\left[\int_{0}^{L_1} T_1(z;\omega)\exp(-\mu_{IR}z)dz + \int_{L_1}^{L_1+L_2} T_2(z;\omega)\exp(-\mu_{IR}z)dz \right.$$
$$\left. + \int_{L_1+L_2}^{\infty} T_3(z;\omega)\exp(-\mu_{IR}z)dz\right]. \quad (3)$$

3 Results and discussion

The results for the PTR frequency scans before and after 2 and 4 days of demineralization are shown in Fig. 3.



a) b)

Fig. 3. PTR frequency scans before and after 2 and 4 days of demineralization treatment. The fitting parameters are: $\mu_{a1} = 41$ m^{-1}, $\mu_{s1} = 40000$ m^{-1}, $\alpha_1 = 4.37 \times 10^{-7}$ m^2/s, $\kappa_1 = 0.91$ W/mK. The assumed parameters are: $\mu_{a2} = 100$ m^{-1}, $\mu_{a3} = 400$ m^{-1}, $\mu_{s2} = 8000$ m^{-1}, $\mu_{s3} = 36000$ m^{-1}, $\alpha_2 = 4.69 \times 10^{-7}$ m^2/s, $\alpha_3 = 2.6 \times 10^{-7}$ m^2/s, $\kappa_2 = 0.91$ W/mK, $\kappa_3 = 0.58$ W/mK.

The theoretical curves were obtained as the best fits of the developed theoretical model to the experimental PTR data. The Downhill Simplex Method in Multidimensions [3] was applied to optimize the multi-parameter fitting process. The low signal magnitude at the high-frequency range caused noisy behaviour, especially of the measured phase, so this region was eliminated from the fitting procedure. As a criterion for best fit we adopted the minimization of the least-squares error between the theory and experiment, averaged for a linear combination of the amplitude and phase. In conclusion, the PTR technique was shown to be a powerful tool for the detection and quantitative analysis of the early enamel demineralization.

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