

Dental Dynamic Diagnostics using Simultaneous Frequency-domain PTR and Laser Luminescence

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Frequency-domain infrared photothermal radiometry is introduced as a dynamic dental diagnostic tool complimentary to laser luminescence for quantifying sound and defective enamel or dentin. A high-spatial-resolution dynamic experimental imaging set-up, which can provide simultaneous measurements of laser-induced frequency-domain infrared photothermal radiometric and luminescence signals from defects in teeth, has been developed.¹ Following optical absorption of laser photons, the new set-up can monitor simultaneously and independently the non-radiative (optical-to-thermal) conversion via infrared photothermal radiometry; and the radiative de-excitation via luminescence emission. In addition, the optical properties of enamel are determined using a three-dimensional luminescence and photothermal model.

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In recent years rapidly increasing research activities have been reported centered on laser-induced luminescence as a probing technique for the detection and quantification of physical and chemical processes associated with carious dental enamel. In general, luminescence suffers from low signal levels and thus in most cases dyes are used to enhance sensitivity². Under laboratory conditions, the results appear satisfactory, yet the use of dyes makes the method difficult for clinical applications. In this work, frequency-domain infrared photothermal radiometry (FD-PTR) and modulated laser luminescence are introduced as complementary dynamic dental diagnostic tools for quantifying sound and defective (cracked) enamel or dentin. The significance to dentistry lies on the conclusions regarding the potential of this technique to monitor dental lesions at the early stages of carious decay where lateral and sub-surface spatial resolution on the order of the crack sizes and sub-surface depths investigated in this work (100-300 μm) may be required.

PTR has the ability to penetrate and yield information about an opaque medium well below the range of optical imaging. Owing to this ability, pulsed-laser PTR has been used with turbid media such as tissue^{3,4} to study the sub-surface deposition localization of laser radiation. The current experimental method is based on low-fluence photothermal radiometric detection microscopy⁵, which detects the emission of infrared radiation from a heated region of the sample without thermally altering it. Infrared radiometric and luminescence images of flat enamel surfaces from teeth with sub-surface lesions (cracks) were obtained at a fixed laser-intensity modulation frequency. Furthermore, a dentin-enamel interface was examined for quantitative comparison with enamel-generated signals. Simultaneous radiometric and luminescence frequency scans for the purpose of depth profiling were performed. A theoretical model was then fitted to the enamel samples to obtain the optical properties of enamel.

Experimental Method

The experimental setup for performing simultaneous FD-PTR and luminescence studies is shown in figure 1. A 488-nm wavelength cw Innova 100 Ar⁺ laser from Coherent is modulated by an external acousto-optic modulator (AOM) at frequency $f = \omega / 2\pi$, where ω is the angular modulation frequency. The laser beam is then focused with a high performance lens onto a sample to a radial ($1/e$) spot size of approximately 30 μm in reflection. The blackbody radiation from the optically excited sample is collected, collimated, and focused to a fine spot size by two axially aligned reflecting objectives onto a liquid-nitrogen-cooled HgCdTe (Mercury-Cadmium-Telluride) detector. The HgCdTe detector has an active square size area of 50 $\mu\text{m} \times 50 \mu\text{m}$ and a spectral bandwidth of 2-12 μm . An anti-reflection coated germanium window with a transmission bandwidth of 2-14 μm is mounted in front of the detector to block any visible radiation from the pump laser. Before being sent to the digital lock-in amplifier, the photothermal radiometric signal is amplified by a pre-amplifier with a frequency bandwidth dc-1MHz. Since both the modulated heating source and the detector are localized, they can be scanned across the sample. To perform PTR imaging the sample is moved in a raster fashion. This process of data acquisition, storage, and scanning is automated. For the simultaneous measurement of luminescence and PTR signal a germanium window was placed between the path of the two reflective objectives. The germanium window was utilized so that wavelengths up to 900nm would be reflected and the infrared radiation would be transmitted to the second reflecting objective focused onto the infrared-detector. The reflected spectrum was focused onto a photodetector of spectral bandwidth 300 nm-1.1 μm . A cut-off colored glass filter was placed in front of the photodetector to suppress scattered laser light and the spectrally integrated enamel luminescence

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following excitation by the 488-nm laser light⁶ was monitored. In order to test if any experimental components showed fluorescence a measurement with a mirror as a sample was performed. The result was negative (no signal).

Following optical absorption of laser photons, the experimental set-up can monitor simultaneously and independently the non-radiative (optical-to-thermal) conversion *via* infrared photothermal radiometry; and the radiative de-excitation *via* luminescence emission. With this experimental set-up two types of experiments can be performed. The first is imaging, where the sample coordinates are scanned at a constant frequency. The second experiment is dynamic, performed at one location on the sample. It generates depth-dependent information by scanning the laser-beam modulation frequency ("a frequency scan").

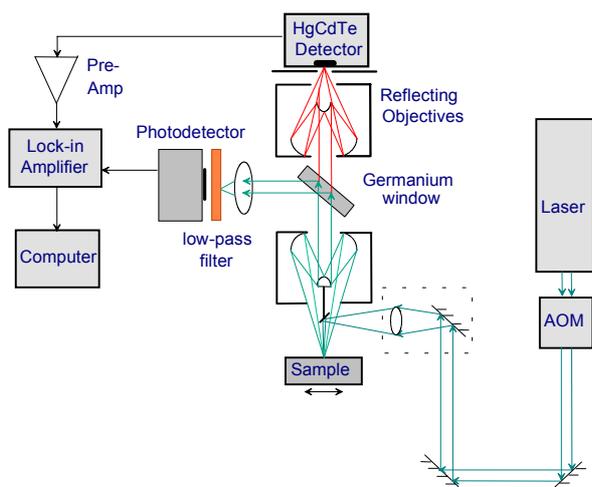


Fig. 1 Frequency-domain photothermal radiometric (FD-PTR) and luminescence imaging instrumentation.

Results and Discussion

PTR and luminescence imaging

Simultaneous PTR and luminescence images were obtained at different modulation frequencies and in the reported image, the signal ranges between high (black) and low (light gray). A flat enamel slice with a single 15 μ m wide transverse crack, 2mm thick and 6mm x 10mm in size is imaged at $f=20$ Hz. The aim is to show the intrinsic features of, and anti-correlation between, PTR and luminescence images. The results of a 0.5mm x 0.5mm image of the flat enamel slice with a near vertical sub-surface crack are shown in figure 2. The luminescence image (fig. 2a) seems to be sensitive to the presence of the crack; in the cracked region the luminescence signal is low (light gray) whereas in the (nearly) intact part of the enamel the luminescence is relatively high (gray). Within the crack region, luminescence photon emission of several wavelengths characteristic of the enamel chromophores is essentially absent due to the material structural destruction. As a result most of the incident energy decays nonradiatively, yielding a strong photothermal radiometric signal. Conversely, in the intact part of the enamel the luminescence is significantly enhanced, while the photothermal contribution is decreased. The two images together represent the expected balance of excited-state energy release between a radiative (luminescence) and a nonradiative (thermal-decay) dynamic process. The PTR image is the result of thermal-wave generation in the tooth and thus consists of two channels; amplitude and phase, Fig. 2 (b-d). In turbid media these channels carry thermal transport information within approximately one thermal centroid below

the surface. The thermal diffusion centroid is determined as the "center-of-mass" among thermal diffusion length, $\mu = \lambda_{th}/2\pi$, optical absorption depth and optical scattering mean-free-path in the bulk of the material. Photothermal amplitude is generally more sensitive to surface property variations, such as the reflectance, whereas phase is largely insensitive to the optical properties of the surface and probes a larger depth range⁷ into the material. In figure 2(b) the PTR amplitude exhibits two "spots" in the defective enamel. These two spots are also seen in phase, figure 2(c), confirming that the extend of these regions of the crack is deeper into the enamel. From optical observation of the tooth after the scan it is estimated that the penetration of the crack spots is 300 μ m.

The luminescence image, figure 2(a), however, shows the crack damage to be uniform throughout the extend of the crack. This is probably due to the influence of enhanced optical scattering at the crack leading to photon diffusion and "blurring" of the luminescence emission from dental enamel and points to the major difference between the two imaging principles: *PTR images depth profiles of sub-surface heat sources; luminescence does not, but is affected by image "blurring" due to photon scattering at the crack. It turns out it is also affected by photon emission delay processes which are characteristic of the material (enamel).* Figure 3 further points to the other major difference between the two techniques: *the superior dynamic range of the PTR amplitude.* For this reason, the image in figure 2(b) is sliced to allow the visualization of other features, the PTR intensity of, which is much lower than the peaks of the defect regions. The sliced image is seen in figure 2(d), whose features are now comparable to the PTR phase, figure 2(c). On the contrary, the luminescence amplitude is essentially continuous along the crack and shows neither the detailed morphology of the cracked region, nor any similarly great signal variations from the surrounding regions.

A major advantage of dental PTR imaging is the localization of features, largely due to the relative insensitivity of this technique to photon scattering. Scanning imaging at different frequencies manifests the dynamic character of modulated imaging (PTR and luminescence).

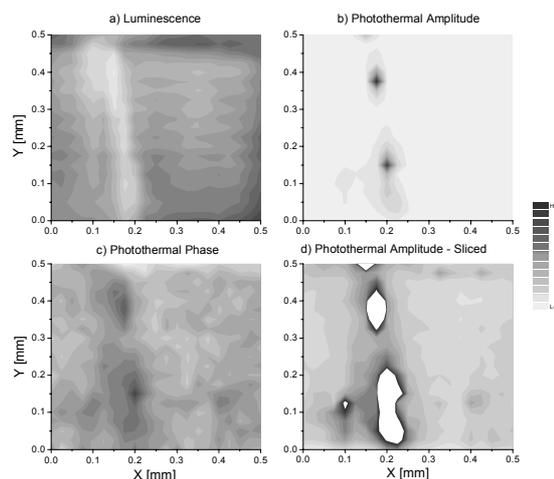


Fig. 2 Simultaneous luminescence and FD-PTR images at $f=20$ Hz. a) luminescence amplitude; b) PTR amplitude; c) PTR phase; and d) PTR amplitude with peaks sliced off.

Frequency scans

To study the dynamic nature (i.e. feature structures depend strongly on modulation frequency) of both luminescence and photothermal methods, frequency scans in the range 10 Hz-10

kHz were performed at different positions along a dentin-enamel interface of a cross-sectioned extracted molar as shown in figure 3. Position 1 is dentin, position 2 is enamel of 0.5mm thickness over the dentin, position 3 is enamel of thickness 1mm, position 4 is enamel of thickness 1.5mm and position 5 is enamel of 2mm thickness. Figure 4 shows the simultaneous photothermal and luminescence frequency scans for the five positions on the tooth. Dentin (pos. 1) exhibits low luminescence amplitude (figure 4a) as compared to the enamel signal (pos. 5). Positions 2 and 3 show similar characteristics (slope) at the high luminescence frequency but differ at the low frequencies. At the low frequency end the luminescence level (signal) of positions 2 and 3 is close to the dentin level (pos. 1). Positions 4 and 5 are at a higher luminescence region signifying a region where only the enamel is detected. The luminescence phase does not show any apparent differences between the positions at the low frequency end. At the high frequencies there are some small variations. The PTR signal contains more detailed information. Position 1 exhibits high signal in both amplitude (figure 4c) and phase (figure 4d). Position 2 is interesting because the sublayer of dentin underneath the enamel is seen as a minimum (interference) in the phase. This clearly shows the profilometric nature of PTR. Position 3, 4 and 5 behave similarly showing that a semi-infinite region has been reached for the enamel. Such a method (interpretation of frequency scans) can be useful for future application since the absence of enamel or deterioration of enamel can determine an early carious region.

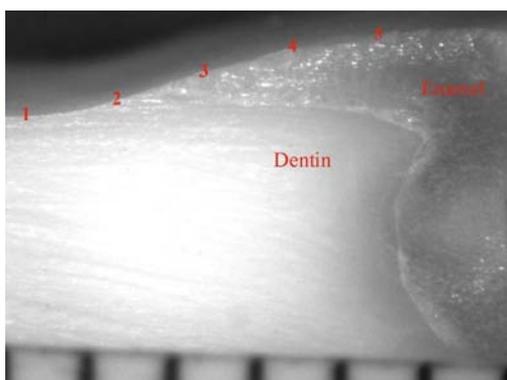


Fig. 3 Side view of dentin-enamel interface of an extracted molar.

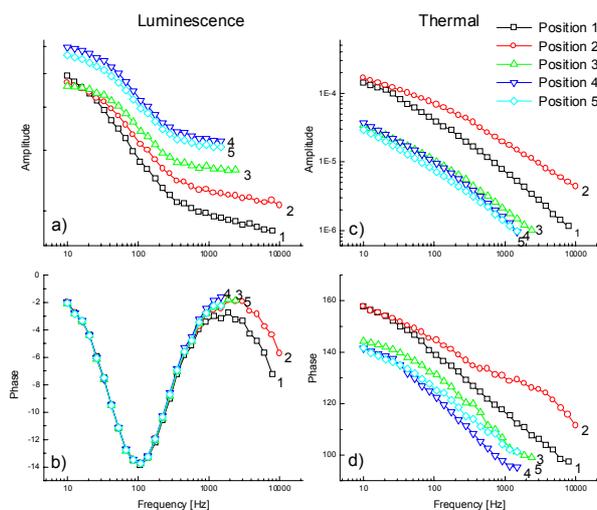


Fig. 4 Simultaneous luminescence and FD-PTR frequency responses at five positions as shown in figure 6. a) luminescence amplitude scan; b) luminescence phase scan; c) PTR amplitude scan; and d) PTR phase scan.

Theoretical Model and Fittings

The frequency scans can be further used for analysis of optical properties of both enamel and dentin. A quantitative theoretical two-lifetime rate model of dental luminescence was advanced and two characteristic lifetimes (τ_1 and τ_2) were measured.¹ The results were then used with a developed quantitative theoretical model⁸ for characterizing the radiometric frequency-domain response. The model was used to perform multiparameter fits for the luminescence and photothermal signals of enamel. The luminescence fitting parameters were the two characteristic lifetimes τ_1 and τ_2 and the PTR fitting parameters were the absorption β_{α} , infrared β_{IR} , and scattering β_S coefficients. To obtain a fit for the PTR signal, a fit for the luminescence signal was first investigated. The minimum in the luminescence phase data was sensitive to the two lifetimes and thus a fit for the phase was first obtained. The amplitude signal was then fitted by varying each parameter to provide a compromised fit for both signals. Trends obtained from the simulations provided a sense of direction in which the best fit would be found. The lifetimes were then used as constants in the PTR signal fittings.

The photothermal signals were fitted by varying the three optical coefficients, β_{α} , β_{IR} , and β_S . The enamel thermal parameters, thermal conductivity $k = 0.9$ W/mK and thermal diffusivity $\alpha = 4.2 \times 10^{-7}$ m²/s were taken from Ref. 9. Simulations of the theoretical model were performed by varying each parameter, while the remaining parameters were kept constant. Trends from these simulations provided information on the relation of the parameters and their tendencies to change the signal output. Increase in the absorption would increase the phase at the very low frequencies; increase in the β_{IR} would increase the signal at the high frequencies, while an increase in the scattering coefficient would decrease the signal in mid frequencies. A convection term, h , was considered in the theoretical model to account for the convection currents at the interface. Simulations were performed where the convection was varied while the remaining parameters were kept constant. This term was found (as expected) to provide a best fit when kept constant for all tooth samples. Finally, best fits for the amplitude and phase PTR signals were obtained by using a three-dimensional least residual analysis as outlined below.

The three optical coefficients, β_{α} , β_{IR} , and β_S were examined in terms of their uniqueness. The convection term h was constant for all positions and the lifetimes were determined from the luminescence signals. A three-dimensional contour was constructed by plotting β_{α} and β_S on the x- and y-axes as a function of the least residuals on the z-axis. The residuals are the sums over the frequency scans of the theoretical data minus the experimental data squared. Several level surfaces were plotted on the same set of axes for different values of β_{IR} . These plots showed that amongst the regions of minima, there was an absolute local minimum. The values obtained from this contour derived the best fit. A search for another neighbouring minimum region was performed by varying β_{α} and β_S on the x- and y-axes. This search showed that the obtained solution of fitting parameters is a unique set, as there were no other neighboring minima to be found.

To illustrate the fitting procedure a healthy enamel tooth was chosen. The fitting for both luminescence and photothermal signals are shown in figure 5. Figure 6 shows the three dimensional contour for three β_{ir} of 1900, 2200 and 2700 cm⁻¹. The absolute local minimum is obtained for $\beta_{ir}=2200$ cm⁻¹ and the optical property fitting parameters are shown in Table 1. A similar fitting procedure for the semi-infinite positions of the extracted tooth was also performed and the results are listed in Table 1. In general, the optical property values are within documented values found with other methods¹⁰⁻¹². It is worth

mentioning that there exist inconsistencies in literature values concerning the optical properties of enamel with a typical error for the scattering coefficient being ~30%, which is representative of the sample variability¹¹.

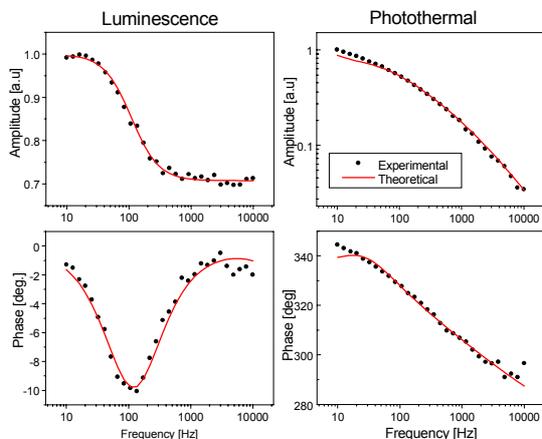


Fig. 5 Luminescence and PTR frequency response for healthy enamel.

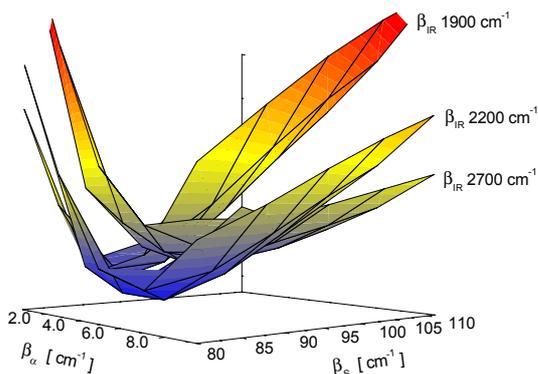


Fig. 6 Three dimensional contour for the optimal solution for healthy enamel.

In conclusion, frequency-domain infrared photothermal radiometry (FD-PTR) was introduced as a non-destructive, non-intrusive method for evaluating sound and defective tooth enamel, and was shown to be a complimentary imaging technique to luminescence. Several advantages of FD-PTR imaging were found including much superior dynamic range of the amplitude signal with regard to the defect state of dental enamel, superior feature localization and resolution, and depth profilometric capabilities. The optical properties of enamel were obtained with a three-dimensional photothermal formulation. Simultaneous radiometric and luminescence frequency scans

and images of case studies with teeth ranging between sound and carious are currently being examined, showing the diagnostic complementarity of the novel integrated frequency-domain instrumentation.

	Healthy Enamel sample	Extracted Molar sample		
		Pos. 3	Pos. 4	Pos. 5
L [mm]	2.0	1.0	1.5	2.0
τ_1 [ms]	1.6	2.00	2.04	2.00
τ_2 [μ s]	0.22	1.00	1.02	1.30
β_α [cm^{-1}]	2.6 \pm 0.5	14.0 \pm 0.5	6.0 \pm 0.5	14.6 \pm 0.5
β_{IR} [cm^{-1}]	2200 \pm 5	440 \pm 5	250 \pm 5	320 \pm 5
β_s [cm^{-1}]	92 \pm 1	75 \pm 1	120 \pm 1	77 \pm 1

Table 1: Values used in the fittings of the luminescence and PTR signals from different positions on the extracted molar.

Acknowledgments

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