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Pulsed photothermal profiling of water-based samples using a spectrally composite reconstruction approach

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Abstract. Pulsed photothermal profiling involves reconstruction of temperature depth profile induced in a layered sample by single-pulse laser exposure, based on transient change in mid-infrared (IR) emission from its surface. Earlier studies have indicated that in watery tissues, featuring a pronounced spectral variation of mid-IR absorption coefficient, analysis of broadband radiometric signals within the customary monochromatic approximation adversely affects profiling accuracy. We present here an experimental comparison of pulsed photothermal profiling in layered agar gel samples utilizing a spectrally composite kernel matrix vs. the customary approach. By utilizing a custom reconstruction code, the augmented approach reduces broadening of individual temperature peaks to 14% of the absorber depth, in contrast to 21% obtained with the customary approach.

1. Introduction
Pulsed photothermal radiometry (PPTR) allows reconstruction of temperature depth profiles induced in layered samples by single-pulse laser exposure. This approach, based on measurement of transient change in mid-infrared (IR) emission, can be applied to profiling of optically scattering biological tissues, provided that validity of one-dimensional approximation is ensured. One relevant example are port wine stain lesions in human skin, where most prominent absorbers (melanosomes in the epidermis and blood capillaries in papillary dermis) are so small and numerous that optical absorption within the interaction volume can be considered laterally uniform.

A major limitation of PPTR temperature profiling is pronounced broadening of distinct temperature peaks, due primarily to low signal-to-noise ratio (SNR) in radiometric signals, combined with ill-posed nature of the involved inverse problem. In early experimental studies involving water-based tissue phantoms the broadening amounted to prohibitive 50–60% of the absorber depth [1].

We hypothesize that a significant part of this artifact results from assuming a fixed IR absorption coefficient of the sample, as is done almost universally to reduce computational complexity in various photothermal radiometric applications. Application of such approximation is particularly controversial in watery biological tissues, which feature a large variation of absorption coefficient \( \mu(\lambda) \) in mid-IR spectral range. Moreover, selection of the effective absorption coefficient value \( \mu_{\text{eff}} \) under such conditions is critical, and determination of optimal \( \mu_{\text{eff}} \) turns out to be non-trivial [2].

Our recent studies showed that suitable narrowing of the spectral acquisition band can improve the accuracy of PPTR temperature profiling in water-based tissues [3,4]. However, the benefits of such approach are inevitably offset by the related reduction of SNR in radiometric signals.
As an alternative approach, numerical studies suggested application of a spectrally composite kernel matrix in the reconstruction process [3,5]. In the following, we present a direct experimental comparison of PPTR temperature profiling using such augmented vs. the customary (i.e., monochromatic) reconstruction approach, performed in dedicated agar gel tissue phantoms.

2. Theoretical background
The basics of PPTR temperature profiling can be found elsewhere [1,3,6]. In its most general form, the radiometric transient, $\Delta s(t)$, is related to temperature rise in the sample, $\Delta T(z,t)$, as [2,3,4]

$$\Delta s(t) = C \int_{\lambda_l}^{\lambda_h} R(\lambda) B'_\lambda(T_b) \mu(\lambda) \int_{z=0}^{\infty} \Delta T(z,t) e^{-\mu(\lambda)z} dz d\lambda$$

(1)

where $\lambda_l$ and $\lambda_h$ define the acquisition spectral band, $R(\lambda)$ marks detector spectral responsivity, and $B'_\lambda(T_b)$ denotes temperature derivative of Planck’s radiation formula at sample baseline temperature $T_b$. The constant $C$ accounts for several other experimental factors, such as sample emissivity, radiation detector size and field of view, losses of collection optics, etc.

By expressing $\Delta T(z,t)$ as a convolution of the laser-induced temperature profile $\Delta T(z,0)$ and Green’s function for one-dimensional heat diffusion equation, Equation (1) can be rewritten as

$$\Delta s(t) = C \int_{\lambda_l}^{\lambda_h} R(\lambda) B'_\lambda(T_b) \int_{z=0}^{\infty} \kappa_\lambda(z,t) \Delta T(z,0) dz d\lambda$$

(2)

The monochromatic kernel function $\kappa_\lambda(z,t)$ for a semi-infinite medium and convective/radiative heat transfer at the surface was derived by Milner et al [6]:

$$\kappa_\lambda(z,t) = \frac{\mu}{2} \exp\left(-\frac{z^2}{4Dt}\right) \left\{ \text{erfcx}(u_-) + \text{erfcx}(u_+) + \frac{2h}{\mu - h} \left[ \text{erfcx}(u_+) - \text{erfcx}(u_1) \right] \right\}$$

(3)

where $D$ and $h$ denote the sample thermal diffusivity and reduced heat transfer coefficient at its surface, respectively, and $\text{erfcx}(u) = \exp(u^2) \text{erfc}(u)$ is the exponential complementary error function with $u_\pm = \mu \sqrt{Dt} \pm z/\sqrt{4Dt}$ and $u_1 = h \sqrt{Dt} + z/\sqrt{4Dt}$.

Calibration of the system, performed by fitting radiometric signal values obtained from a black body with varying temperature to Planck’s radiation formula, eliminates the experimentally specific factors in Equation (2), thus enabling absolute measurements of temperature rise in the sample [4]. Calibrated PPTR signals assume a form

$$\Delta S(t) = \int_{z=0}^{\infty} K(z,t) \Delta T(z,0) dz$$

(4)

where the kernel function $K(z,t)$ equals $\kappa_\lambda(z,t)$ in the limit of monochromatic detection.

3. Materials and Methods
3.1. Agar gel tissue phantoms
Seven tissue phantoms evaluated below consist of 1-2 mm thick agar gel substrate layer, one optically absorbing layer, and a thin superficial agar gel layer.

Details of the agar gel layer preparation were presented elsewhere [7]. The absorbing layer consists of a very thin (~7 μm), colored polyethylene foil, which provides a repeatable and spatially uniform optical absorption. The thickness of the superficial agar layer varies between ~40 μm and 0.9 mm (samples A–G, respectively).
To prevent trapping of air bubbles, which might disturb heat transfer between adjacent layers, the samples were constructed in a water bath.

3.2. Experimental setup

Each PPTR measurement involves sample irradiation with a single 1 ms pulse from a Nd:YAG/KTP laser at 532 nm and radiant exposure of 0.35 J/cm$^2$. The IR radiation emitted from the center of irradiated area is collected by Si lens (Galvoptics, Essex, UK) condenser with magnification $M = 1$. The lenses are coated for high transmission in the acquisition spectral band of the InSb radiation detector (P5968-100, Hamamatsu; $\lambda = 3.0$–5.6 μm). The latter has a diameter of 1 mm, field of view of 45°, and peak spectral sensitivity $R_p = 2.5$ A/W at $\lambda_p = 5.3$ μm (Figure 1).

Radiometric signal transients following laser irradiation were acquired for 1.5 s at a rate of 50,000 s$^{-1}$. The PPTR signals $S$ were obtained by calibrating the raw data using a computer-controlled black body (BB701, Omega Engineering, Stamford, CT), subtracting the baseline value, and computationally reducing the sampling frequency to 1000 s$^{-1}$.

![Figure 1](image)

**Figure 1.** Absorption coefficient of agar gel in mid-IR (solid line), and spectral responsivity of the InSb radiation detector, $R(\lambda)$, relative to its peak value, $R_p$ (dashed).

3.3. Reconstruction of the initial temperature profiles

With the experimental PPTR signals represented as vectors $S$, Equation (3) converts to simple multiplication of the initial temperature profile $T$ with a kernel matrix $K$; $K_{ij} = K(z_i, t_j) \Delta z$. Nevertheless, reconstruction of $T$ from a given signal $S$ presents a severely ill-posed inverse problem [6], which is most commonly solved by iterative minimization of the residual norm $\|S - KT\|^2$. In our case, the laser-induced temperature profiles $T$, represented by 300 temperature values uniformly distributed over a depth interval of 1.5 mm, were reconstructed using a custom implementation of projected $\nu$-method with adaptive regularization [8].

The reconstructions were performed first within the customary monochromatic approximation. Elements of the kernel matrix $K = \kappa$ were calculated using the effective absorption coefficient value $\mu_{\text{eff}} = 27.4$ mm$^{-1}$. This value was determined by following a recently developed procedure [2], taking into account the IR spectral properties of the sample absorption and detector responsivity (Figure 1).

Subsequently, the same experimental signals were analyzed also using a spectrally composite kernel matrix $K$. The matrix elements were computed by dividing the acquisition spectral band ($\lambda = 3.0$–5.6 μm) into intervals of width 0.02 μm and adding their contributions [4]:

$$K_{i,j} = \sum_{n=1}^{N} R(\lambda_n) B_{\lambda_n} \cdot (T_b) \kappa_n(z_j, t_j; \mu_n) \Big/ \sum_{n=1}^{N} R(\lambda_n) B_{\lambda_n} \cdot (T_b)$$

(5)
Here, $\lambda_n$ is the central wavelength of the $n$-th spectral interval, $\mu_n$ is the corresponding agar gel absorption coefficient, and $R(\lambda_n)$ is spectral responsivity of the InSb detector (Figure 1). The thermal parameters of agar gel were estimated to $D = 0.143 \text{ mm}^2/\text{s}$ and $h = 0.02 \text{ mm}^{-1}$.

4. Results

The signal-to-noise ratio (SNR) in the acquired PPTR signals decreases nearly exponentially with absorbing layer depth, and amounts to $110-1350$. This corresponds to a noise-equivalent temperature rise of $\text{NE}\Delta T = 2.2 \text{ mK}$.

Figure 2 presents statistical analyses of the reconstruction results for all seven samples (A–G, see the labels). Solid lines connect the average temperatures and gray bars indicate standard deviations. The reconstructed laser-induced temperature is broadened progressively with increasing depth of absorption layer ($Z$), in agreement with earlier reports [1,2,4,9]. However, when applying the augmented, spectrally composite approach to the reconstruction process (Figure 2b), the broadening is markedly reduced in comparison with the customary monochromatic approximation (Figure 2a), in all tested samples.

**Figure 2.** Average temperature profiles (solid lines) and standard deviations (gray bars) obtained from 10 PPTR signals acquired from each agar tissue phantom (see labels A–G). The reconstruction process was performed using (a) the monochromatic approximation, and (b) spectrally composite approach.

In Figure 3, we present full widths at half maximum ($W$) of the reconstructed temperature profiles as a function of peak temperature depth ($Z$). For either reconstruction approach, the widths increase approximately linearly with $Z$ (dashed lines), except at depths below ~0.5 mm. For the shallower absorbers (samples A–D), the broadening effect is smaller or comparable to the actual width of the initial temperature profile. (Note that heat diffusion during the laser pulse must be taken into account.)
Figure 3. Full widths at half maximum of reconstructed temperature peaks ($W$) as a function of peak temperature depth ($Z$) when using the monochromatic approximation (open circles) and spectrally composite approach (solid) in the reconstruction process. Vertical bars mark standard deviations.

For the samples with deeper absorbers, conversely, the measured widths $W$ indicate directly the amount of broadening. By using the spectrally composite approach (solid circles), the broadening amounts to $\sim 0.14 \, Z$, a significant improvement over the monochromatic reconstruction results obtained from the same experimental signals ($\sim 0.21 \, Z$; open circles).

5. Discussion

With introduction of spectrally composite kernel matrix $K$, broadening of reconstructed temperature peaks in water-based layered tissue phantoms has reduced to $\sim 14\%$ of their depth. This is significantly below the value obtained from the same experimental signals by using the customary reconstruction approach and much less than in earlier experimental attempts [1,4,6,7]. Due to the earlier mentioned inherent limitations of the problem, however, this broadening is still rather large.

We believe that the discussed advantage applies also to PPTR profiling in human skin, where water is again the primary chromophore in mid-IR spectral region. However, the somewhat weaker mid-IR absorption in skin makes the reconstruction problem slightly more ill-posed, likely leading to larger broadening than demonstrated here in agar gel phantoms.

Additional incremental improvement of PPTR profiling accuracy and robustness may be achieved by introducing non-uniform signal binning and/or depth discretization [1,10].

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