GLOBAL RESEARCH IMMERSION PROGRAM FOR YOUNG SCIENTISTS

Modelling Temperature rise for Frequency-Domain Thermoreflectance

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Introduction

Frequency-Domain Thermoreflectance (FDTR) is a non-invasive technique used to determine the thermal properties of both bulk and thin film materials. It operates by measuring changes in the thermoreflectance of a material caused by the modulation frequency of a pump laser with a probe laser. This allows thermal properties such as thermal conductivity to be determined (Yang 2016).

Predicting the temperature rise in the sample due to both the pump and probe lasers is crucial due to the sensitivity of thermal properties with temperature changes. Accurate prediction provides insights into the experimental conditions during FDTR measurements and validates the temperature conditions of the results obtained.

The main source of heating in the FDTR setup (Fig 1) is the two CW lasers: the pump (488 nm) and the probe (532 nm). The pump laser, which is frequency modulated, primarily heats the sample. In contrast, the steady state probe laser is less intense and is used for data collection.

FDTR samples are often coated with a metal transducer layer, complicating the determination of the actual temperature rise in the underlying sample. Therefore, it is necessary to develop a model that accurately reflects the temperature rise in the actual sample beneath the transducer layer.

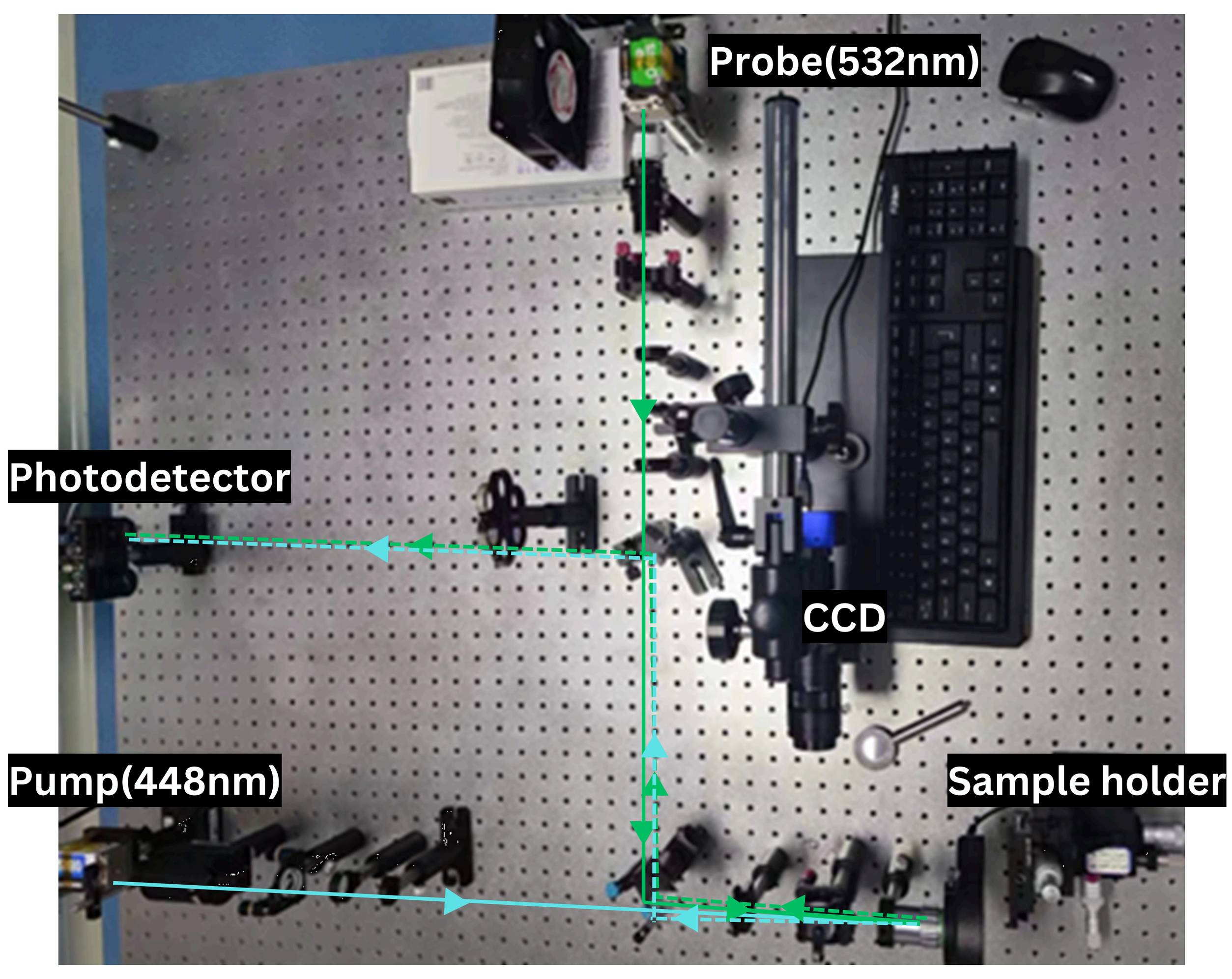

Figure 1. Experimental set up of the FDTR system in Thermal Transport and Energy Conversion Lab (USTC), with the pump laser (448 nm) and the probe laser (532 nm)

Temperature rise model

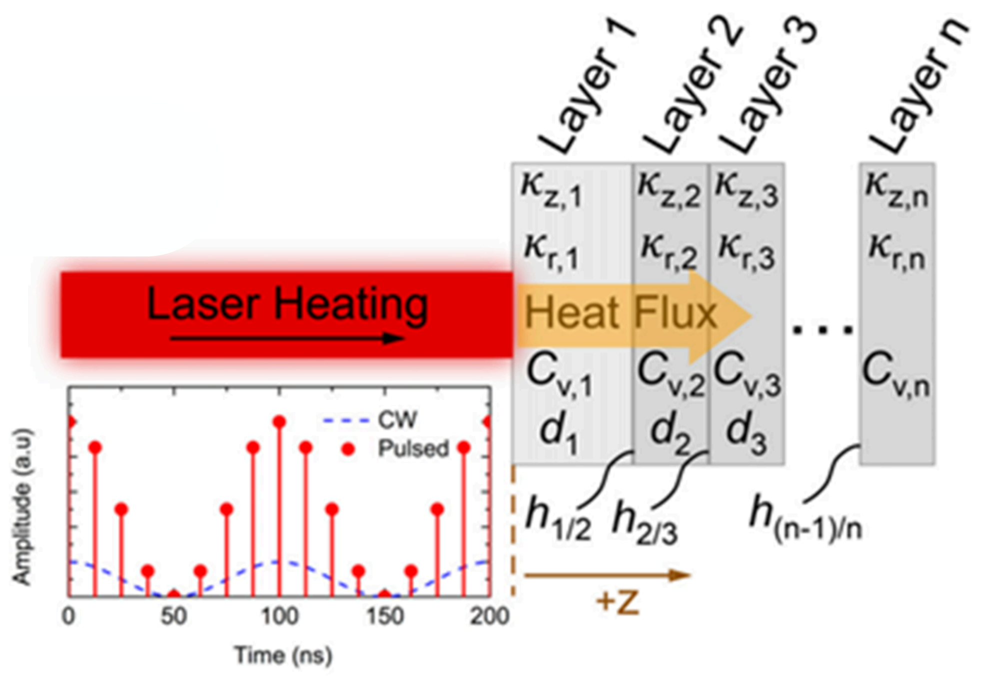

Figure 2. FDTR sample schematic under a multi-layer insulated boundary condition where n represents the number of layers (Braun and Hopkins 2017)

The temperature rise model for the FDTR stemed from the study conducted by Braun and Hopkins in 2017. The model was derived from the diffusive heat equation with radial symmetry:

$$\kappa_r \left\{ \frac{1}{r}\frac{\partial T(z,r,t)}{\partial r} + \frac{\partial^2 T(z,r,t)}{\partial r^2} \right\} + \kappa_z \frac{\partial^2 T(z,r,t)}{\partial z^2} = C_v \frac{\partial T(z,r,t)}{\partial t},$$

where κ_r, κ_z are the respective in-plane and perpendicular heat conductivities, **r** the inplane radius, **T(z, r, t)** the relative temperature with respect to specific time (**t**) and penetration depth (**z**), C_v the volumetic heat capacity (Braun and Hopkins 2017). Specifically, the model states that once the surface temperature (**Ttop**) and heat flux (**Qtop**) of the top layer are known, the temperature and flux of subsequent layers in the sample can be determined (schematic of FDTR sample and heat flux in Fig 2.). This is achieved through the equation below, after taking the Hankel and Fourier transform of both the surface temperature and heat flux.

$$\begin{bmatrix} \tilde{T}_n(z) \\ \tilde{Q}_n(z) \end{bmatrix} = \begin{bmatrix} \cosh(q_n z_n) & -\frac{1}{q_n \kappa_{z,n}} \sinh(q_n z_n) \\ -q_n \kappa_{z,n} \sinh(q_n z_n) & \cosh(q_n z_n) \end{bmatrix} \times \prod_{j=n-1,n-2,\ldots}^{j=1} \mathbf{M}_j \mathbf{N}_j \begin{bmatrix} \tilde{T}_{top} \\ \tilde{Q}_{top} \end{bmatrix} = \begin{bmatrix} \tilde{A} & \tilde{B} \\ \tilde{C} & \tilde{D} \end{bmatrix} \begin{bmatrix} \tilde{T}_{top} \\ \tilde{Q}_{top} \end{bmatrix} \quad (1)$$

In particular:

$$\tilde{Q}_{top} = \frac{1}{2\pi} \exp\left(-\frac{k^2 r_0^2}{8}\right) \tilde{G}(\omega),$$

where $\tilde{G}(\omega)$ was the fourier transform of:

$$G_{CW}(t) = \alpha A \left(e^{i\omega_0 t} + 1\right).$$

Taking the assumption that the sample is an 1D semi-dimensional sample, we have an expression for **Ttop** in the Fourier domain witj **Jo(kr)** the zeroth Bessel function:

$$\tilde{T}_{top}(r,\omega) = \int_0^\infty -\left(\frac{\tilde{D}}{\tilde{C}}\right) \tilde{Q}_{top} J_0(kr) k \, dk = -\frac{\tilde{G}(\omega)}{2\pi} \int_0^\infty \left(\frac{\tilde{D}}{\tilde{C}}\right) \exp\left(-\frac{k^2 r_0^2}{8}\right) J_0(kr) k \, dk = \tilde{L}(r,\omega) \tilde{G}(\omega),$$

Finally, taking the inverse Fourier transform, we obtain our expression for **Ttop** composed of a steady state component induced by the CW lasers, and an alternating component modulated through the modulation frequency **w0.**

$$T_{top,CW}(r,t) = \alpha A (\tilde{L}(r,\omega_0) e^{i\omega_0 t} + \tilde{L}(r,0))$$

MATLAB Model

The code provided by Braun et al on the single temperature rise approximation of laser induced heating has been edited to produce the average and maximum temperature rise for the FDTR system in the lab as a function of spot radius (Braun et al. 2018), as seen in Fig 3 and 4.

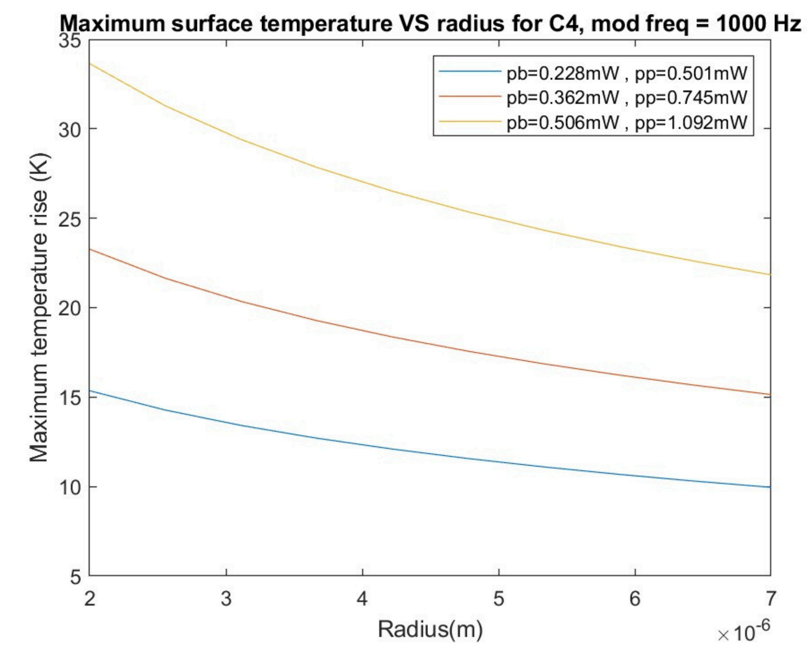

Figure 3. Maximum temperature rise of the lab FDTR system with a pump laser (488nm) (absorption rate = 0.63) and a probe laser (532nm) (absorption rate = 0.35) under different output power conditions with respect to spot size.

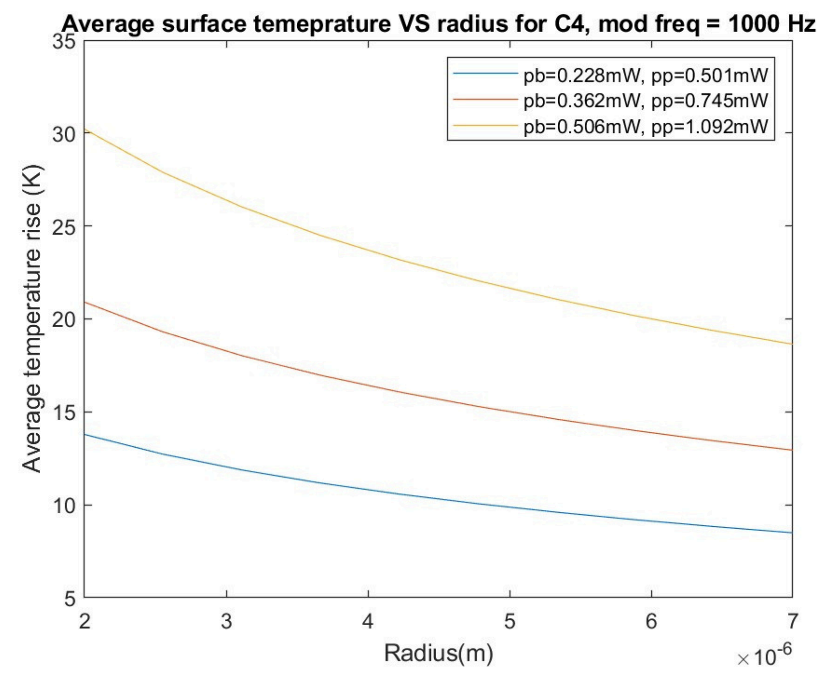

Figure 4. Averaged temperature rise of the lab FDTR system with a pump laser (488nm) (absorption rate = 0.63) and a probe laser (532nm) (absorption rate = 0.35) under different output power conditions with respect to spot size.

Discussion

The MATLAB code by Braun et al utilised a single temperature rise approximation. This was made as the typical alternating contribution was found to be two magitudes smaller than the steady state contribution in laser heating. Hence, under the assumption that the alternating thermal penetration depth induced by the modulation frequency was much less than the steady state component, the single temperature estimation can be made (Braun et al 2018)

Furthermore, the absorption rates of gold used in Fig. 3 and 4 were 0.64 and 0.35 for the pump and the probe respectively (Poopakdee 2021). These values were derived from literature and not experimentally tested on the inhouse FDTR. A more acurate temperature rise estimate should use the tested experimental absorption rates.

Reference

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