Finite Element Modeling of Beam Deflection in Photothermal Deflection Spectroscopy

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BACKGROUND: Photothermal Deflection Spectroscopy (PDS) measures the deflection of a laser beam (probe beam) due to a change in the index of refraction caused by the excitation of an adjacent thin film by a broadband light source (pump beam).

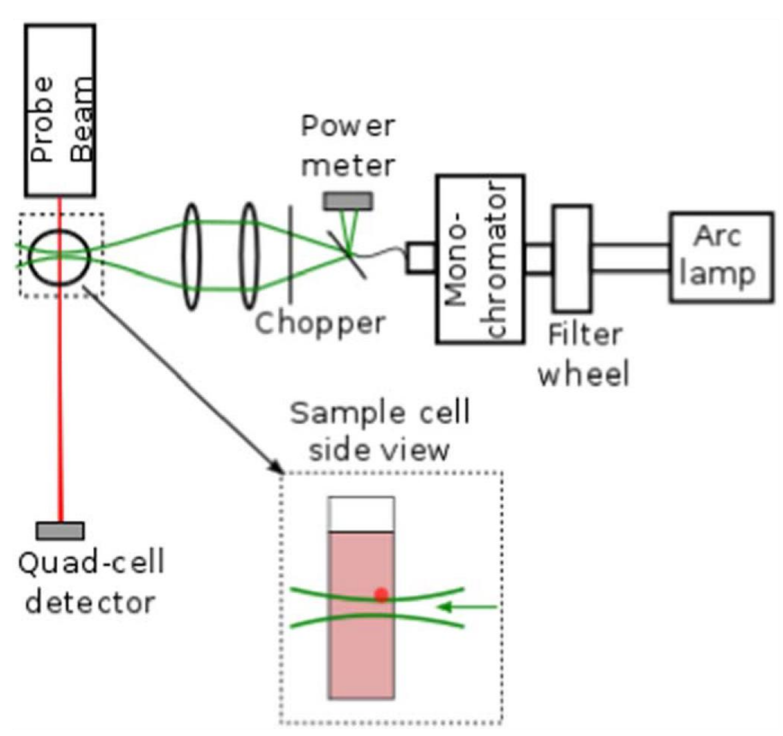
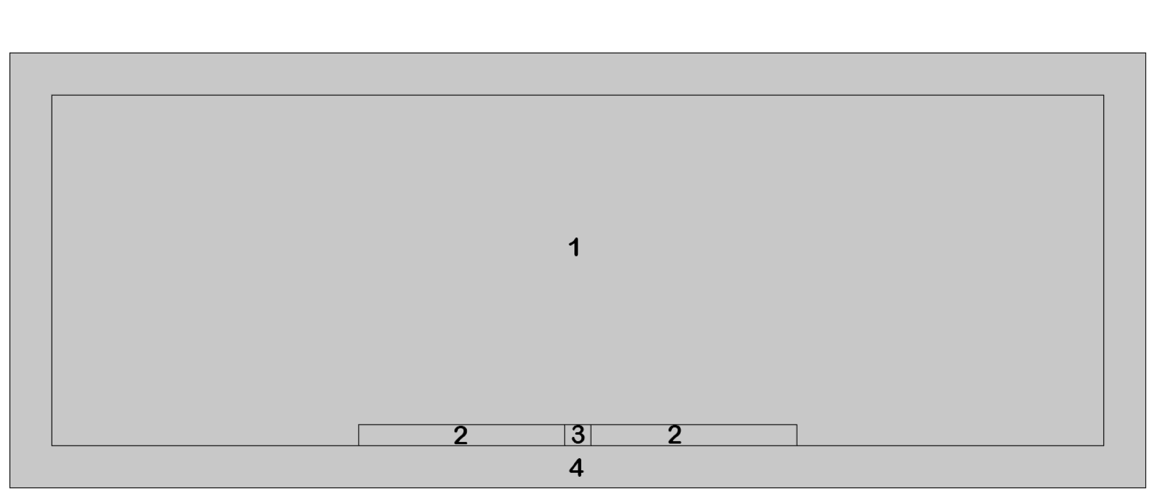


Figure 1. PDS Schematic[1]

COMPUTATIONAL METHODS: The pump beam was modeled using the Radiative Beam in Absorbing Media physics. This was then used as a heat source in the Heat Transfer in Solids and Fluids physics, which modeled the temperature dispersion throughout the cuvette. An analytic function was created to link the temperature of the FC-72 to the index of refraction. This was then used with the Geometrical Optics physics to model the deflection of the probe beam through the cuvette. The position of the rays were then exported into MATLAB using COMSOL LiveLink for MATLAB, and the signal was calculated. This ray tracing was repeated at multiple time steps using LiveLink for MATLAB and graphs were created (Fig. 4-5) for the signal generated as a function of time as well as the simulated signal generated by the lock-in amplifier as a function of time. The signal is created by taking the total intensity of the Gaussian probe beam on one side of the detector subtracted from the other, which is found in MATLAB using the equation Signal = $\mathrm{erf}\left(\frac{\mu}{\sigma\sqrt{2}}\right)$. These graphs will be used to compare with theory and link the model with experiments.



1: Fluorinert™ FC-72
2: Sample
3: Area on sample excited by pump beam
4: Cuvette Walls

Figure 2. Model Geometry

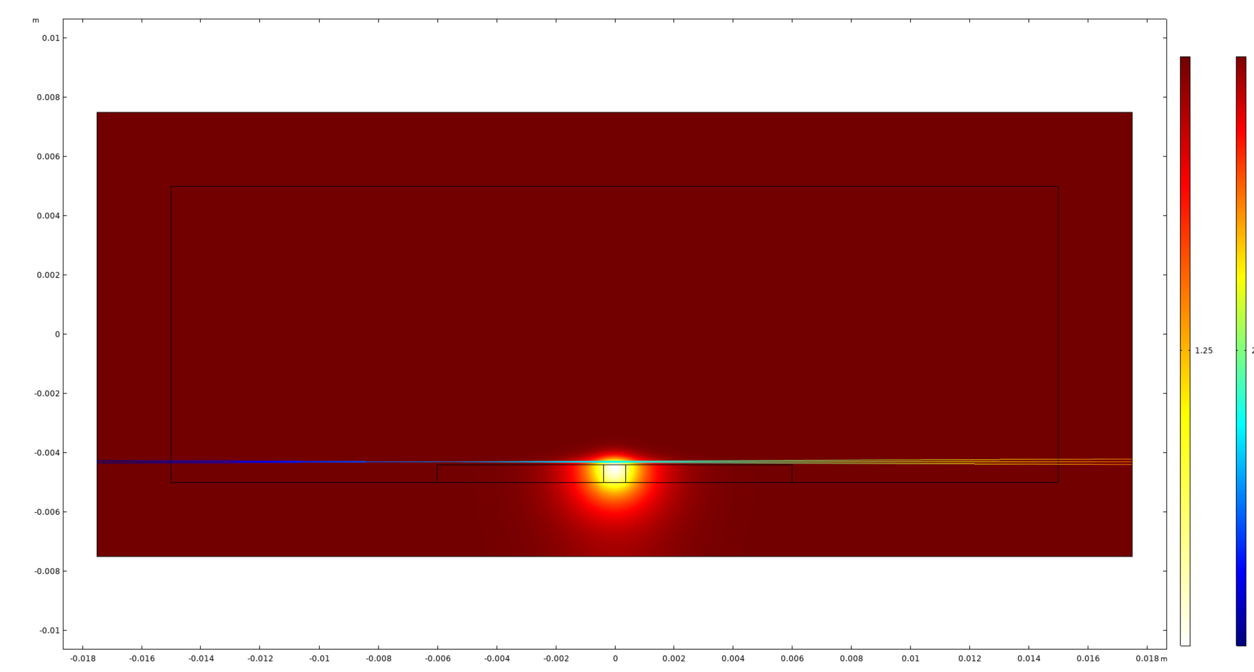


Figure 3. Ray trace through index of refraction gradient

RESULTS: Below are the graphs for signal vs time and simulated lock-in signal vs time. Figure 3 matches very well with theory, save for what are likely to be mesh and time stepping artifacts in the first second of the model. The lock-in signal, as expected, converges after ~1s. The signal dies off quickly as the probe beam is moved away from the sample, which also matches well with our experiments.

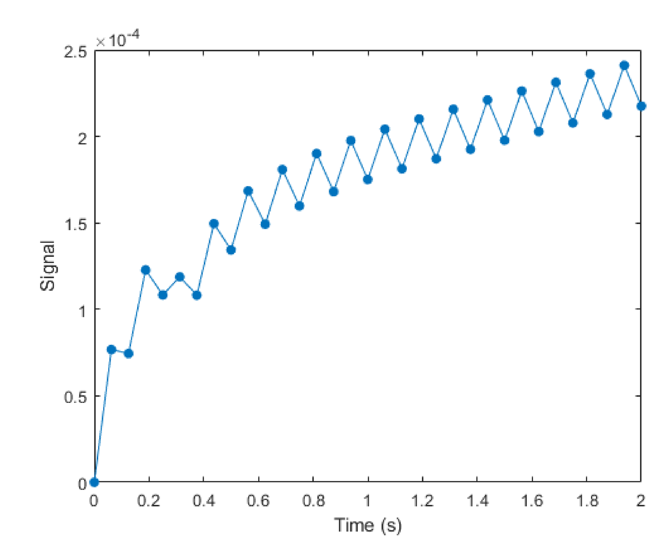


Figure 4. Detector signal vs time

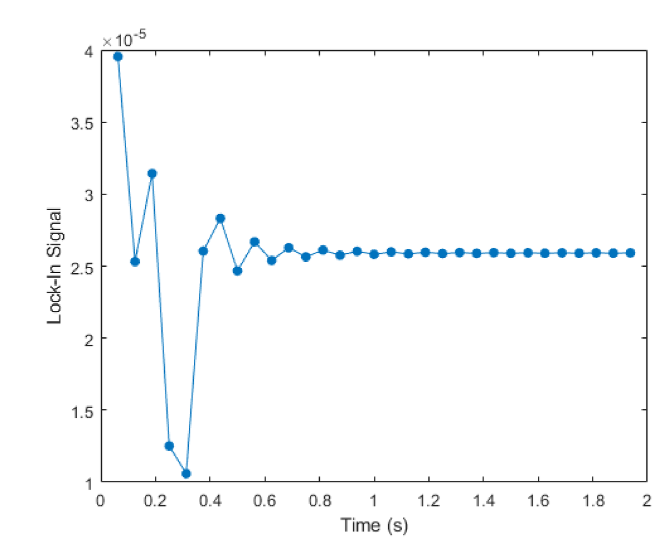


Figure 5. Simulated lock-in amplifier signal vs time

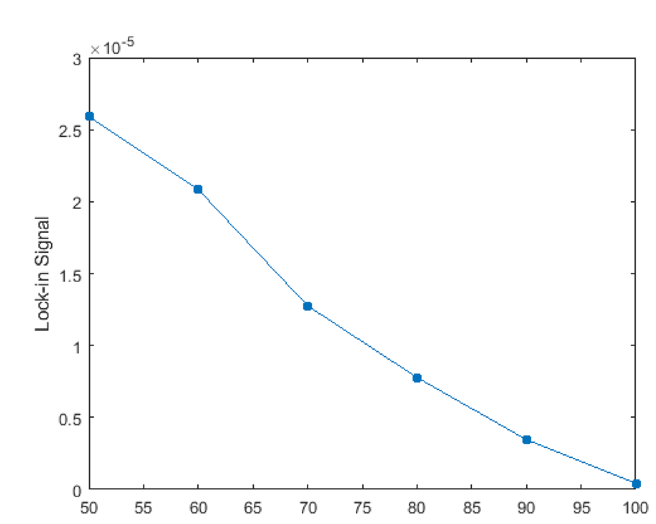


Figure 6. Simulated lock-in amplifier signal vs probe beam offset

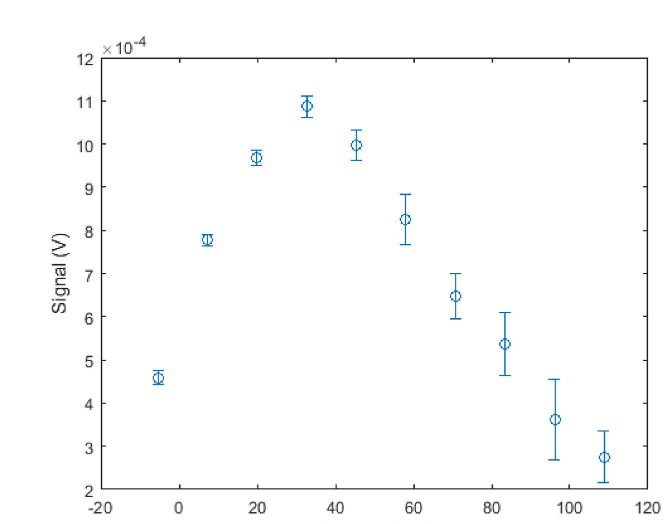


Figure 7. Experimental signal vs probe beam offset

CONCLUSIONS: The results are very encouraging but not quite complete. Ray traces were only done immediately before and after the pump beam hits the sample, which is not necessarily in phase with the temperature diffusion. Additionally, the model does not account for the drift of the probe beam during measurements. The results match very well with theory, although further work is needed to improve the model to link with experiments.

REFERENCES:

1. Johnson et. al, Absolute fluorescence quantum yield determined by photothermal deflection spectroscopy, Methods and Applications in Fluorescence, vol. 7 (2018)