Analytical method for estimating chemical composition of bio-samples under photothermal investigation

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Thermal Lens spectroscopy is a photo-thermal technique used for detection and quantification of analytes in liquid samples. The technique boosts from high detection sensitivity and relatively simple instrumentation. However, reproducibility of photo-thermal signals is a challenge and depends on the tightness of alignment of optical elements and use of similar experimental design and reference sample standards for calibration purposes. In this paper we report the development of a simple but universal analytical method that determines the ratio of changes of specific molar extinction coefficients $(\frac{\Delta\varepsilon_{\lambda 1}}{\Delta\varepsilon_{\lambda 2}})$ for a sample being probed with light of wavelength (λ_3) and alternately pumped up to optical saturation using optical beams of wavelengths (λ_1, λ_2). The model takes as its inputs, the acquired photo-thermal signals (I_1 and I_2) obtained upon sample excitation with the two pump beams. The output, $(\frac{\Delta\varepsilon_{\lambda 1}}{\Delta\varepsilon_{\lambda 2}})$ is a parameter that is related to the chemical composition of the sample and therefore can aid in identification of biomarkers of interest present. The model is independent of the design of the photothermal setup. The model was applied in detection of hemozoin present in malaria infected blood probed using a simple photo-thermal setup comprising of a RGB light emitting diode and a 3D printed optical microscope fitted with a Raspberry Pi camera. After incorporating the model in processing the acquired photothermal signals, a machine learning classification was performed and a classification accuracy of 100% between malaria infected and non-infected samples was attained.

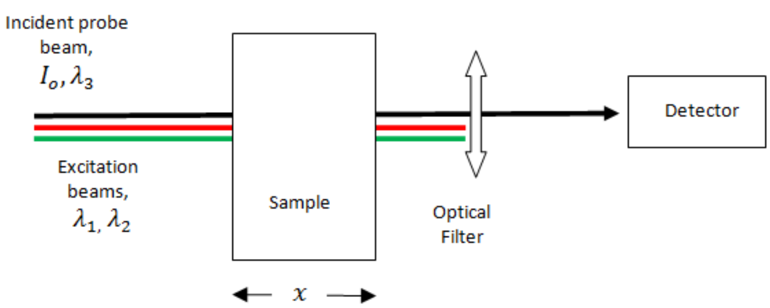

Fig. 1. Schematic diagram showing the required setup for implementation of the photo-thermal model.

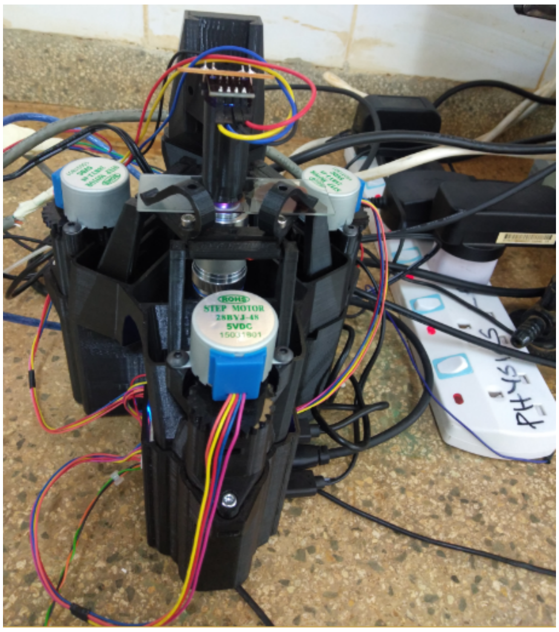

Fig. 2. An Image of the actual instrumentation setup used in the implantation of the model.

Equation (1) shows how the parameter $\frac{\Delta\varepsilon_{\lambda 1}}{\Delta\varepsilon_{\lambda 2}}$, is to be computed using the measured photo-thermal signals

$$\frac{\Delta\varepsilon_{\lambda 1}}{\Delta\varepsilon_{\lambda 2}} = \ln\left(\frac{I_1 - I_2}{I_3}\right) \qquad \text{Eqn. 1}$$

Table 1. Results showing the classification accuracies for photo-thermal signals processed according to equation 1.

	Precision	Recall	F1-Score
Negative	1.00	1.00	1.00
Positive	1.00	1.00	1.00