GLOBAL RESEARCH IMMERSION PROGRAM
FOR YOUNG SCIENTISTS

Uncertainty Analysis of Frequency Domain Thermoreflectance

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1.Introduction

Frequency Domain Thermoreflectance (FDTR)[1] is a cutting-edge technique used to measure the thermal properties of materials at the nanoscale. Utilizing a continuous-wave laser, FDTR creates a modulated heat source on the sample surface, while a probe beam detects temperature fluctuations via changes in reflectivity. This method is critical for analyzing the thermal conductivity and thermal boundary conductance in advanced materials like thin films and nanostructures, which are essential for the development of nanoelectronics and other high-tech applications. Uncertainty analysis[2] is critical in FDTR experiments as it ensures the accuracy and reliability of thermal property measurements. By identifying and quantifying potential errors, we can enhance precision, validate theoretical models, and optimize experimental designs. This process not only facilitates accurate comparisons across different studies but also bolsters the scientific credibility of the research findings.

2.Method: Analytical formula

The least-square minimization technique[3] is employed to analyze the fitting uncertainty in phase lag from the thermal model and experimental data.

$$\phi = f(\omega, X_U, X_C) \quad (1)$$

The above equation (1) represents the thermal model where modulation frequency is the independent variable. It includes two sets of parameters: unknown parameters and controlled parameters.

$$R = \sum_{i=1}^{M} [\phi_i - f(\omega_i, X_U, X_C)]^2 \quad (2)$$

Following the least square minimization procedure, we sum the residual squares as shown in equation (2). By taking the partial derivative for each parameter, we get the expression for $\widehat{X}_U$.

$$\frac{\partial R(X_U, X_C)}{\partial x_u}|_{\widehat{X}_U} = 0, u = 1, 2, ..., p \quad (3)$$

$f(\omega_i, X_U, X_C)$ can be approximated by a first-order Taylor expansion around both $X_U^\star$ and $X_C^\star$.

$$f(\omega_i, X_U, X_C) \approx f(\omega_i, X_U^\star, X_C^\star) + \sum_{u=1}^{p} \frac{\partial f(\omega_i, X_U, X_C)}{\partial x_u}|_{X_U^\star, X_C^\star}(x_u - x_u^\star)$$
$$+ \sum_{c=p+1}^{N} \frac{\partial f(\omega_i, X_U, X_C)}{\partial x_c}|_{X_U^\star, X_C^\star}(x_c - x_c^\star), i = 1, 2, ..., M \quad (4)$$

By substituting Eq.(4) into the resultant form from Eq.(3), we have Eq.(5). The summations of partial derivatives can be written in Jacobian matrices Eq.(6), Eq.(7) to simplify and manipulate to the final expression for $\widehat{X}_U$, Eq.(8).

$$\sum_{i=1}^{M}([\phi_i - f(\omega_i, X_U^\star, X_C^\star) - \sum_{u=1}^{p} \frac{\partial f(\omega_i, X_U, X_C)}{\partial x_u}|_{X_U^\star, X_C^\star}(\hat{x}_u - x_u^\star)$$
$$- \sum_{c=p+1}^{N} \frac{\partial f(\omega_i, X_U, X_C)}{\partial x_c}|_{X_U^\star, X_C^\star}(x_c - x_c^\star)] \frac{\partial f(\omega_i, X_U, X_C)}{\partial x_u}|_{X_U^\star, X_C^\star}) = 0 \quad (5)$$

$$J_U^\star = \begin{pmatrix} \frac{\partial f(\omega_1, X_U, X_C)}{\partial x_1}|_{X_U^\star, X_C^\star} & \cdots & \frac{\partial f(\omega_1, X_U, X_C)}{\partial x_p}|_{X_U^\star, X_C^\star} \\ \vdots & \ddots & \vdots \\ \frac{\partial f(\omega_M, X_U, X_C)}{\partial x_1}|_{X_U^\star, X_C^\star} & \cdots & \frac{\partial f(\omega_M, X_U, X_C)}{\partial x_p}|_{X_U^\star, X_C^\star} \end{pmatrix} \quad (6)$$

$$\text{and } J_C^\star = \begin{pmatrix} \frac{\partial f(\omega_1, X_U, X_C)}{\partial x_{p+1}}|_{X_U^\star, X_C^\star} & \cdots & \frac{\partial f(\omega_1, X_U, X_C)}{\partial x_N}|_{X_U^\star, X_C^\star} \\ \vdots & \ddots & \vdots \\ \frac{\partial f(\omega_M, X_U, X_C)}{\partial x_{p+1}}|_{X_U^\star, X_C^\star} & \cdots & \frac{\partial f(\omega_M, X_U, X_C)}{\partial x_N}|_{X_U^\star, X_C^\star} \end{pmatrix} \quad (7)$$

$$\widehat{X}_U = (J_U^{\star\prime} J_U^\star)^{-1} J_U^{\star\prime}(\Phi - F(X_U^\star, X_C^\star) - J_C^\star(X_C - X_C^\star)) + X_U^\star \quad (8)$$

As our focus is on uncertainties in unknown parameters, we calculate the variance-covariance matrix of $\widehat{X}_U$ from Eq.(8) to obtain the variances of the individual elements of $\widehat{X}_U$, Eq.(9).

$$\mathrm{Var}[\widehat{X}_U] = (J_U^{\star\prime} J_U^\star)^{-1} J_U^{\star\prime}(\mathrm{Var}[\Phi] + J_C^\star \mathrm{Var}[X_C] J_C^{\star\prime}) J_U^\star (J_U^{\star\prime} J_U^\star)^{-1} \quad (9)$$

3. Uncertainty Analysis

In the fitting process, several gold (Au) properties, such as thermal conductivity, heat capacity, thermal boundary conductance, and the probe and pump beam radii are controlled parameters with their corresponding uncertainties. Using the returned fitted parameters, we apply the formula Eq.10 for correlation coefficients[5] to assess the relationships between these parameters. Finally, we calculate the percentage uncertainties of the fitted parameters, providing insight into the precision and reliability of the measurements.

$$r = \frac{cov(xy)}{\sigma_x \sigma_y} \quad (10)$$

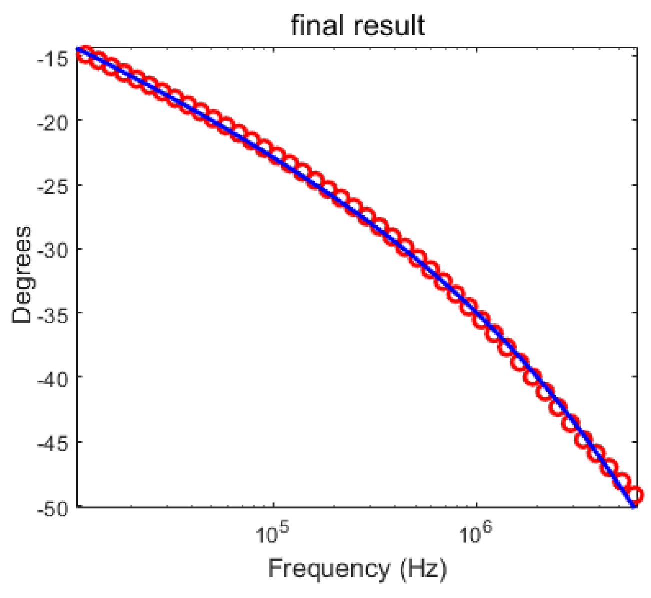

Figure 1: The experimental phase lag (represented by red circles) fitted with the phase lag from the thermal model (depicted as a blue line).

Frequency range	Correlation coefficient			Uncertainty (%)		
(Hz)	$r(G, C_{SiO_2})$	$r(G, \kappa_{SiO_2})$	$r(C_{SiO_2}, \kappa_{SiO_2})$	G	C_{SiO_2}	κ_{SiO_2}
$5000 - 3\times10^7$	0.4691	−0.4195	−0.0785	11.88	4.53	8.12

Table 1: Correlation coefficients and calculated uncertainties for a three-parameter fit

From Table 1, we can infer that within the given frequency range, thermal conductivity and thermal boundary conductance exhibit a positive correlation. This positive correlation results in a significant increase in the uncertainty associated with G . Moreover, for the purpose of fitting the data, we have assumed a constant phase noise of 0.3 degrees[4] for all measurements.

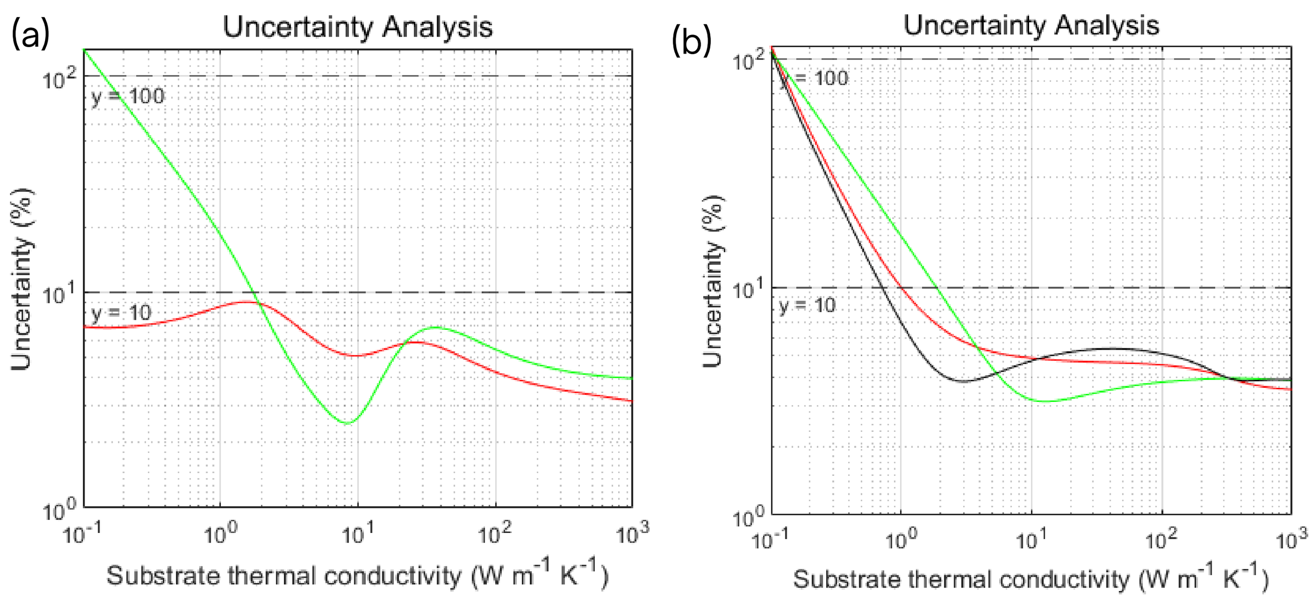

Figure 2: Calculated uncertainties for two and three parameter fits of a bulk substrate, plotted as a function of substrate thermal conductivity.

The two plots compare two- and three-parameter fits with the magnitude of substrate thermal conductivity varying from 0.1 to 1000 on a logarithmic scale to test the effect of uncertainty on different substrate thermal conductivity. In Fig 2 (a), the uncertainties for k and G are the smallest for a substrate thermal conductivity around 10W/mK.

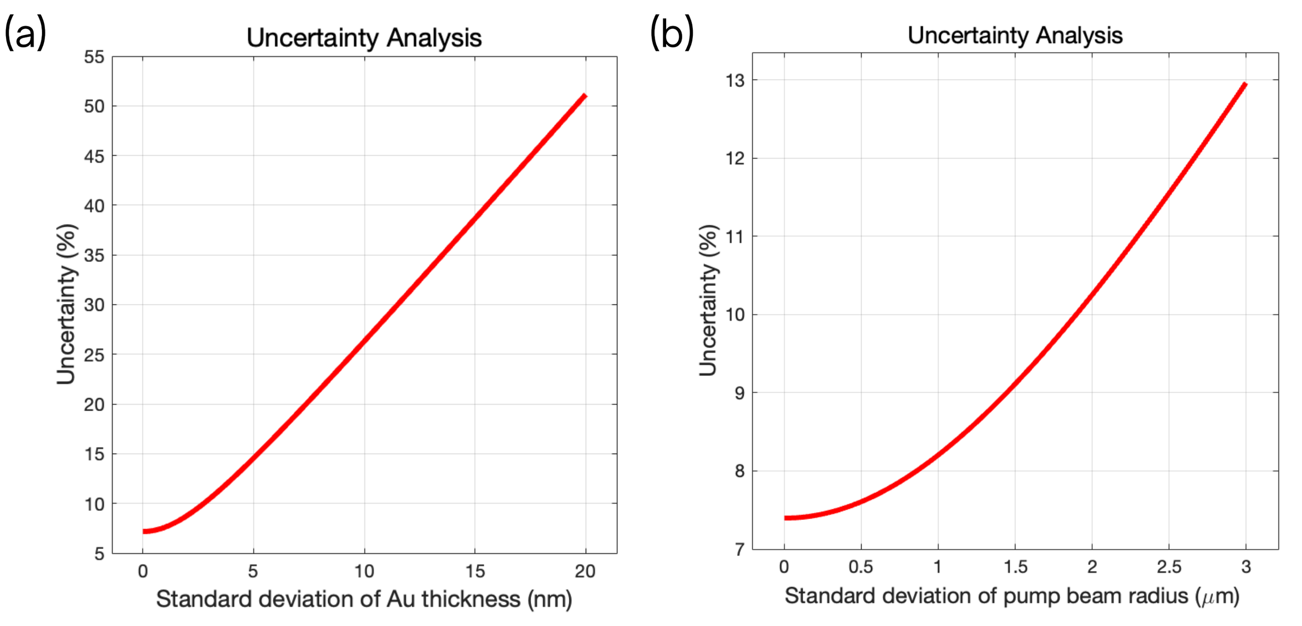

Figure 3: Uncertainty in substrate thermal conductivity determined by FDTR with two-parameter fits of Ks and G, plotted as a function of (a) the uncertainty of the transducer thickness, and (b) the uncertainty of the pump spot 1/e2 radius

Figure 3 illustrates the impact of varying the uncertainty in different controlled parameters on a specific fitted parameter. The results demonstrate the importance of accurately determining the uncertainties in these quantities. Notably, the thickness of the gold layer has a significant effect on the final fitted parameter, highlighting the critical nature of precise measurements in this aspect.

4. Discussion

The plots in this poster illustrate that small changes in the frequency range can drastically alter the fit and shape of the graphs. This underscores the importance of carefully selecting and maintaining the frequency range.
Additionally, the provided parameters are approximations, introducing uncertainties into the results. Accurate determination of these parameters is crucial, as highlighted in Figure 3, where the thickness of the gold layer significantly impacts the fitted parameter. Improving the precision of these parameters will enhance the reliability of the measurements and the overall conclusions.

5. Conclusion

This study emphasizes the crucial role of accurately determining and controlling parameter uncertainties in Frequency Domain Thermoreflectance (FDTR) measurements. The sensitivity of the fitting process to changes in the frequency range demonstrates that even minor adjustments can significantly alter the results. Additionally, the approximations used for parameters such as thermal conductivity and gold layer thickness introduce notable uncertainties into the final outcomes.
Our analysis shows that precise measurement and control of these parameters are essential for minimizing uncertainty and improving the reliability of the measurements. Future efforts should focus on refining these input parameters to achieve more consistent and accurate results. This improvement is vital for advancing the understanding and application of thermal properties in materials, particularly in fields like nanoelectronics and other high-tech applications.

Reference

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