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Technical Summary

Development of a program for uncertainty analysis in multiparameter model optimisation

In summer 2022, I worked as an intern in the University of Bristol Centre for Device Thermography and Reliability (CDTR) for four weeks. I created a Python application which calculates the thermal properties of thin layered structures by fitting a theoretical model to experimental Frequency Domain Thermoreflectance (FDTR) data. The application calculates the uncertainty in the fitted parameters using an analytical formula, avoiding the need for lengthy statistical simulations. The code and accompanying documentation is publicly available in the git repository at: `https://git.sr.ht/~callum/thermref`.

Background

Heat management is critical to the performance, efficiency, and longevity of semiconductor devices. However, measuring the thermal properties of multilayer structures, such as the one illustrated in Figure 1, is difficult, if not impossible, with conventional thermometry. In thermoreflectance techniques, samples are coated with a thin metal layer, for which the optical reflectivity is proportional to temperature, and a "probe" laser is reflected off of the surface. The phase shift of the probe laser is dependent on the reflectivity of the surface, so can be used to measure temperature.

In frequency domain thermoreflectance, a "pump" laser is used to periodically heat the surface. The surface temperature at a set time after each pump depends on the thickness, heat capacity, and thermal conductivity of each layer, the thermal boundary resistance between layers, and the pump frequency. Therefore, by measuring the probe phase shift as the pump frequency is varied, and fitting this data with a theoretical heat diffusion model, the thermal properties of the layers in the sample can be determined.

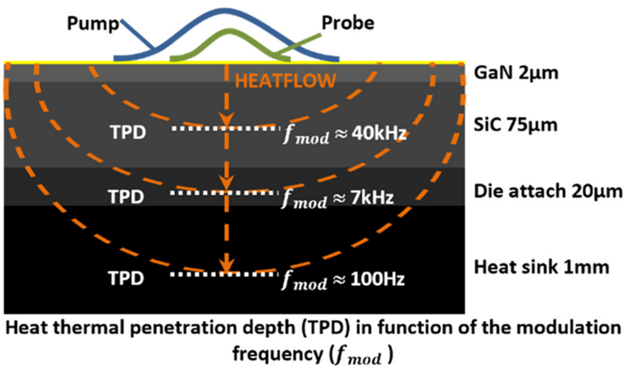

Figure 1: Illustration of the heat flow in a multilayer device, showing the increase in thermal penetration depth with pump modulation frequency. Reproduced unchanged from Ref. [1] under CC BY 4.0.

For each layer, the temperature (T) and heat flux (F) on the bottom surface (b) can be calculated from those on the top surface (t) by:

$$\begin{bmatrix} T_b \\ F_b \end{bmatrix} = M \begin{bmatrix} T_t \\ F_t \end{bmatrix} \quad , \tag{1}$$

where M is a matrix which depends on the thickness, heat capacity, and thermal conductivity of the layer, and the pump frequency. The temperature and heat flux on the bottom surface of the nth layercan be written in terms of those on the top of the first layer:

$$\begin{bmatrix} T_{b_n} \\ F_{b_n} \end{bmatrix} = M_n \dots M_2 M_1 \begin{bmatrix} T_{t_1} \\ F_{t_1} \end{bmatrix} = \widetilde{M} \begin{bmatrix} T_{t_1} \\ F_{t_1} \end{bmatrix} \quad . \tag{2}$$

Finally, the phase shift of the probe laser (which is what is measured) is given by:

$$\Delta\phi = \text{arg}\left(\int_0^\infty f\left(\widetilde{M}, w, k\right) dk \right) \quad , \tag{3}$$

where the integrand, f, is dependent on the effective spot radius of the pump and probe lasers, w, and the Hankel transform variable, k. For a more detailed summary, see Refs. [1] and [2].

Project aims

Analysis of the uncertainty in the fitted parameters is usually done by a Monte Carlo simulation. However, this method is computationally intensive and therefore slow, or expensive. Yang *et al.* derived a formula for analytically calculating the uncertainty in parameters fitted using least-squares algorithms, and validated it using Monte Carlo simulations [3]. The aim of my internship was to efficiently implement this formula for multilayer FDTR data, providing flexibility on which parameters to fit.

Implementation

The existing implementation of the heat diffusion model used by the CDTR hardcoded the matrix $\widetilde{M}$, which had been manually pre-calculated for a set number of layers. This method, while computationally efficient, is impractical for use with the uncertainty formula, which requires the calculation of the derivatives of the phase shift: respect to all known and unknown (fitted) parameters (Jacobian matrices). Therefore, the first step was to generate the model for a variable number of layers, in a form which would permit computational symbolic differentiation.

Symbolic integrand and least-squares fitting

I used the SymPy computer algebra Python library, to do the matrix multiplication to find $\widetilde{M}$, and generate a symbolic expression for the integrand, f. This can be done in advance of any data fitting, which retains the performance benefits of manually hardcoding the integrand, while allowing variability in the number of layers. This approach could be easily extended to different thermal models of similar form.

After conversion of the symbolic integrand to a function for use in the numerical integration methods of SciPy, I used lmfit, a non-linear least-squares minimisation library, to fit the model to experimental data, keeping fixed the known parameters specified in a configuration file.

Calculation of uncertainties

To calculate the phase shift Jacobians for controlled and variable parameters, Equation 3 needs to be differentiated. By applying the chain and quotient rules, I moved the derivative inside the integral and calculated it symbolically using SymPy. This method avoids the computational error which would be introduced by slow numerical differentiation, and allows the unknown (fitted) parameters to be changed without additional work. More detail on the calculation of the derivative can be found here.

Finally, I used these Jacobians, along with with the experimental uncertainty in the phase shift data and the known uncertainty in the controlled parameters, to calculate the uncertainty in the fitted parameters using the formula in Ref. [3].

Conclusion

After only the first year of my degree, I quickly built a working understanding of an advanced measurement technique and the statistical maths required for multiparameter uncertainty analysis. I wrote performant, well documented, and extensible code using previously unfamiliar libraries, which is still in use by the CDTR team today.

References

[1] Nathawat Poopakdee et al. “In situ Thermoreflectance Characterization of Thermal Resistance in Multilayer Electronics Packaging”. In: *ACS Applied Electronic Materials* 4.4 (2022), pp. 1558–1566. DOI: `10.1021/acsaelm.1c01239`.

[2] Puqing Jiang, Xin Qian, and Ronggui Yang. “Tutorial: Time-domain thermoreflectance (TDTR) for thermal property characterization of bulk and thin film materials”. In: *Journal of Applied Physics* 124.16 (Oct. 2018), p. 161103. ISSN: 0021-8979. DOI: `10.1063/1.5046944`.

[3] Jia Yang, Elbara Ziade, and Aaron J. Schmidt. “Uncertainty analysis of thermoreflectance measurements”. In: *Review of Scientific Instruments* 87.1 (Jan. 2016), p. 014901. ISSN: 0034-6748. DOI: `10.1063/1.4939671`.