Vassar College | Undergraduate Research Summer Institute (URSI) Symposium | 2020

Using Matlab Simulations to Study Heat Flow In Thin Films

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Introduction

We use Matlab to simulate experiments in which an ultra-fast laser pump-probe method is used to measure the thermal conductivity of thin films that are less than a few micrometers in thickness. The laser emits pulses that are less than a picosecond in duration; the pump pulses heat the thin film and the probe pulses act as a picosecond time sensitive thermometer. We studied Matlab simulations published by researchers at the University of Illinois found here: https://cahill.matse.illinois.edu/software-and-data/.[1] We used the simulations to design the ideal experimental set up for studying the thermal conductivity of $MoSe_2$.

Experiment

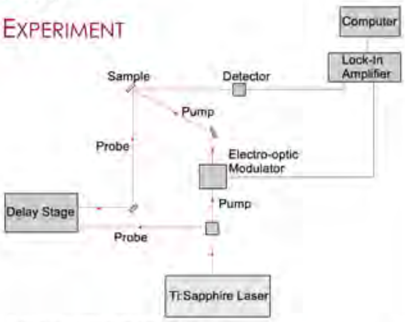

Figure 1a. The experimental set up.

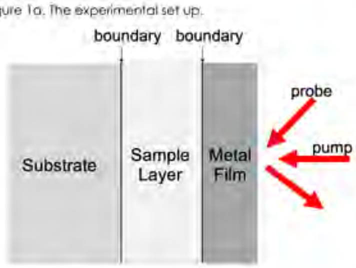

Figure 1b. The material set up.

In Figure 1a, the Ti:Sapphire laser splits into pump and probe beams and the pump pulses are chopped by the electro-optic modulator (EOM) before hitting the sample. The probe pulses go to a delay stage, and then reflect off the sample to the detector. The lock-in amplifier amplifies the signal from the detector that is in phase with the EOM. In Figure 1b a metal film is deposited on top of a sample layer which is grown on a substrate. The pump pulses heat the metal film and then the probe pulses are used to measure the change in reflectivity of the metal film. For our experiment, the metal film is Al, the sample layer $MoSe_2$, and the substrate is Si.

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Simulations

Thermal Conductivity Simulations

While the cooling curves appear straightforward, it is a complex problem as the metal film is reheated about a 100 times per ns by the pump beam while the pump beam is also modulated by the EOM every 1 ns.

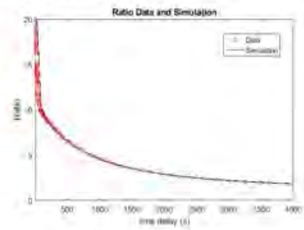

Figure 2a. The ratio data and fitted simulation cooling curves. Data taken from researchers at the University of Illinois.

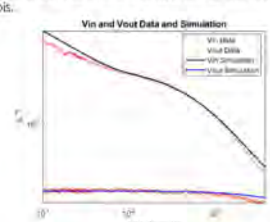

Figure 2b. Vin and Vout for the cooling curve in Figure 2a. Plotted on a log scale to show variation in Vout.

The researchers at University of Illinois developed the method of looking at the ratio to create cooling curves instead of just Vin. Vin is the signal that is in phase with the EOM and amplified by the lock-in amplifier, while Vout is the signal out of phase with the EOM. The ratio (-Vin/Vout) tells us about the change in temperature of the metal film (Vin) while also compensating for inconsistencies in the experimental set-up (Vout).

Sensitivity Simulations

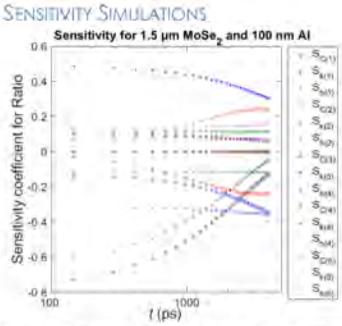

Figure 3. Sensitivities for 1.5 um MoSe2 with 100 nm Al film and laser parameters of 5 um spot size and 1.4 MHz Modulation frequency.

A subset of Matlab simulations allows for testing the sensitivities of the material parameters for the metal film, sample layer, and substrate, and the two boundaries.

Figure 3 shows sensitivities of each parameter computed as a function of time, so we wrote a program that computed the time averaged sensitivity of each parameter as seen in Table 1.

Time Averaged Sensitivities

	Heat Capacity	Thermal Conductivity	Thickness
Al	0.3618	0.0845	0.2495
Boundary 1	0.0001	0.1849	0.1851
$MoSe_2$	0.2424	0.3935	0.3377
Boundary 2	0.0000	0.1134	0.1142
Si	0.0702	0.1429	0

Table 1. Time averaged sensitivities for each parameter shown in Figure 3. The thermal conductivity of $MoSe_2$ is the most sensitive parameter. The thickness of Si is not sensitive as the simulation assumes all heat leaves through the bottom layer.

Results

We tested sensitivity at different thickness of $MoSe_2$ and at different spot sizes. We expect that most of our $MoSe_2$ films will be between 500 nm to 1 μm thick, but a 1.5 μm thickness would result in optimized sensitivity to the thermal conductivity of the sample layer.

Changes in Modulation Frequencies at Different Spot Sizes for 1 μm $MoSe_2$

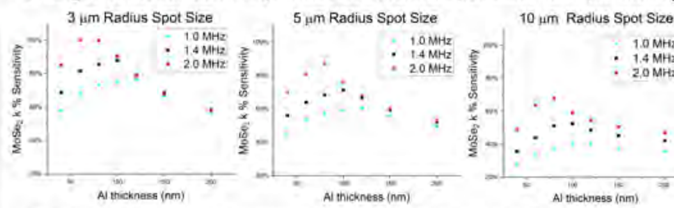

Figure 4a. Sensitivity to the thermal conductivity (k) of $MoSe_2$ decreases as spot size increases.

Changes in Modulation Frequency at Different Thicknesses of $MoSe_2$ for 10 μm Spot Size

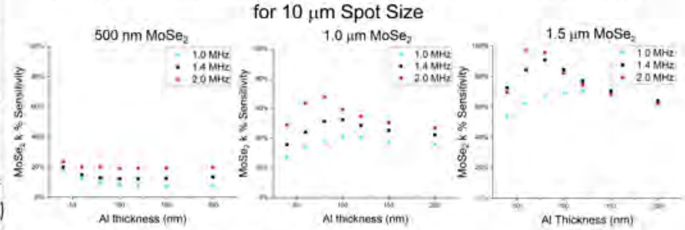

Figure 4b. Sensitivity to k increases as the thickness of $MoSe_2$ increases.

For 1 μm $MoSe_2$, the ideal experimental set up that optimizes sensitivity to thermal conductivity is at 3 μm radius spot size, 2.0 modulation frequency, and 60 or 80 nm Al. An 80 nm thickness increases certainty of the Al thickness measurement and reduces dependence on the boundary; however the time averaged sensitivity value is higher for 60 nm Al than 80.

Discussion

It is possible that a 3 μm spot size and 2 MHz modulation frequency cannot be achieved with our experimental set up. Small spot sizes also increase misalignment errors. Researchers at MIT suggest using a larger pump and smaller probe spot size to reduce misalignment errors.[2] We did a preliminary investigation that suggests this might be advantageous for $MoSe_2$ films less than 1 μm.

References and Acknowledgments

Thank you to Vassar for making remote URSI possible. Thank you to the Cahill research group at the University of Illinois for making the simulations and data accessible to all.

1. Cahill, D. (n.d.). Cahill Research Group: Software and Data. Retrieved from https://cahill.matse.illinois.edu/software-and-data/

2. Collins, Kimberlee C., Maznev, Alexei A., Cuffe, John, Nelson, Keith A., & Chen, Gang. *Examining thermal transport through a frequency-domain representation of time-domain thermoreflectance data*. United States. doi:10.1063/1.4903463.