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Photothermal Deflection Spectroscopy (PDS) for PV material characterisation

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Various new materials are under investigation for making cheaper and more efficient solar cells. Understanding the bandgap and sub-bandgap levels of these new materials is absolutely essential for advancing new technologies as they determine most of the optoelectronic properties in the resulting solar cells. Photothermal Deflection Spectroscopy (PDS) is an ultra-sensitive characterisation method that has been widely used for this end, especially, since the advent of perovskite thin-films in photovoltaics[12].

PDS is capable of measuring the weak absorption in the sub-bandgap regime and thus can characterise non-radiative defects and Urbach energy tails in organic and inorganic thin solid films [34]. This can be used to determine the quality of the material. However, this method has been mostly used as a qualitative measurement technique, largely due to the lack of accurate fitting models for the PDS signals. The existing models are based on Jackson's analytical work[5] and do not take into account the complexities of optical pathways inside the sample, especially in the sub-bandgap regime where most of the light travels through the sample and reflects from the sample-substrate interface, causing interference patterns.

In this work, we develop a robust mathematical model for accurately predicting the optical and thermal properties of the sample. The parameters in the model are varied to:

- characterise the defects at the interfaces and bulk
- Interpret the interference peaks in the PDS signal
- Estimate the refractive index and the thickness of the thin film.
- Determine the thermal conductivity of the sample
- Identify the thermal vs electronic contribution to PDS signal

The model is fitted to PDS characterisation results on thin silicon samples.

Setup and Methodology

The PDS setup is shown in the block diagram in Figure-1. The pump beam from the monochromator and the probe beam from the laser source are aligned perpendicularly on the sample. The pump beam wavelength is scanned from 400 nm to 2000 nm to probe different energy levels in the material and the deflections in the probe beam (or the PDS signal) is captured for each wavelength using a position detector. The PDS signal is connected to a lock-in amplifier to increase the signal-to-noise ratio of the results. The pyro detector

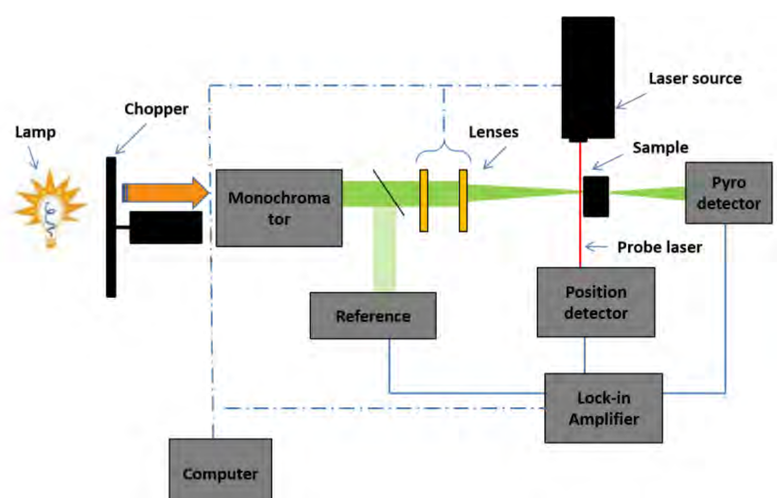

Figure 1: The PDS setup block diagram

and the reference detector normalises the PDS signal with the input power.

The mathematical model is developed in MATLAB using the Transfer Matrix Method (TMM) from travelling wave equations. Multiple reflection paths between the sample surface and the interface between the sample and the substrate are modelled. The thermal properties are modelled using the heat conduction equations and are implemented numerically. The Least Mean Square (LMS) algorithm is used for fitting purposes.

Results

Figure-2 (left) shows the different contribution of the thermal and electronic mobility parameters on the silicon sample by varying the pump beam chopping frequency. This characterisation technique is readily transferrable to nanocrystal as well as quantum dot samples, where the device performance is limited by mobility (right).

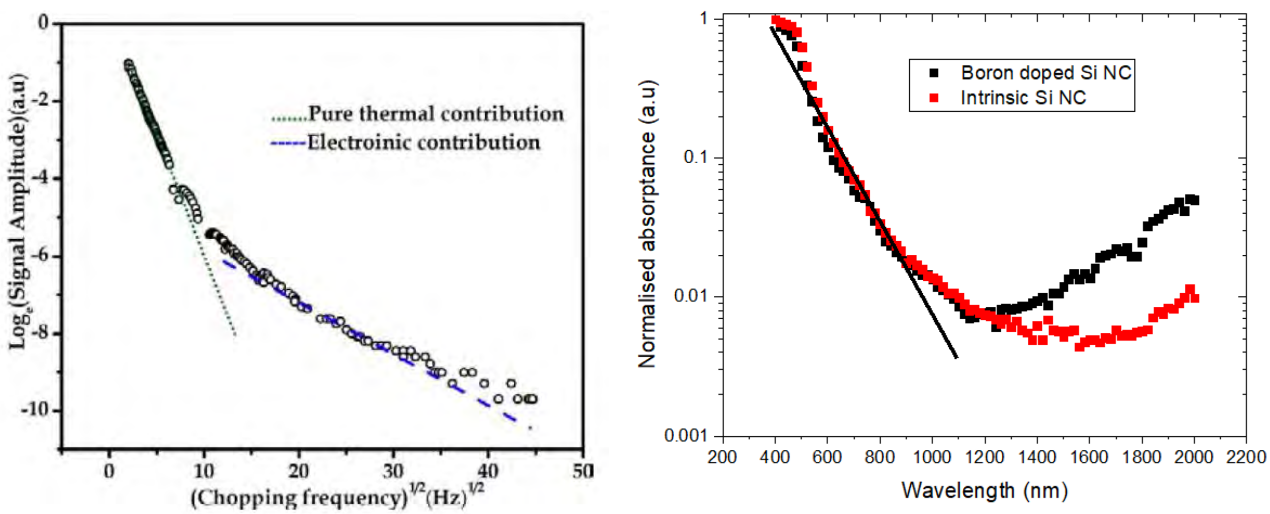

Figure 1: (left) Thermal vs Electronic contribution to PDS signal on a silicon sample, (right) Normalised PDS signal from silicon nanocrystal sample.

Our major findings and conclusions will be presented in the paper and at the conference.

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