Inverse modelling for determination of thermal conductivity of layered samples

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Introduction

- Project aim: "to improve the understanding and use of continuous modelling packages, and to improve model users' confidence in the accuracy of their results"
- Focus on computationally efficient sensitivity, optimisation and uncertainty methods.
- General investigation using small problems.
- Illustrate with case studies:
  - Charge transport in organic LEDs.
  - Laser flash experiment.

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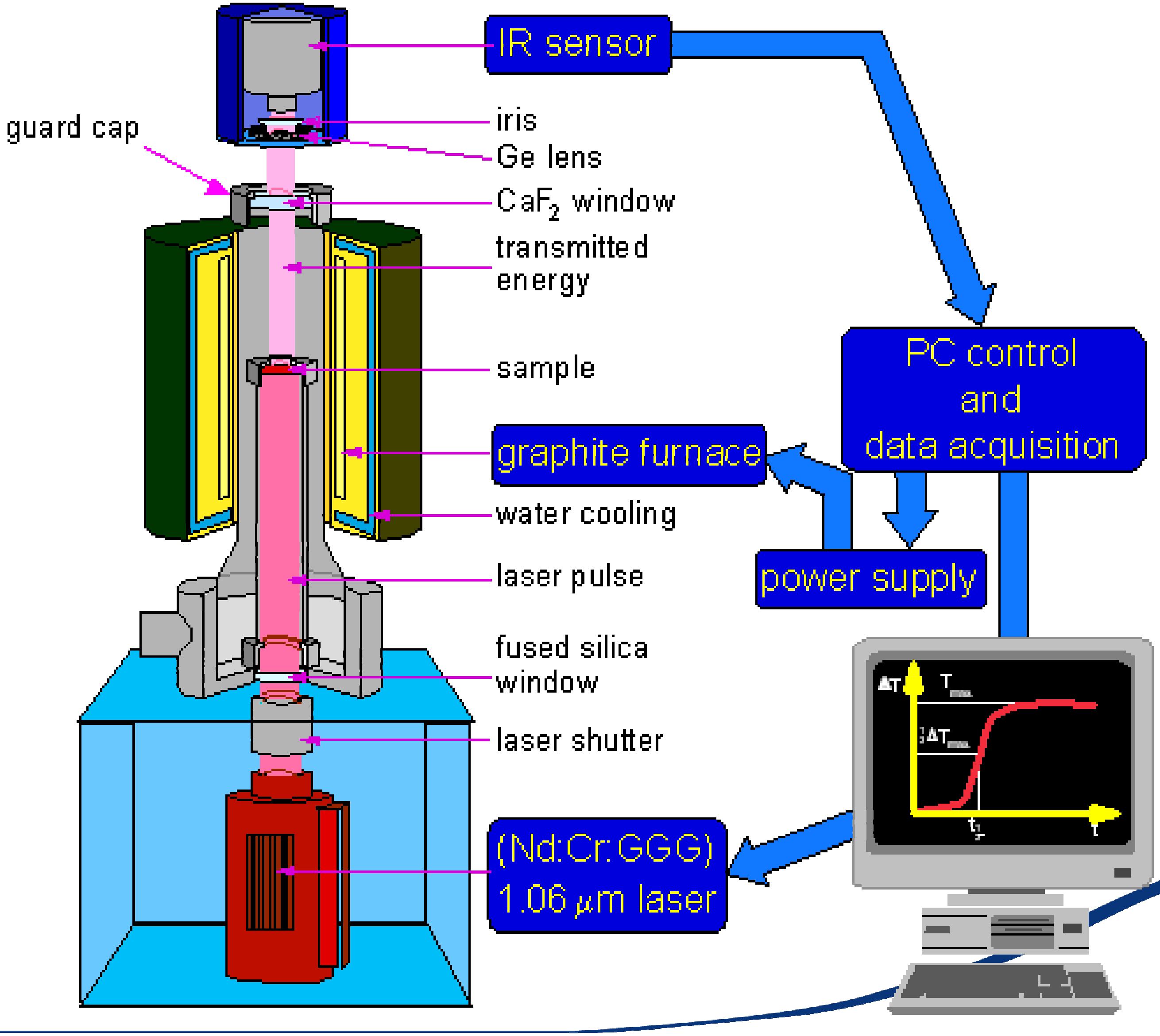
Thermal conductivity

- Key parameter for simulation of heat transfer.
- Determined from thermal diffusivity α for materials of known density ρ and specific heat capacity c_p: $\lambda = \alpha \rho c_p$
- Thermal diffusivity measured using laser flash thermal diffusivity (LFTD) experiment.

Experimental set-up



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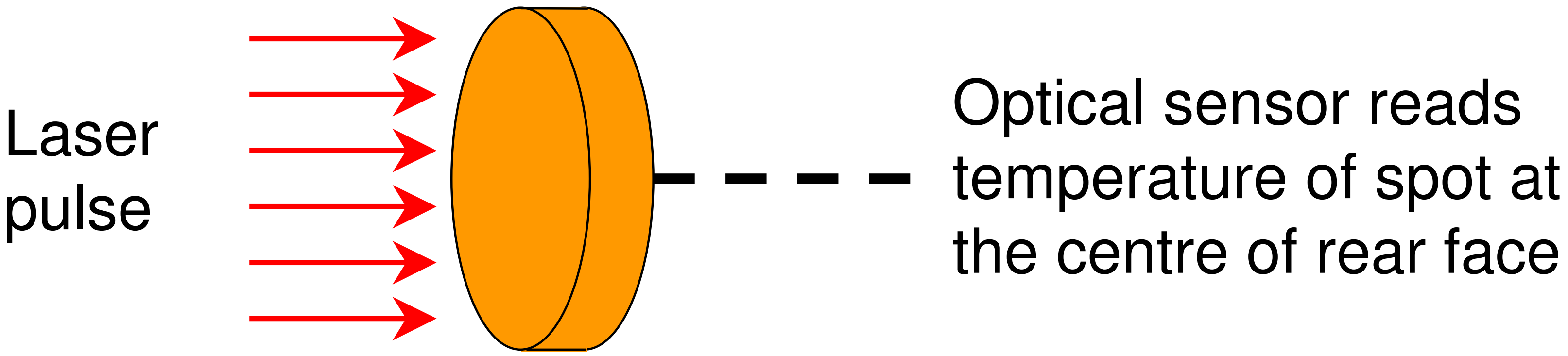
Idealisation of experimental set-up



Optical sensor reads temperature of spot at the centre of rear face

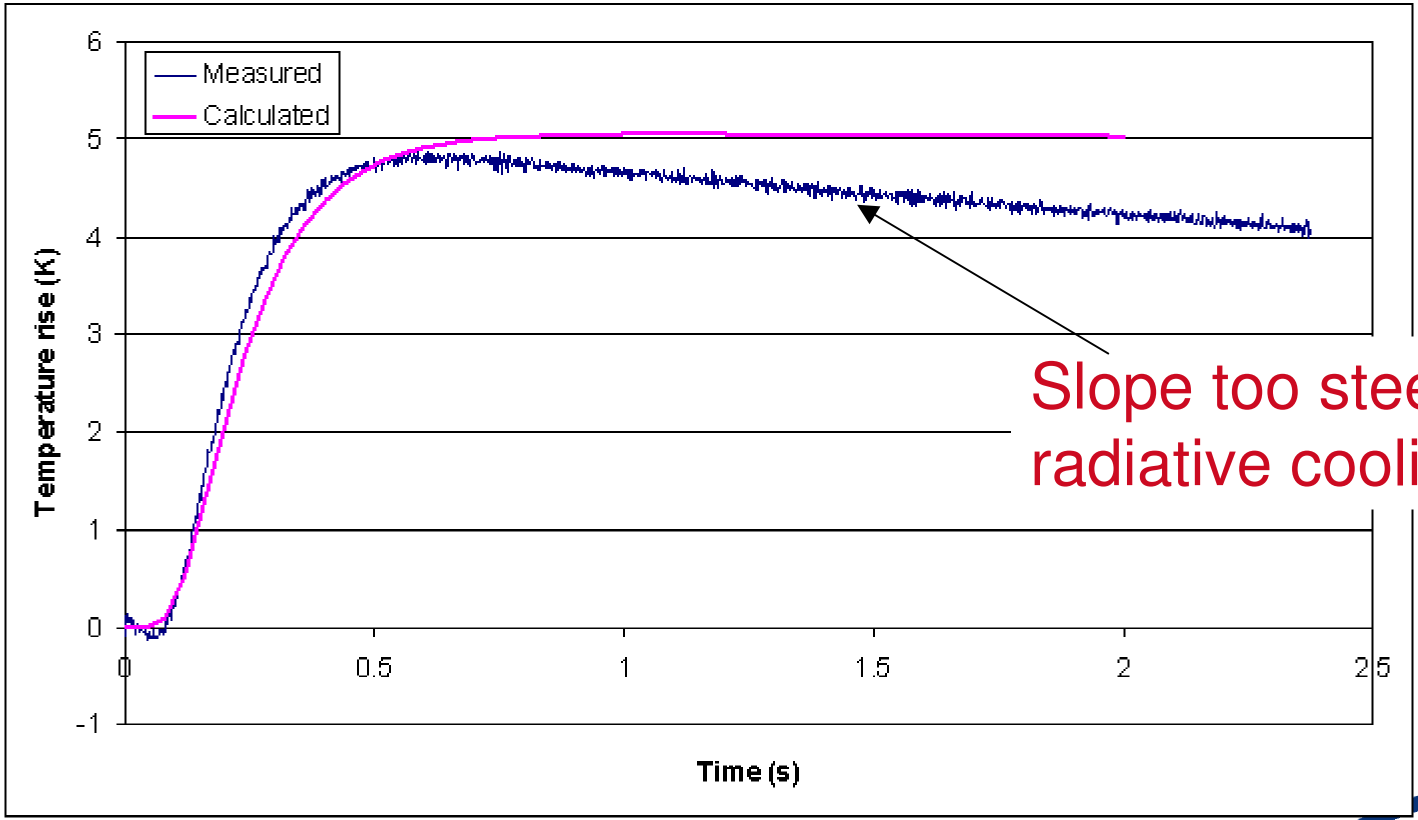
- Sample is on pins in vacuum so only radiative losses.
- Known fixed ambient temperature maintained by furnace.
- Laser pulse nearly instantaneous.
- Laser power is unknown.
- Typical temperature rise is less than 5 K.

Data processing

- Record temperature rise vs. time data.
- Diffusivity determined from time for temperature rise to reach half of maximum.
  - Corrections applied to diffusivity value for radiative losses from faces and for non-instantaneous laser pulse.
- Relies on assumptions
  - Uniform homogeneous sample.
  - Constant material properties.
  - No conductive or convective losses.
  - Small temperature rise.
  - Spatially uniform laser flash.

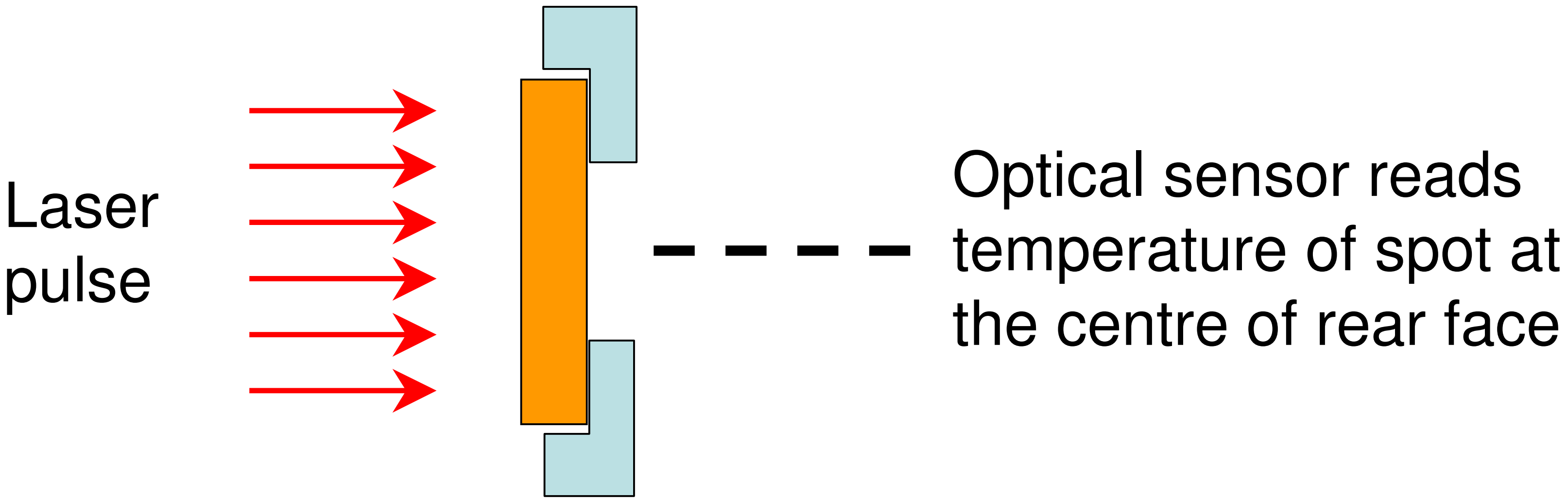
Data set of interest

Earlier work calculated $\lambda = 2.1\ \mathrm{W\ m^{-1}\ K^{-1}}$, $I = 1.6\times10^{8}\ \mathrm{W\ m^{-2}}$



Slope too steep for purely radiative cooling!

Altered idealisation of experimental set-up



- Possible contact between guard cap and sample.
- Particularly likely if thermal expansion is high.
- Assume a perfect thermal bond between cap and rear face of sample.

Problem of interest

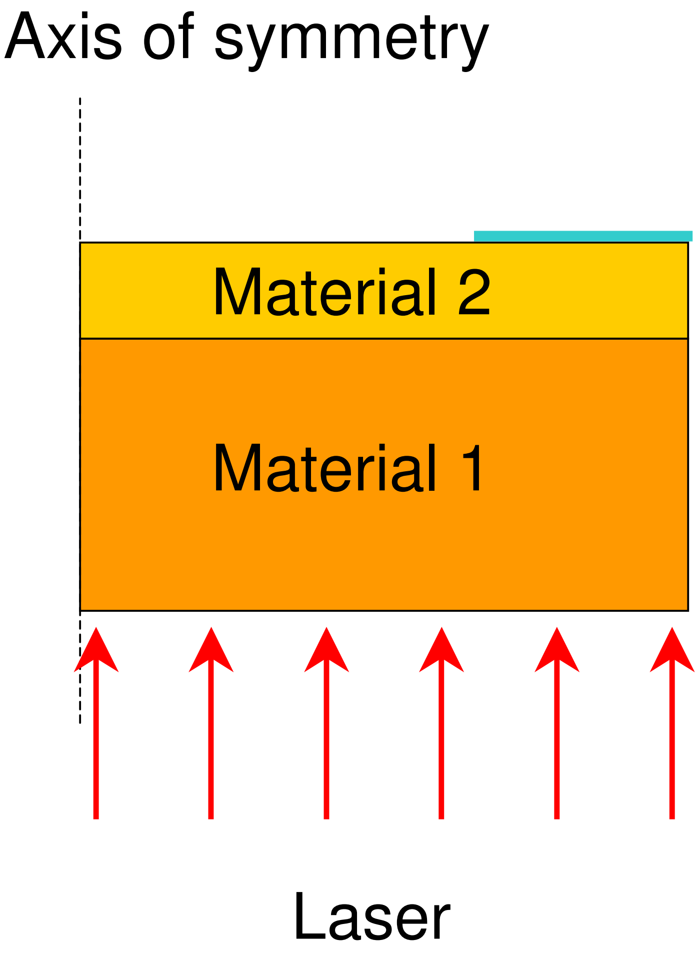
- Materials at high temperature in corrosive environments form surface layers.
- Such layers cannot be created separately from their parent materials.
  - Generally too fragile to remove and form into a sample for LFTD.
- LFTD as it stands requires homogeneous materials.
- Need a new approach.

New approach

- Finite volume approach to solve heat flow within a layered system.
  - Assume axisymmetry, uniform laser profile, homogeneity within each layer.
- Use an optimisation method to match model results to experimental data.
  - Estimate thermal conductivity, emissivity, laser power.
- Ideally, compute uncertainties associated with parameter estimates.
  - Requires goodness of fit to be consistent with experimental uncertainties.

Initial model

$$\frac{\partial}{\partial t}\left(\rho c_p T\right) = \nabla.\left(\lambda \nabla T\right) + Q$$



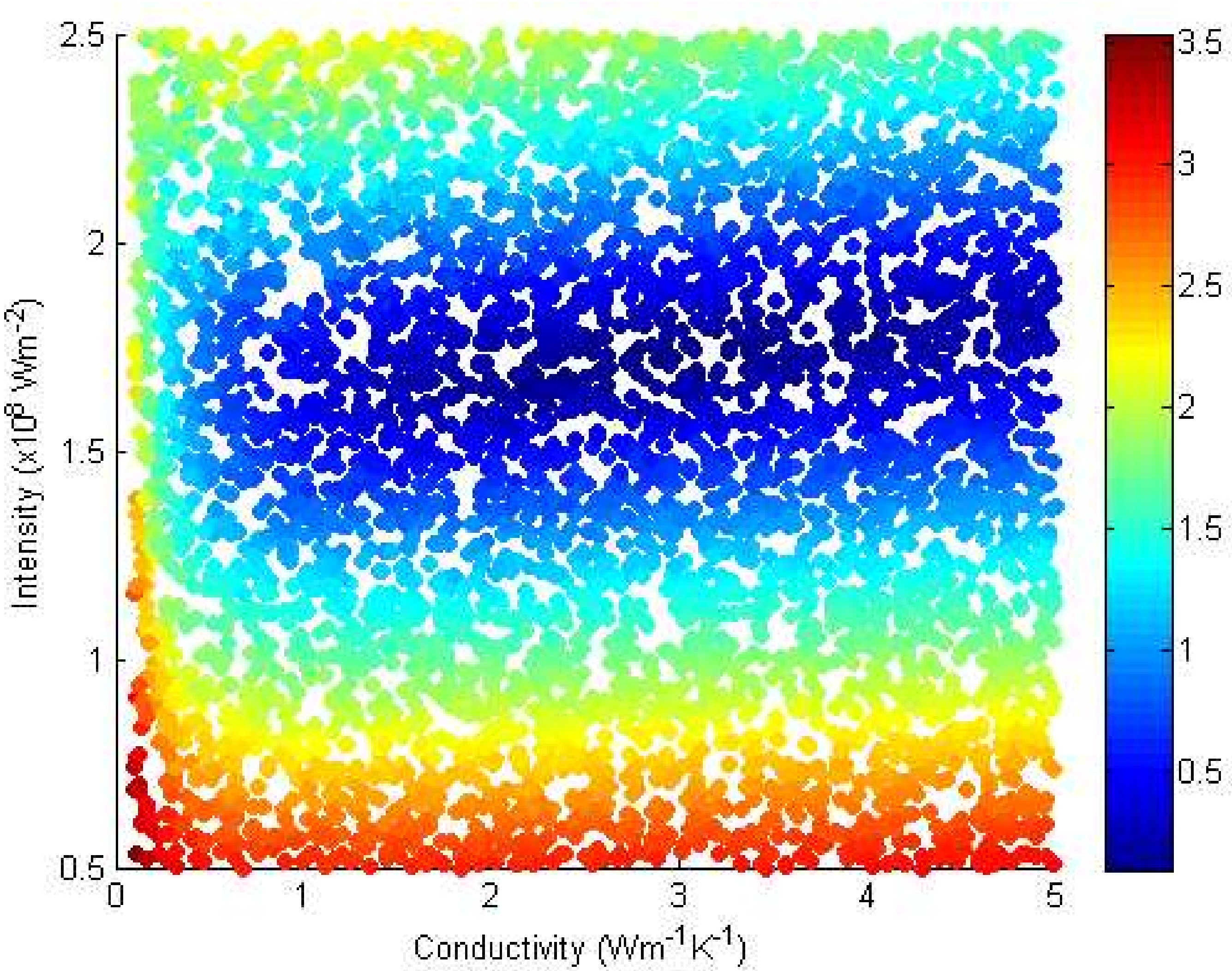
Temperature initially uniform.

All faces not in contact with guard cap lose heat to the surroundings through radiation (dependent on ε).

Region in contact with guard cap (marked in blue) assumed to be at ambient temperature.

Q is a heat source term and depends on *I*.

Sensitivity analysis



Morris OAT sensitivity indices

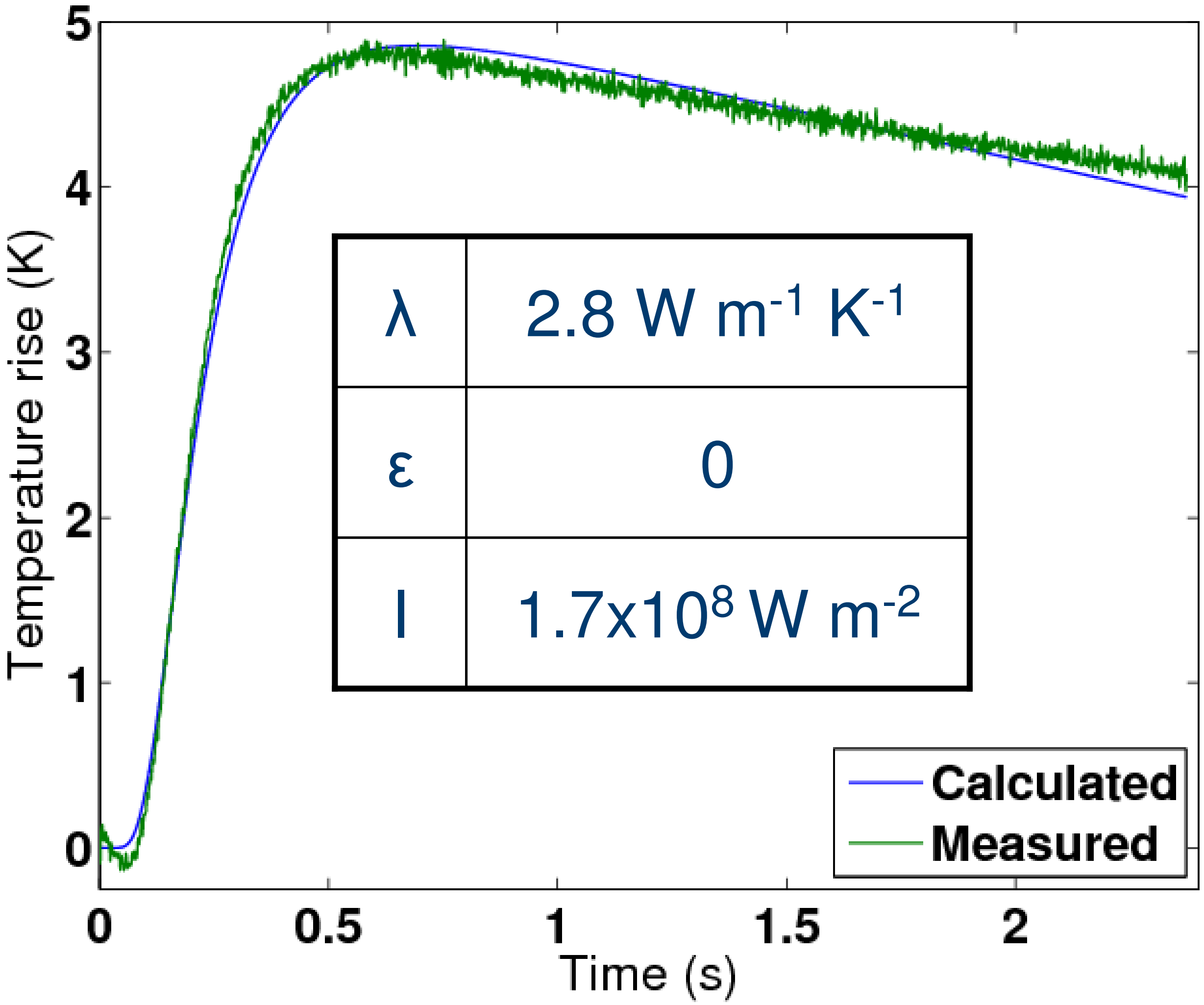
Parameter	Mean EE	St dev EE	Mean abs(EE)
λ	-0.087	0.195	0.158
ε	-0.003	0.045	0.038
l	-0.522	0.697	0.741

EE=elementary effect

Optimisation

- Minimise root mean square difference between measured and calculated temperature rise.
- Three unknowns: laser power, emissivity and thermal conductivity of material 2.
  - Bounds on all values.
- Sensitivity analysis suggests a smooth unimodal response surface.
- Use Levenburg-Marquardt implementation that requires function values only.
  - Performs well for smooth surfaces.
  - Matlab routine lsqnonlin.

Initial optimisation results



λ	2.8 W m^{-1} K^{-1}
ε	0
I	1.7x10^8 W m^{-2}

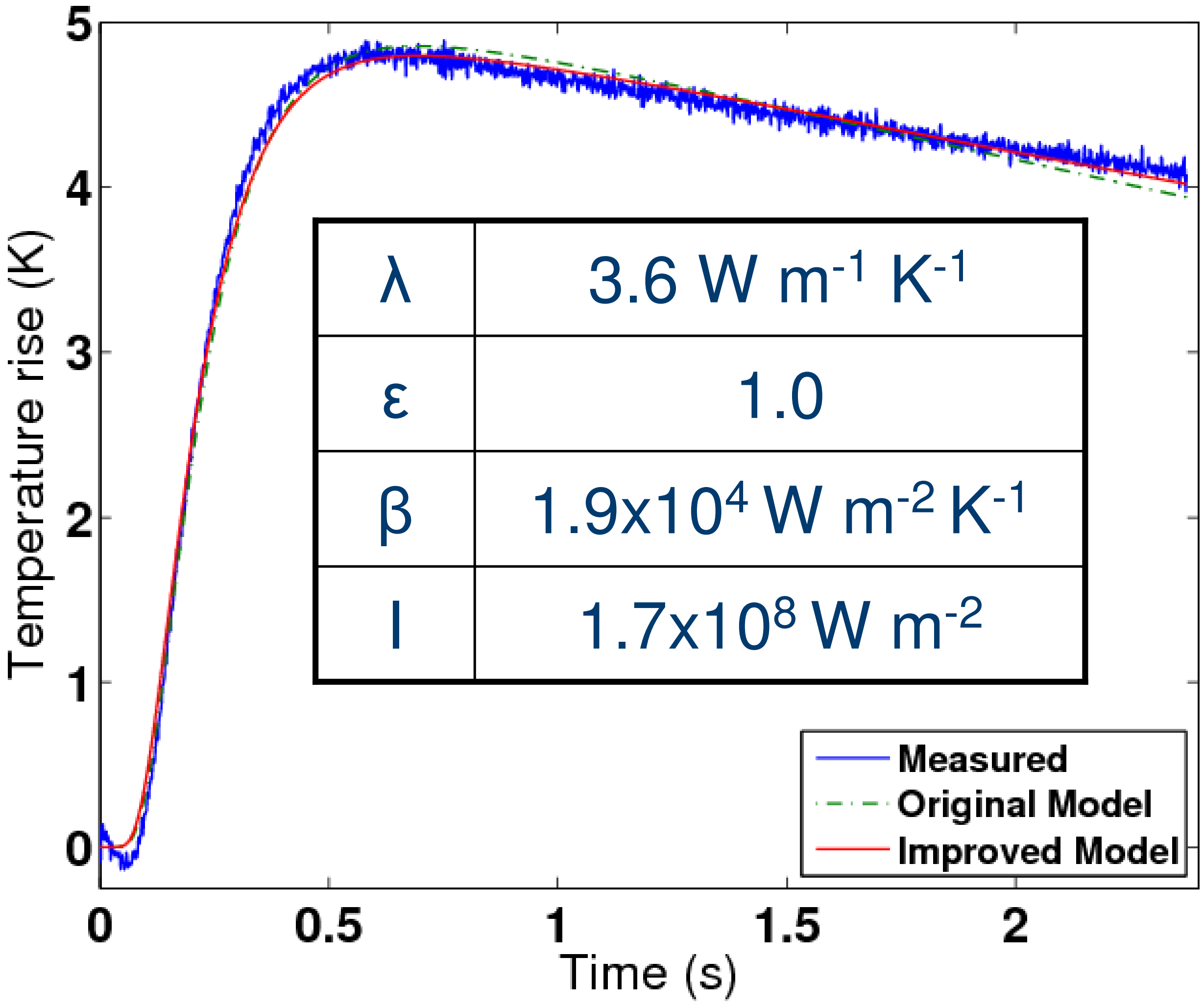
Typical optimisation run required 32 evaluations of the objective function.

Literature suggests λ is between 2.6 and 6 W m^{-1} K^{-1} for flakes of same oxide.

Model improvements

- Fit is good but not within measurement noise.
- Cooling part is worst.
- Try using an imperfect thermal bond between sample and guard cap.
  - Define imperfect bond as an extra layer between sample and guard cap.
  - Characterise bond quality with a parameter β.
  - Test runs show $\beta = 100$ is equivalent to no bond and $\beta = 10^6$ is equivalent to a perfect thermal bond.
  - Include β in optimisation.

Improved model results



λ	3.6 W m^{-1} K^{-1}
ε	1.0
β	1.9x10^{4} W m^{-2} K^{-1}
I	1.7x10^{8} W m^{-2}

Typical optimisation run required 126 evaluations of the objective function

Still not within measurement noise.

Conclusions

- Applied an inverse modelling approach to estimate unknown values.
  - Sensitivity analysis identified important parameters and showed smoothness of response surface.
  - Well-chosen optimisation algorithm gave good results quickly and repeatably.
- Improvements in model gave better fit to data
  - Still not perfect: inclusion of guard cap in model possibly next step.

Further information

- Further information on sensitivity, optimisation, and this case study will be available in NPL report form soon.
- Please contact Louise Wright (louise.wright@npl.co.uk) if you want to be informed when the reports are ready for download.

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