Thermal conductivity and thermal boundary resistance of diamond heat spreaders

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Thermal conductivity and thermal boundary resistance (TBR) of diamond heat spreaders

Challenges for thermal conductivity measurements. (5)

Time-domain thermoreflectance and thermo-optic phase spectroscopy. (4)

When is thermal boundary resistance (TBR) important? (7)

For a heat spreader we want the lateral thermal conductance, i.e., product of thermal conductivity and thickness (W/K), to be high

Can’t beat diamond for high isotropic thermal conductivity.

isotopically enriched single crystal diamond	3300 W/(m K)
single crystal diamond	2200
thick CVD diamond	1700
best diamond/metal-matrix composite	960
cubic SiC and BP	500
Si	140

Graebner (1992); Olson (1993); Weber (2008); Zheng (2018); Cheng (2022)

Vast phase space of measurement methods for thermal transport

Heat source

- Joule
- Peltier
- Absorption of EM radiation

Thermometer

- Electrical resistance
- Seebeck
- Infrared radiation
- Thermoreflectance (intensity)
- Optical index gradient
- Expansion/displacement

Temporal

- Steady-state (cw)
- Pulsed
- Step
- Modulated (ac)

Dimensionality

- Planar (1D), high and low aspect
- Radial (2D)
- 3D

Diamond is uniquely challenging because of the high thermal conductivity

Thermal resistance of the diamond is small compared to the contact resistances in the measurements (heaters, thermometers, heat sinks, transducer coatings)

- *Temperature drops in the diamond are small, resulting in large systematic errors (e.g., from black body radiation)*
- *Difficult to source and sink large heat currents*

Thermal diffusivity of diamond is large, $D = 1000$ mm^2/s.

- *Thermal diffusion times τ_D are short. For $L = 10$ mm, $\tau_D = 0.1$ sec; for $L = 0.3$ mm, $\tau_D = 0.1$ msec.*

Difficult (for most people) to fabricate precisely shaped samples needed for steady-state measurement.

Can be done of course but typically in a well-equipped laboratory with a lot of expertise.

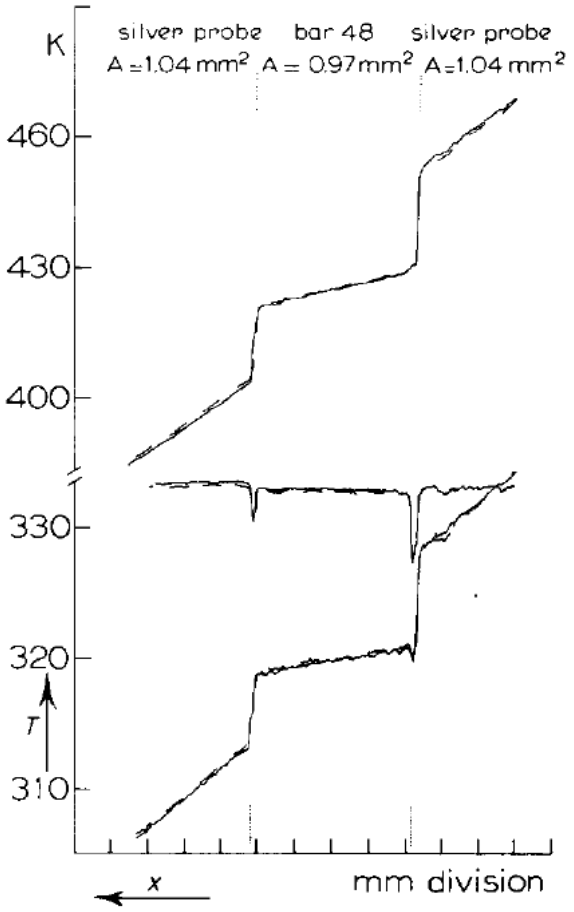
Berman (1975). Conventional longitudinal measurements on small cross-sectional area (1x1 mm^2) bar-shaped samples.

Bergmeister (1975). Heat flow meter on plate shaped using radiation thermometry to measure the temperature gradients in the heat flux sensor (Ag) and the diamond crystal. Small cross section (1x1 mm^2)

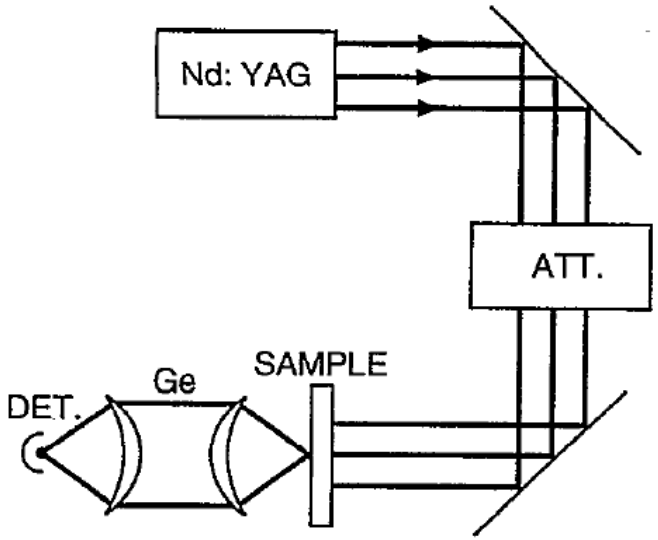
Graebner (1992). CVD diamond films. In-plane using evaporated metal heaters and thermocouples; cross-plane using flash-diffusivity with a Q-switched laser, a fast HgCdTe detector, and replacing the conventional graphite films with Ti metal films.

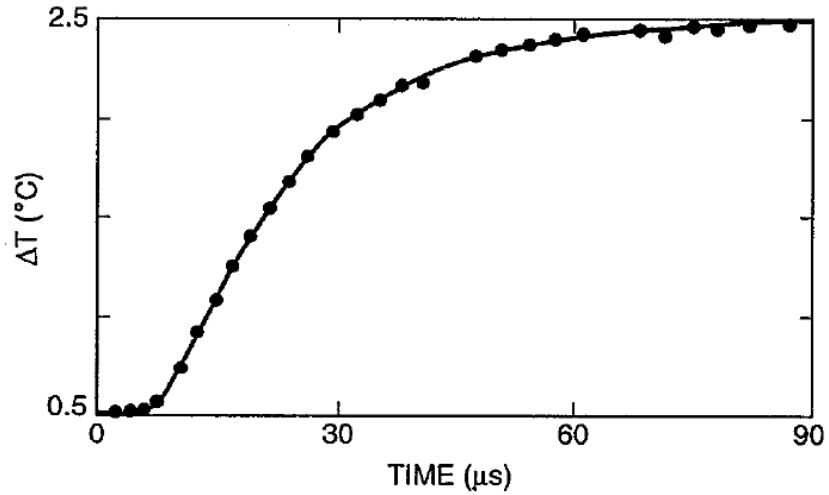
Can be done of course but typically in a well-equipped laboratory with a lot of expertise.

Bergmeister Ag-diamond-Ag



Graebner flash diffusivity



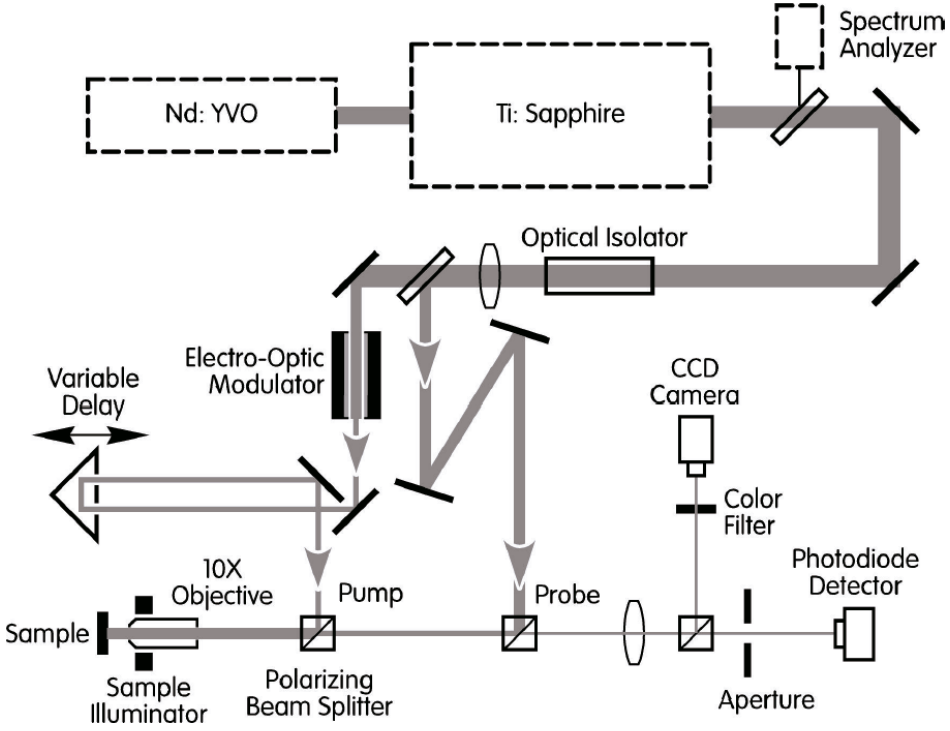


TDTR was developed to study interfaces and thin films but is also applicable to bulk crystals including diamond

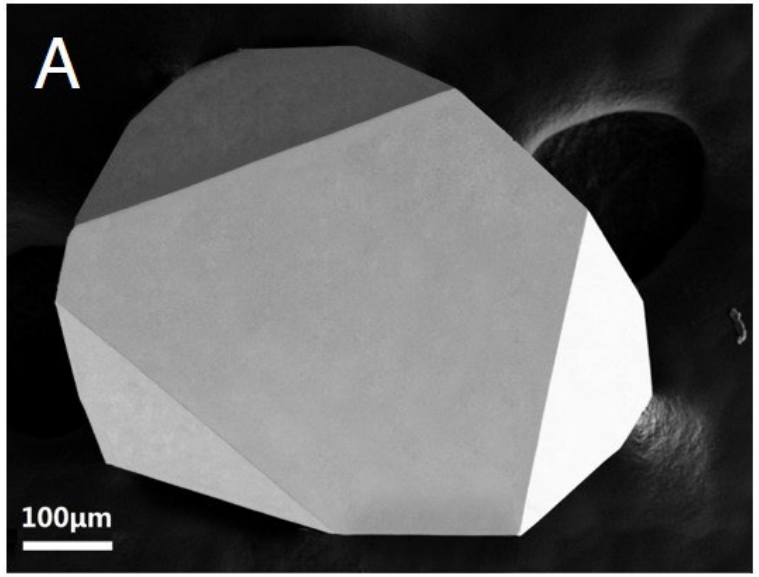
Time-domain thermoreflectance (TDTR) provides a near universal method for any sample with a smooth surface. Provides micron-scale spatial resolution.

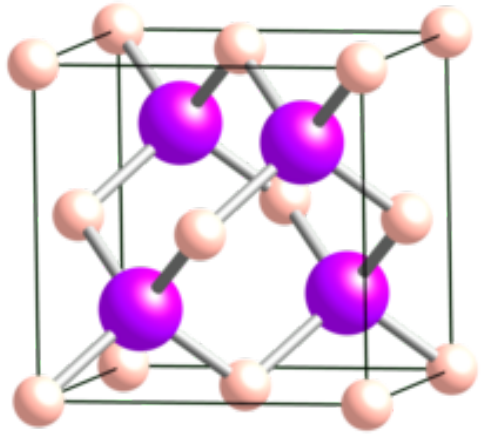
Expensive and requires significant training to collect and analyze data.

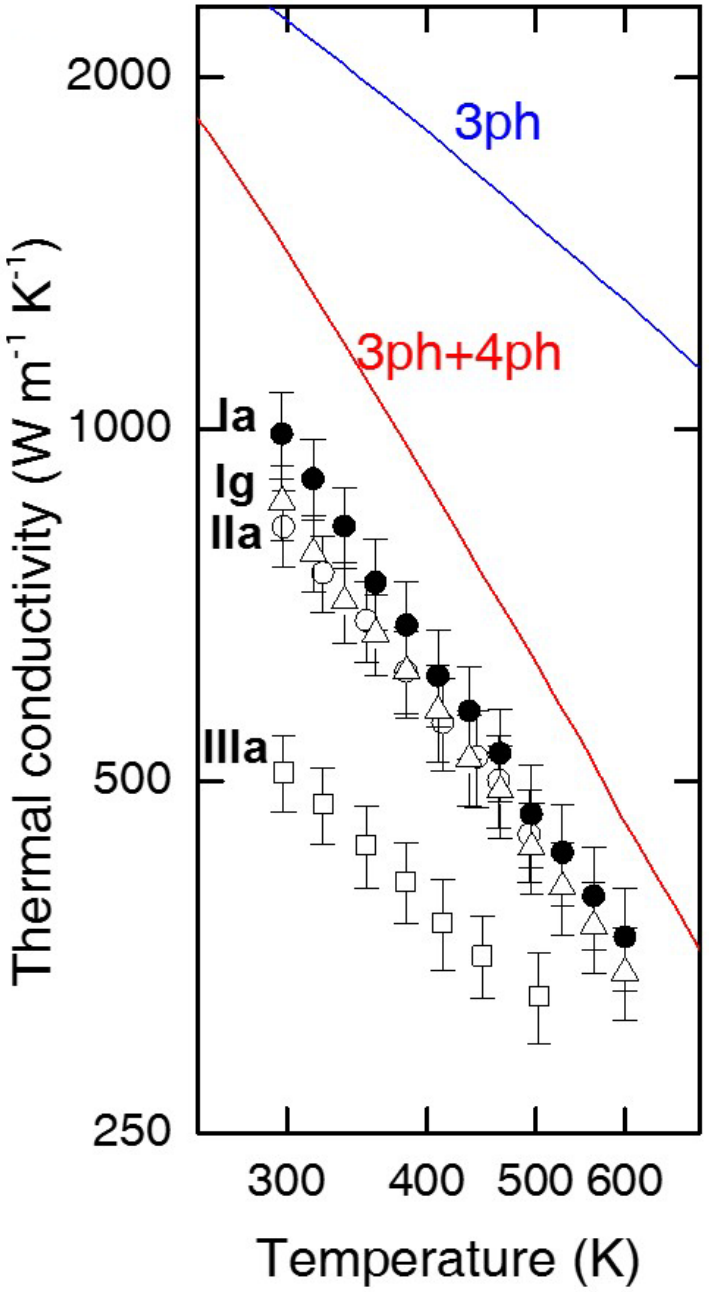
TDTR makes use of a combination of frequency domain and time domain responses that allow for good separation of the TBR of the transducer/sample interface and the thermal conductivity of sample. That separation is difficult to achieve in the pure frequency domain version (FDTR) or the near-steady-state version (SSTR).



Thermal conductivity of BAs is limited by four-phonon scattering







Li, Zheng *et al.*, *Science* (2018)

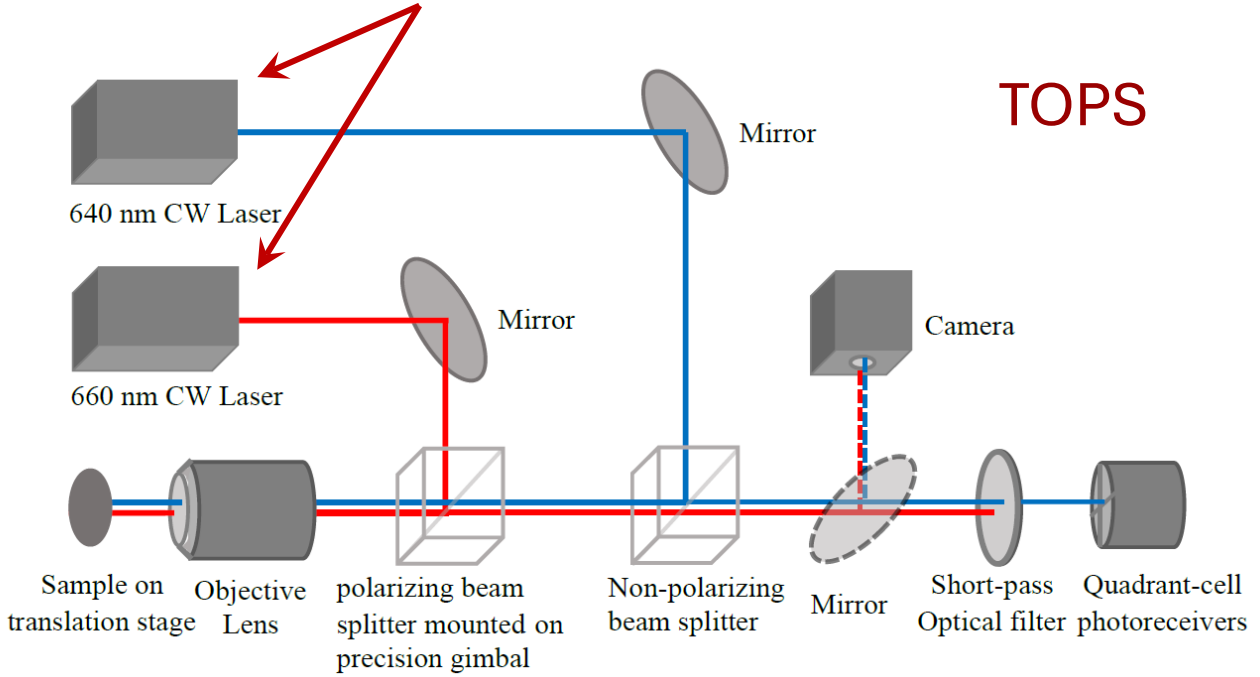
Thermo-optic phase spectroscopy (TOPS) uses essentially the same instrument as frequency-domain thermoreflectance (FDTR)

The photodiode used in FDTR is replaced by a quadrant photocell.

Advantages are higher signal-to-noise and less sensitivity to artifacts created by rough surface morphology.

Mostly sensitivity to in-plane thermal diffusivity. Need an independent measurement of heat capacity or effusivity.

Recently changed to fiber-coupled super-luminescent diodes to further reduce noise



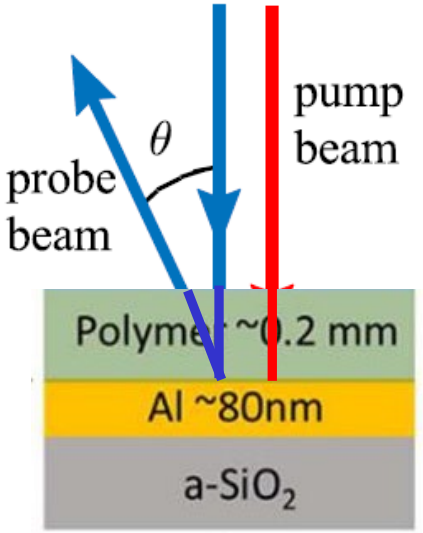
Lv et al. *ACS Applied Polymer Materials*, 2021a

Two main categories of TOPS: immersion-TOPS (mirage effect) and displacement-TOPS (photothermal displacement)

I-TOPS works well for transparent, i.e., fully amorphous polymers and liquids.

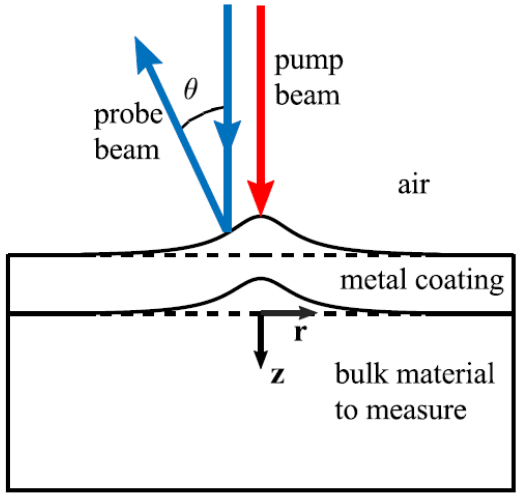
We also use I-TOPS with a known transparent material (liquid or elastomer) to study an unknown sample. We are pursuing this approach for high thermal conductivity materials and their TBR.

I-TOPS



D-TOPS is now our go-to method for bulk polymer samples and small inorganic crystals.

D-TOPS



Lv et al. *ACS Applied Polymer Materials*, 2021a
Sun et al. RSI, 2023; APL 2024

We typically want the thermal boundary resistance (TBR) to be low

TBR = 1/(thermal conductance per unit area).

lowest (Al/MgO at 60 GPa)	1 $(m^2 K)/GW$
intrinsic value for Al/diamond (at 5 GPa)	5
best direct-bonded interfaces to diamond	10
highest (Bi/H-terminated diamond)	140
For comparison:	
100 μm thick Si die	700
5 μm thick, 3 W/(m K) thermal interface material	1700

Costescu (2002); Lyeo (2006); Hohensee (2015); Wilson (2015); Cheng (2022)

Consider the system of a Si die bonded to diamond

How low of TBR is needed for the Si/diamond bond?

Need to consider the size and geometry of the heat source

3D: Gaussian heat source at the surface of a semi-infinite material, power P, radius w_0 , thermal conductivity κ. In steady-state

$$\Delta T \approx \frac{\mathrm{P}}{4\mathrm{w}_0\kappa}$$

2D: Gaussian heat source at the surface of a thin slab of thickness $h < \mathrm{w}_0$ with heat sink at a radial distance R from the source.

$$\Delta T \approx \frac{\mathrm{P}}{2\pi h\kappa}\ln\left(\frac{\mathrm{R}}{\mathrm{w}_0}\right)$$

Need to consider the size and geometry of the heat source

1D: Planar heat source of area A, semi-infinite materials does not have a steady-state. Temperature increases as $\sqrt{t}$. E is effusivity $\sqrt{\kappa C}$

$$\Delta T \approx \frac{\mathrm{P}\sqrt{t}}{\mathrm{A}E}$$

The next level of the thermal management is also critical: how is heat removed from the heat spreader?

Keep in mind the principles of linearity and superposition

If the temperature excursion is not too large (on an absolute scale), then the diffusion equation (or in steady-state Laplace's equation) is a linear differential equation.

The temperature excursion created by a sum of an ensemble of heat sources is the same as the sum of the temperature excursions created by the individual heat sources.

Convert TBR to characteristic lengths to provide insight on when TBR is important.

How thick of a piece of diamond (or Si, depending on the geometry) has the same thermal resistance as the interface? The materials physics community calls this the Kapitza length, L_K

$$L_K = \kappa(TBR)$$

The intrinsic value of L_K for an ideal strongly bonded interface is small, 15 μm in diamond or 1 μm in Si assuming TBR = 7 m^2-K/GW

For an isolated hot spot radius of radius $w_0 \ll L_K$, TBR dominates, and the high thermal conductivity of diamond does not help with thermal management.

What if the heat source is on the other side of the die?

Then we only need $L_K < h$ (h is the thickness of the die)

$$TBR < \frac{h}{\kappa} \approx \frac{100\ \mu\mathrm{m}}{140\ \left(\frac{\mathrm{W}}{\mathrm{m\ K}}\right)} \approx 700\ (\mathrm{m^2\ K})/\mathrm{GW}$$

A metallic thermal interface material with a thickness of a few microns should be sufficient

Fin-effect length scale for a heat spreader further relaxes requirements on TBR if the heat source is large

For 2D heat spreading (radius of heat source larger than Si thickness), the fin effect length gives us another view of what TBR is needed to take advantage of the high thermal conductivity of diamond.

$$L_f = \sqrt{(TBR)h\kappa}$$

We do not need for this length to be smaller than the size of the heat source, w_0. Use that condition as a criteria.

$$TBR < w_o^2/(h\kappa)$$

This relaxes the requirements on TBR by a large factor, the square of the ratio of the size of the heat source to the die thickness. Even a relatively thick metallic thermal interface materials (TIM) should be fine.

Concluding comments

- Accurate measurements of thermal conductivity of diamond heat spreaders are challenging. TDTR can provide spatially resolved measurements, including anisotropy, but requires a high level of expertise
- Thermo-optic phase spectroscopy has the potential of simplifying the measurements. (See also recent work by Prof. Amy Marconnet on dynamic infrared microscopy.)
- The geometry of the problem dictates what value of thermal boundary resistance (TBR) is needed for a diamond heat spreader to be an effective solution for thermal management.
- TBR dominates for isolated hot spots with a spatial extent smaller than the Kaptiza length, at best 15 microns in diamond.