## Supplementary Information:

# Depth Thermography: Noninvasive 3D Temperature Profiling Using Infrared Thermal Emission

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#### S1: Fourier-transform spectrometer (FTS) calibration

The measured thermal-emission signal is inevitably mixed with a background because every component of the FTS measurement system emits thermal radiation. The background could come from the instrument and the surrounding environment and can be sample-dependent. For example, there could be background emission from the room where the instrument is located that is reflected or scattered into the FTS beam path. In general, the measured signal from an emitter x can be expressed by the following expression:

$$S_x(\lambda) = m(\lambda)[I_x(\lambda) + B_x(\lambda)], \qquad (S1)$$

where  $I_x(\lambda)$  is the true emission spectrum from the emitter,  $B_x(\lambda)$  is the background emission, and  $m(\lambda)$  is the system response, including the collection efficiency of the setup and the responsivity of the detector. A non-scattering opaque emitter can only affect the background through reflection. In this case, we can write  $B_x(\lambda) = R_x(\lambda, T)B_1(\lambda) + B_2(\lambda)$ , where  $R_x(\lambda, T)B_1(\lambda)$  and  $B_2(\lambda)$  represent the sample-dependent and sample-independent contribution of the background emission, respectively. Therefore, Eq. S1 becomes the following for an opaque and non-scattering emitter:

$$S_{x}(\lambda) = m(\lambda)[I_{x}(\lambda) + R_{x}(\lambda, T)B_{1}(\lambda) + B_{2}(\lambda)].$$
(S2)

If all parts of the emitter that we are measuring are in thermal equilibrium (i.e., the entire emitter has a single uniform temperature), then the emission spectrum from the emitter can be written as:  $I_x(\lambda) = \epsilon_x(\lambda, T)I_{BB}(\lambda, T)$ , where  $\epsilon_x(\lambda, T)$  is the emissivity and  $I_{BB}(\lambda, T)$  is the blackbody spectrum at sample temperature *T* given by Planck's law. In this case, Eq. S2 becomes:

$$S_{\chi}(\lambda, T) = m(\lambda) [\epsilon_{\chi}(\lambda) I_{BB}(\lambda, T) + R_{\chi}(\lambda, T) B_{1}(\lambda) + B_{2}(\lambda)].$$
(S3)

Looking at Eq. S2, to extract the true emission signal  $I_x(\lambda)$  from the measured data  $S_x(\lambda)$ , one needs to determine  $m(\lambda)$ ,  $B_1(\lambda)$ ,  $B_2(\lambda)$  and  $R_x(\lambda)$ . The first three terms are related to the FTS and can be determined by measuring two known non-scattering, opaque references  $\alpha$  and  $\beta$ , whose emissivity and reflection coefficient do not change significantly with temperature, as follows:

#1: The system response function can be obtained from thermal emission measured from reference  $\alpha$  at two different temperatures  $T_1$  and  $T_2$ :

$$m(\lambda) = \frac{S_{\alpha}(\lambda, T_1) - S_{\alpha}(\lambda, T_2)}{\epsilon_{\alpha}(\lambda)[I_{BB}(\lambda, T_1) - I_{BB}(\lambda, T_2)]}$$
(S4)

#2: With the known system response function  $m(\lambda)$ , the total backgrounds for  $\alpha$  and  $\beta$  can be obtained from thermal emission measured at temperature  $T_1$  (or  $T_2$ ):

$$B_{\alpha}(\lambda) = \frac{S_{\alpha}(\lambda, T_{1})}{m(\lambda)} - \epsilon_{\alpha}(\lambda)I_{BB}(\lambda, T_{1})$$
(S5)

$$B_{\beta}(\lambda) = \frac{S_{\beta}(\lambda, T_1)}{m(\lambda)} - \epsilon_{\beta}(\lambda) I_{BB}(\lambda, T_1)$$
(S6)

#3:  $B_1(\lambda)$  and  $B_2(\lambda)$  can then be determined from  $B_{\alpha}(\lambda)$  and  $B_{\beta}(\lambda)$ :

$$B_1(\lambda) = \frac{B_\alpha(\lambda) - B_\beta(\lambda)}{R_\alpha(\lambda) - R_\beta(\lambda)}$$
(S7)

$$B_2(\lambda) = B_\alpha(\lambda) - R_\alpha(\lambda)B_1(\lambda)$$
(S8)

We measured thermal emission from polished wafers of fused silica and sapphire—known references to calibrate our measurements. We characterized the two references by measuring their emissivity  $\epsilon(\lambda)$  by taking the difference of emission at two temperatures (60 and 100 °C, where the emissivity of both fused silica and sapphire does not change) and normalizing to that of the blackbody reference:

$$\epsilon(\lambda) = \epsilon_{BB}(\lambda) \frac{S(\lambda, T_1) - S(\lambda, T_2)}{S_{BB}(\lambda, T_1) - S_{BB}(\lambda, T_2)}$$
(S9)

Their reflectances are obtained as  $R(\lambda) = 1 - \epsilon(\lambda)$  according to Kirchhoff's law [S1]. Note here at these low temperatures, the temperature gradient can be safely neglected. Figure S1(a) shows the measured raw (but Fourier-transformed) thermal-emission signal from wafers of sapphire and fused silica at 50 and 75 °C. In the measurement, the samples were tilted by 10° to avoid multiple reflections between the sample and the interferometer [S2]. The calibrated system response  $m(\lambda)$  and the backgrounds  $B_1(\lambda)$  and  $B_2(\lambda)$  are plotted in Fig. S1 (b, c). Note that our calculated  $B_2$  is negative because in our setup the constant background emission originates from components after the interferometer [S2]. Also note that the artificial peaks in  $B_1(\lambda)$  and  $B_2(\lambda)$  near 7 and 11  $\mu$ m come from the fact that the reflection of sapphire and fused silica are very close to each other near these two wavelengths, leading to sharp features. The calibrated values of  $B_1(\lambda)$  and  $-B_2(\lambda)$  can be well represented by thermal emission from room-temperature emitters with effective emissivity values of 0.95 for  $B_1$  and 0.94 for  $B_2$ , as shown by the dotted black curves in Fig. S1(c). The effective emissivity of  $B_1$  (0.95) is expected because the sample is placed inside a sample compartment in our FTS; the enclosure of the sample compartment can be approximately treated as a blackbody with emissivity close to unity [S3]. The effective emissivity of  $B_2$  (0.94) indicates that there is a significant amount of background after the interferometer in our FTS [S2].



Figure S1. (a): Measured thermal emission from polished wafers of sapphire (solid) and fused silica (dotted) at 50

(blue) and 75 °C (red). (b): Calibrated system response  $m(\lambda)$  of our FTS. (c): Calibrated  $B_1$  (purple) and  $B_2$  (cyan) of our measurement system. Dotted lines show the corresponding fitting of  $B_1$  and  $B_2$ .

#### S2. Reflectance measurement of the fused-silica window

As shown in Eq. S2, the reflection coefficient of the fused-silica window needs to be determined to obtain the true thermal-emission signal. The reflectance of the 1-mm fused silica was measured with our FTS using a reflective microscope objective with NA = 0.4. Figure S2 shows the measured reflectance at room-temperature, 200 and 300 °C. As shown here, the reflectance of fused silica changes with temperature [S4]. The peak between 8 and 10  $\mu$ m decreases as temperature increases, but the change in reflectance (and, we assume, all optical properties) is negligible away from the vibrational resonances.



Figure S2. Measured temperature-dependent reflectance of the 1-mm-thick fused silica.

Note that our microscope reflectance measurements were performed with an objective with NA = 0.4 centered around the normal, whereas our emission setup had NA = 0.05 centered around an angle of 10°. Despite these differences, the measured reflectance using the microscope setup is very close to the reflectance of the fused-silica window in the emission setup. This is because the averaged p- and s-polarized reflectance does not change within a small range of angles near the normal direction. To demonstrate this, we calculated the expected reflectance of 1-mm-thick fused silica using the optical properties extracted from spectroscopic ellipsometry measurement at 300 °C (Fig. S5). The polarization-averaged reflectance does not change appreciably with incident angle for angles less than  $25^{\circ}$ .



Figure S3. Calculated reflectance averaged over p- and s-polarization for the 1-mm-thick fused-silica window using the optical properties extracted from spectroscopic ellipsometry at 300 °C.

#### S3: Measuring surface temperature with a commercial infrared camera

To double check the surface temperature of the samples obtained by fitting the measured thermalemission spectra, we used a mid-infrared camera (FLIR A325sc with software from FLIR). Our infrared camera has a bandwidth from 7.5 to 13  $\mu$ m, where both the fused-silica window and the CNT blackbody reference are opaque [S5]. The infrared-camera software returns a map of temperature once a wavelength-integrated emissivity value is assigned in the camera software (we refer to this as  $\epsilon_{set}$ ).

To measure the surface temperature of both samples when heated by a 300 °C heater, we first heated both samples to 50 °C, putting the samples in firm contact with the heater stage. At 50 °C, the temperature gradient between the top and the bottom of these samples can be safely neglected, so we adjusted  $\epsilon_{set}$  such that the camera reading returns 50 °C. We found  $\epsilon_{set}$  of 0.89 for fused silica and 0.97 for the CNT blackbody led the camera software to return 50 °C [Figure S4(a) and (c)]. Then both samples were further heated up by setting the heater temperature to 300 °C. The corresponding temperature readings from the camera are shown in Figure S4(b) and (d). As shown here, the measurements from the infrared camera (surface temperature of 283.0 °C for the fused-silica window and 282.3 °C for the CNT blackbody) agree quite well with the values obtained by fitting the emission spectrum (surface temperature of 283 °C for fused silica and 282 °C for CNT blackbody, Fig. 3).

Note that the infrared-camera software also has several assumptions to aid in the temperature-extraction process, such as the surrounding temperature, the humidity and transmittance of the atmosphere, etc.



Figure. S4. Infrared camera image of the fused-silica window (a-b) and the CNT blackbody (c-d) when the heater temperature was set to 50 (left) and 300 °C (right). The color bar is the measured temperature, assuming  $\epsilon_{set}$  of 0.89 for fused-silica window and 0.97 for the CNT blackbody.

#### S4: Obtaining material properties from ellipsometry measurements

To extract the temperature from the measured thermal-emission spectrum, we needed precise values of  $n(\lambda)$  and  $\kappa(\lambda)$  of our sample at different temperatures. Therefore, we performed ellipsometry measurements on our fused-silica window with incident angles of 35, 45 and 55°, for free-space wavelengths from 4 to 15  $\mu$ m, at 50, 200 and 300 °C. The complex refractive indices were then extracted by fitting the raw data ( $\Psi$  and  $\Delta$ ), assuming an infinitely thick sample with uniform temperature. The assumption of uniform temperature is reasonable considering the limited temperature gradient and the anticipated modest change in  $n/\kappa$  as a function of temperature. Figure S5 shows the results, where the amplitude of the vibrational resonances near 9  $\mu$ m becomes slightly smaller and the resonance width becomes slightly broader as the temperature increases. Away from the vibrational resonances, the changes in n and  $\kappa$  from room temperature to 300 °C are negligible.



FIG. S5. Real (solid) and imaginary (dotted) parts of the refractive index of our 1-mm-thick fused-silica window, extracted using spectroscopic ellipsometry at room temperature (blue), 200 (green), and 300 °C (red).

#### S5: Detailed description of the temperature-extraction process

#### S5.1 Temperature extraction assuming no instrument limitations

In the ideal case without noise, the extraction of the temperature distribution from the thermal-emission spectrum is very robust because there is a unique combination of temperatures corresponding to a specific spectrum (*i.e.* there is a unique solution of Eq. 4). We demonstrate this point numerically here.

As in the main text, we consider a 1-mm-thick fused-silica window, assuming its temperature drops linearly from 300 °C at the bottom surface to 283 °C at the top surface, and calculate its corresponding thermal emission spectrum [Fig. S6(a)]. In the calculation, the 1-mm-thick fused silica was modeled as an 11-layer structure, with each layer having the same optical material properties, but different temperatures.

Then, we used the calculated emission values at 11 different wavelengths, and sent them into a nonlinear equation solver [lsqnonlin(fun,  $x_0$ ) in Matlab] to solve the 11 different temperatures. This solver starts at  $x_0$  and finds a minimum of the sum of squares of the functions in "fun", which is Eq. 4 in the main text. In solving temperature, we set an upper and lower bound of 330 and 250 °C, respectively. At first, all 11 spectral points were chosen in the opaque region of fused silica [black dots, Fig. S6(a) for  $\lambda > 8$   $\mu$ m]. In this case, the inversion process was only able to recover the temperature of the top layer [Fig. S6(b)], as expected. Then, all 11 spectral points were chosen in the semitransparent region [red dots, Fig. S6(a) for  $\lambda > 8 \mu$ m], and all 11 temperatures were easily recovered from the spectral data [Fig. S6(c)]. In this extraction process, we did not need to make any assumptions about the shape of the temperature distribution.



FIG. S6. (a): Calculated thermal-emission spectrum from a 1-mm-thick fused-silica window, assuming a linear temperature drop from 300 to 283 °C from the bottom surface to the top surface. (b) Recovered temperatures from the emission data taken from the opaque region [ $\lambda > 8 \mu$ m, black dots in (a)] of fused silica. (c) The same as (b) but using the semitransparent region [ $\lambda < 8 \mu$ m, red dots in (a)].

In the absence of noise, this inversion process works for arbitrary temperature profiles. As an example, the 1-mm-thick fused-silica window is assumed to have some arbitrary temperature distribution shown in Fig. S7(b). The corresponding thermal-emission spectrum is shown in Fig. S7(a). In this case, the nonlinear equation solver is still able to recover all the temperatures [Fig. S7(b)] from the calculated spectrum.



FIG. S7. (a): Calculated thermal-emission spectrum from a 1-mm-thick fused-silica window with an arbitrary temperature distribution along the vertical direction, as indicated by the green line in (b). Recovered temperature using the emission spectrum within the semitransparent spectral region of fused silica (red symbols).

#### S5.2 Temperature extraction in realistic experimental conditions with noise

In any experimental setting, the measured thermal-emission spectra are inevitably noisy. Extracting temperature distributions from noisy spectra is much more difficult. To demonstrate this, we calculated the emission spectrum with  $\Delta \lambda = 100$  nm and added random fluctuations with relative amplitude of 1% to each wavelength points of the exact spectrum [*i.e.*,  $I_{noisy}(\lambda_i) = I(\lambda_i)(0.99 + 0.2\text{rand})$ , where "rand" returns a uniformly distributed random number in the interval (0,1)], as shown in Fig. S8 (a). The extracted temperatures using the nonlinear equation solver [i.e., the temperature profile that returns the minimum error in Eq. 4] in the bounded region between 240 and 350 °C using the noisy spectrum are plotted using red crosses in Fig. S8(b). As shown here, the extracted temperatures are drastically different from the input. The reason behind this is that the one-to-one relationship between temperature and thermal-emission spectrum breaks down when noise is present. In this case, there is no exact solution to Eq. 4 and there are many possible combinations of temperatures resulting emission spectra that have similar error with respect to the noisy spectrum. The extracted temperature distribution from the nonlinear equation solver, which tries to find the minimum error of all these possible combinations in a certain temperature range, depends very sensitively on the exact value of noise.



FIG. S8. (a): Calculated thermal-emission spectrum from a 1-mm-thick fused-silica window assuming a linear temperature drop from 300 to 283 °C from the bottom surface to the top surface, as indicated by the green line in (b). 1% of random noise is added into each wavelength point of the spectrum (black dotted line; also see inset). (b): Recovered temperature profiles from the noisy emission spectra within the semitransparent region of fused silica. The extractions from emission spectra with different random noise are quite different from one another, and

from the input temperature distribution.

To further demonstrate this point, we generated the 1% random noise with a different random seed, and plotted the extracted temperatures using black circles in Fig. S8(b). The extracted temperatures look drastically different not only from the input linear distribution, but also from the temperatures extracted from the previous noisy spectrum with a different seed for the noise. Hence, extraction of temperature distribution from non-ideal thermal-emission spectra is not trivial.

One approach that enables a more robust temperature extraction is to use more spectral points (M) in the thermal-emission spectrum to solve the temperatures (N): i.e., M > N. One can understand why this works by considering the extreme case where there is an infinite number of wavelength points, but the noise level per point remains the same. In this case, the spectrum that minimizes the error in Eq. 4 would be the exact spectrum due to the random nature of the noise. If, on the other hand, M is not big enough, the spectrum that has the minimum error can be different from the exact spectrum. Hence the extracted temperature can be different from the actual temperature. In reality, the noise level increases as the resolution increases because a finite signal is divided into more wavelength, leading to an increase of the relative noise level. Here we assume such relative noise level does not change with the number of "bins" for simplicity.

To demonstrate this point, we consider a relatively simple case: a two-layer model. In this simple model, the 1-mm-thick fused-silica window is assumed to be at 280 °C for the top half and 290 °C for the bottom half, with an abrupt transition at the interface. The local emissivity of the top and bottom layers were calculated using the scattering-matrix method. Then we added random noise to the spectrum and performed a brute-force (exhaustive) sweep of different combinations of  $T_{top}$  and  $T_{bottom}$  to find the combination that returns the global minimum error:

$$Error(T_{top}, T_{bottom}) = \sum_{\lambda_1}^{\lambda_2} \{I_{noisy}(\lambda) - \bar{\epsilon}_{top}(\lambda)I_{BB}(\lambda, T_{top}) - \bar{\epsilon}_{bottom}(\lambda)I_{BB}(\lambda, T_{bottom})\}^2$$
(S10)

Error maps with four different random noise seeds and two different numbers of spectral points M are shown in Fig. S9. In Fig. S9,  $\lambda_1 = 4.8$  and  $\lambda_2 = 5 \ \mu m$  are fixed, and the wavelength points (*i.e.*,  $\lambda$  in Eq. S10) are picked uniformly between  $\lambda_1$  and  $\lambda_2$  with  $\Delta \lambda = 50$  nm for the top row and  $\Delta \lambda = 0.1$  nm for the bottom row. Therefore, only 5 different wavelength points were used to generate the top panels, while 2000 wavelength points were used to generate the bottom panels. The magnitude of the noise added here is 1% for each of the 5 and 2000 wavelength points [*i.e.*,  $I_{noisy}(\lambda_i) = I(\lambda_i)(0.99 + 0.2rand)$ ].

As shown from the top panels in Fig. S9, the combination of  $T_{top}$  and  $T_{bottom}$  that returns the minimum error changes significantly when different random noise is added to the exact spectrum. This is because only 5 wavelength points are used. On the other hand, if enough wavelength points are used (bottom figures of Fig. S9), the combination of  $T_{top}$  and  $T_{bottom}$  that returns the minimum error overlaps with

the input temperature and does not change when different random noise is added on top of the exact spectrum. Such temperature extraction is very robust.



FIG. S9. (a-d): Distribution of  $\log_{10}(Error)$  for different values of  $T_{top}$  and  $T_{bottom}$  from Eq. S9 (with  $\lambda_1 = 4.8$ ,  $\lambda_2 = 5 \ \mu m$  and  $\Delta \lambda = 50$  nm so that M = 5) for the same level of random noise per wavelength but with different random seeds. The temperatures that generate the exact spectrum are marked with red crosses. (e-h): same as (a-d) but with  $\Delta \lambda = 0.1$  nm and M = 2000.

One can do similar analysis for more complicated cases, such as with three or more layers. As the layer number increases, the number of unknown temperatures that needs to be determined increases. Consequently, the number of wavelength point needed for robust temperature extraction for a fixed amount of noise per wavelength point increases as well. In other words, temperature extraction from a noisy spectrum must sacrifice resolution with robustness in the case of limited number of wavelength points. For the experimentally measured thermal-emission spectrum from the fused-silica window, we have about 450 wavelength points with a noise level of about 1% per wavelength point. We found that robust temperature extraction is possible for the experimental data assuming four layers [Fig. 4(c)]. When more layers are included (i.e., assuming a 5 or more-layer structure for the fused-silica window), temperature extraction becomes much more challenging.

One way to make temperature extraction much more robust without improving the experimental data is to put constraints onto the potential temperature distributions. For example, some functional form with a few parameters can be assumed to describe the temperature vs. depth. In this case, instead of solving for N unknown independent temperatures, only the parameters of the assumed functional form need to be determined.

One example demonstrated in the main text is the case of a piece of fused silica on top of a heater. Assuming no radiative heat transfer, Fourier's law of heat conduction tells us that the temperature profile inside the fused silica is a linear function of depth when it is in a steady state:

$$T(z) = T_{top} + \alpha z \tag{S11}$$

Therefore, only two parameters need to be determined:  $\alpha$  and  $T_{top}$ . As shown in [Fig. 4(c)], the

extracted temperature from the experimental spectrum after making the assumption in Eq. S11 is very close to the true value.



FIG. S10. (a): Calculated thermal-emission spectrum from a 1-mm-thick fused-silica window assuming a Gaussian temperature distribution along the depth direction, as indicated by the green line in (b). 1% of random noise is added into each wavelength points ( $\Delta \lambda = 12.5$  nm) of the exact spectrum [*i.e.*,  $I_{noisy}(\lambda_i) = I(\lambda_i)(0.99 + 0.2\text{rand})$ ] (black dotted line). (b): Recovered temperature profiles with different seeds of 1% random noise are shown by different markers.

As a further demonstration of this approach, we consider the case of Gaussian-like temperature distribution. Such a temperature distribution may be found in active devices such as the light-emitting diodes (LEDs) [S6] and quantum cascade lasers [S7], [S8]. Due to the electron-hole recombination process, the active layer of such devices is expected to be much hotter than the surrounding regions. As a numerical example, a 1-mm-thick fused silica window is assumed to have a Gaussian distribution in the depth direction:

$$T(z) = T_{top} + \alpha e^{-(z-z_0)^2/\beta}$$
(S12)

An input temperature distribution with the following parameters was assumed for the fused-silica window:  $T_{top} = 300$  °C,  $\alpha = 50$  °C,  $z_0 = 0.4$  mm, and  $\beta = 0.06$  mm<sub>2</sub>. The temperature distribution is shown using the green line in Fig. S10(b) and the corresponding thermal-emission spectrum is shown using the green line in Fig. S10(a). In the calculation, we picked  $\lambda_1 = 4.8$  and  $\lambda_2 = 10 \ \mu m$ , with  $\Delta \lambda = 12.5$  nm, so there were total of ~400 wavelength points. 1% of random noise was added onto each wavelength points of the calculated exact emission spectrum [*i.e.*,  $I_{noisy}(\lambda_i) = I(\lambda_i)(0.99 + 0.2rand)$ , black dotted line in Fig. S10(a)] and the noisy spectrum was then sent into the nonlinear equation solver to extract the temperature profile. In the extraction, even though the fused-silica window was divided into 11 layers, only 4 parameters needed to be determined. As shown in Fig. S10(b), the extracted temperature profile is very robust against noise, as the extraction does not change too much when the same level of noise with different random seeds was added into the spectrum.

#### S6: Simultaneous extraction of temperature and refractive index

In this section, we show numerically that our method can be extended to extract both temperature and refractive index of multiple layers from thermal-emission spectra. The basic idea is related to optical ellipsometry, but with no external light source: the optical material properties (n and  $\kappa$ ) and temperature can be extracted from the thermal emission spectra at different angles and in different polarization states. Here we consider a numerical example of a three-layer structure sitting on top of a heated surface, as shown in Fig. S11.



Fig. S11: Schematic of the test system for demonstration of simultaneous extraction of refractive index and temperature from thermal-emission spectra at multiple angles and in multiple polarization states.

Here, the heater is assumed to comprise aluminum at a temperature of  $T_0 = 573$  K (selected arbitrarily). We assumed that each layer in the three-layer structure has a thickness of 100 nm ( $d_1 = d_2 = d_3 = 100$  nm), each with different *n*,  $\kappa$ , and *T*. To demonstrate the retrieval of these parameters, we consider for simplicity the use of the thermal-emission spectrum at 11 different wavelengths ( $\lambda_i$ , i = 1, 2, ..., 11). Please note that we chose this number of wavelengths as a demonstration; using a higher-resolution spectrum would provide even more information and can, in principle, result in more-precise retrieval of the unknown parameters.

There are a total of 69 unknowns for this system  $(n_{1i}, \kappa_{1i}, n_{2i}, \kappa_{2i}, n_{3i}, \kappa_{3i}, \text{ with } i = 1, 2, ...11$ representing 11 wavelengths, and  $T_1, T_2, T_3$ ). In order to solve for these 69 unknowns, we assume that we need at minimum 69 equations of the following type:

$$I^{s,p}(\lambda_i,\theta_k) = \sum_{j=1}^3 \bar{\epsilon}^{s,p}{}_j(\lambda_i,\theta_k) I_{BB}(\lambda_i,T_j)$$
(S13)

Eq. (S13) is adapted from Eq. (4) in the main manuscript. Note that the effective emissivity of each layer for both s- and p-polarization  $\bar{\epsilon}^{s,p}{}_{j}(\lambda_{i},\theta_{k})$  is a function of  $n_{i}$  and  $\kappa_{i}$  for all three layers. For each specific angle and polarization state, we have thermal emission at 11 different wavelengths. Therefore, we can use the 'measured' thermal emission in the s- and p-polarizations from four different angles, which gives us a total of 88 known emission data points to solve the 69 unknowns.

To see how this works, we assigned random values of n (uniformly chosen between 1 and 4) and  $\kappa$  (uniformly chosen between 0.1 and 0.5) to three different layers at 11 wavelengths (here we choose 4,

4.5, 5, ..., 9 micron). For simplicity, we assumed no relationship between *n* and  $\kappa$ , though in reality there must be a relationship, as encoded in the Kramers-Kronig relations. We assigned three randomly selected values of temperatures (uniformly chosen between 500 and 600 K) to these three layers. One example of the input parameters is shown in Tab. S1. The s- and p-polarized thermal-emission spectra from this structure at four different angles (arbitrarily chosen) were calculated using Eq. (S13)—this is the forward calculation. The resulting thermal-emission spectra for emission angles of 10, 25, 45, and 50° for both s- and p-polarization are plotted in Fig. S12.

	<i>n</i> <sub>1</sub>	κ <sub>1</sub>	<i>n</i> <sub>2</sub>	κ2	$n_3$	κ3		
$\lambda_1$	2.62	0.47	1.62	0.12	1.66	0.34	$T_1$	529
$\lambda_2$	1.98	0.16	1.29	0.44	3.24	0.17	$T_2$	540
:	:	:	:	:	:	:	$T_3$	586
$\lambda_{11}$	1.68	0.23	2.05	0.33	1.86	0.43		

Table S1: One example of input parameters, including real (*n*) and imaginary ( $\kappa$ ) parts of the refractive index for three different layers at three of the 11 different wavelengths (remaining input parameters not shown for brevity), and temperatures for the three layers in Kelvin.



Fig. S12: Forward calculation. Calculated thermal-emission spectra at emission angles of 10, 25, 45, and 50° for both s- and p-polarizations for the structure in Fig. S11 using the material and thermal parameters in Tab. S1.

To set up the inversion process, the forward calculation was formulated into a function with 69 variables (33 pairs of  $(n, \kappa)$  and three temperatures). Then, these 69 unknowns were solved using the forward-calculated thermal-emission spectra shown in Fig. S12 as the input for the function using the nonlinear equation solver "fsolve" in Matlab. The output of this inversion is shown in Tab. S2, which verifies fully recovering both the refractive index and temperature. At this step, we assumed that the thermal-emission spectra were perfectly known, with no uncertainty.

	<i>n</i> <sub>1</sub>	κ1	n <sub>2</sub>	κ2	$n_3$	κ3		
$\lambda_1$	2.62 <mark>(2.39)</mark>	0.47 <mark>(0.44)</mark>	1.62 <b>(1.53)</b>	0.12 <mark>(0.11)</mark>	1.66 <mark>(1.71)</mark>	0.34 <mark>(0.32)</mark>	$T_1$	529 <mark>(530)</mark>
$\lambda_2$	1.98 <mark>(2.11)</mark>	0.16 <mark>(0.18)</mark>	1.29 <mark>(1.29)</mark>	0.44 <mark>(0.40)</mark>	3.24 <mark>(3.23)</mark>	0.17 <mark>(0.15)</mark>	$T_2$	540 <mark>(543)</mark>
:	:	:	:	:	:	:	$T_3$	586 <mark>(592)</mark>
$\lambda_{11}$	1.68 <mark>(1.81)</mark>	0.23 <mark>(0.25)</mark>	2.05 <mark>(2.20)</mark>	0.33 <mark>(0.36)</mark>	1.86 <mark>(1.75)</mark>	0.43 <mark>(0.41)</mark>		

Table S2: Extracted *n*,  $\kappa$ , and *T* using the exact thermal-emission spectra in Fig. S12. The numbers in parentheses (red) are the extracted values when the noise-added spectra in Fig. S12 were used. In the extraction, restrictions were added to *n* and  $\kappa$  such that they were only solved in a range that is within 10% of their input values.

We tested this process by using different combinations of randomly selected material properties (n and  $\kappa$ ) and layer temperatures (T). Each time, the nonlinear solver could fully and uniquely recover the values of n,  $\kappa$ , and T using the corresponding thermal-emission spectra from four different angles and two polarization states. Although we have not proven here the unique relationship between the n,  $\kappa$ , T and the corresponding thermal-emission spectra, these numerical tests appear to indicate the one-to-one relationship between the thermal-emission spectra and the features of the material system (n,  $\kappa$ , and T).

Similar to the situation of extracting temperature with known optical material properties (the effective emissivities), the noise in the measured emission spectrum makes the extraction of n,  $\kappa$ , and T less robust. Much more robust extraction can be achieved if we have some (even if imprecise) prior knowledge of the refractive index of the materials in the sample. It is easy to imagine many practical situations where the refractive indices of the materials in a test system are known approximately, but not precisely. In the following, we demonstrate temperature extraction from noisy spectra with imprecisely known refractive index values.

Like before (Fig. S11), we are exploring a three-layer structure and using the emission spectrum sampled at 11 different wavelengths. As one example, we used the initial input parameters in Tab. S1. The calculated thermal-emission spectra in Fig. S12 were modified with the addition of random noise with magnitude that is 1% of the spectra power [i.e.,  $I_{noisy}(\lambda_i) = I(\lambda_i)(0.99 + 0.2\text{rand})$ , where "rand" returns a uniformly distributed random number in the interval (0,1)]. The 1% of noise level is similar to our current measurement for each wavelength.

The noisy spectra generated from the exact forward-calculated spectra were used to perform the inversion process. In this process, we constrained the possible n and  $\kappa$  to be within a range of their actual values—in essence, we assumed that we knew the approximate values of n and  $\kappa$ , but we did not know them precisely. This is quite realistic: often, literature values of n and  $\kappa$  are known but do not fully represent the actual materials in the sample, or perhaps materials characterization was performed at one temperature but the n and  $\kappa$  have some temperature dependence. In one example, we restricted the solution of n and  $\kappa$  to be within 10% of the input values shown in Tab. S1. The outputs of the extraction process are shown by the red numbers in parentheses in Tab. S2. Note here, we still used the nonlinear equation solver "fsolve" in Matlab, which may be a non-ideal way of solving this problem.

The extracted temperature values depend on the initial input values for n,  $\kappa$ , and T, as well as the random noise. Therefore, to test the dependence of the robustness of temperature extraction on the uncertainty in material properties, we performed a series of simulations using different combinations of randomly selected input parameters (n,  $\kappa$ , and T) and, for each set of input parameters, the corresponding thermal-

emission spectra were modified by adding different sets of random noise at the same noise level. Finally, the temperature extraction error  $|(T_{extracted} - T_{input})/T_{input}|$  was obtained by taking the average value of these simulations. We tested the method using different numbers of wavelengths in the "measured" spectrum and different magnitudes of uncertainties in the values of *n* and  $\kappa$  of the layers. The results for four different angles and a 1% noise level for each wavelength in the emission spectra are shown in Tab. S3. As expected, the extraction error increases when the uncertainty in *n* and  $\kappa$  increases, while it decreases when the number of wavelengths increases. For the case of 11 wavelengths, robust temperature extraction (extraction error < 1%) can be achieved for a 10% of uncertainty in materials properties *n* and  $\kappa$ , and 1% of noise level in the emission spectra.

Number of wavelength	Uncertainty in n and κ (%)	Averaged extraction error(%)
3	1	1.64
3	5	3.55
3	10	5.62
5	1	0.55
5	5	2.29
5	10	2.75
11	1	0.33
11	5	0.81
11	10	0.96

Tab. S3: Averaged temperature-extraction error for different combinations of the number of "measured" wavelengths in the emission spectrum and the uncertainty level in n and  $\kappa$ .

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