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Calculated Transmission Using a Portable Spectroreflectometer

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LIST OF ACRONYMS

AO	atomic oxygen
ASTM	American Society for Testing and Materials
LPSR	laboratory portable spectroreflectometer
UV	ultraviolet

NOMENCLATURE

a	ρ_{mirror}
b	$\rho_{\mathrm{sample}}\rho_{\mathrm{mirror}}$
c	$\rho_{\mathrm{sample}}-x$
s	solar
x	reflectance of sample measured with reflective backing
α_{mirror}	solar absorptance of reflective backing
α_{s}	solar absorptance
α_{sample}	absorptance of sample with blackbody backing
α_{x}	absorptance of sample with reflective backing
ε	thermal emittance
ρ	reflectance
ρ_{gold}	reflectance of gold puck
ρ_{mirror}	reflectance of reflective backing
ρ_{sample}	reflectance of sample measured with blackbody backing, proportion transmitted by sample
τ	transmission
τ_{s}	solar transmittance
τ_{sample}	proportion transmitted through sample

TECHNICAL PUBLICATION

CALCULATED TRANSMISSION USING A PORTABLE SPECTROREFLECTOMETER

1. INTRODUCTION

Under normal circumstances, a spectrophotometer is used to measure transmission of material samples. However, a sample may be too large to fit into the spectrophotometer chamber, or a field inspection may be required. This Technical Publication describes the procedure for using measurements made with a portable spectroreflectometer to calculate transmission. A similar procedure is used to calculate infrared transmission using measurements from a portable infrared reflectometer.

2. TEST SETUP

A variety of materials were chosen for both direct transmission measurements and reflectance measurements, including narrow-band filters, clear polymer films, clear polymer films with coatings (particularly ones with interference patterns), polymer films made translucent by atomic oxygen (AO) erosion, and window materials. An example of field inspection was using the portable spectroreflectometer to measure transmission of various materials used in the International Space Station Microgravity Science Glovebox ground unit. These measurements were made prior to installing light-emitting diodes of 275-nm wavelength for sterilization of the flight unit. For astronaut safety, transmission measurements of the work volume materials were needed to ensure that no harmful amount of ultraviolet (UV) radiation would be transmitted through the Lexan shield.

Direct transmission measurements were made with a PerkinElmer® LAMBDA 1050 spectrophotometer (fig. 1). The LAMBDA 1050 is a double-beam, double-monochromator, ratio-recording spectrophotometer usually operated in the 200- to 2,400-nm wavelength range. The integrating sphere is 150 mm in diameter and can accommodate 6-by-6-in samples up to 1 in thick. Thicker-yet-smaller samples have been measured. The LAMBDA 1050 is capable of spectral resolution from 0.05 to 5 nm in the UV and visible wavelengths and spectral resolution from 0.2 to 20 nm in near infrared. For these measurements, a 5-nm interval was chosen.

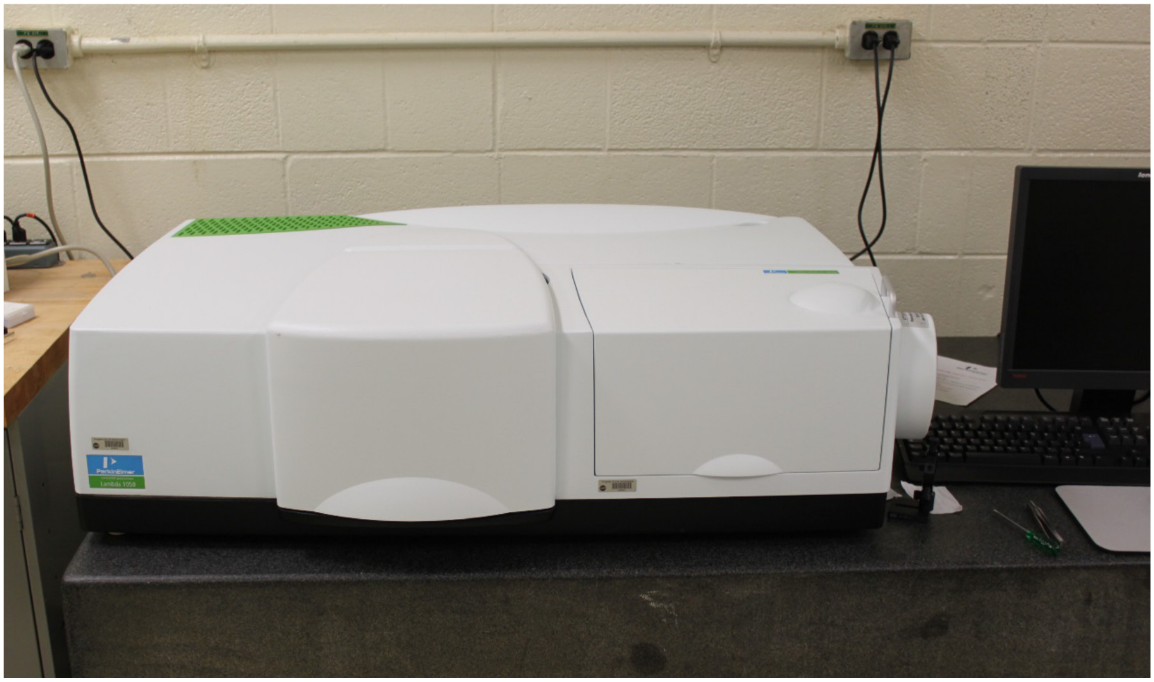

Figure 1. PerkinElmer spectrophotometer.

Reflectance measurements were made with an AZ Technology Laboratory Portable Spectroreflectometer (LPSR) model 300 (fig. 2). The automated program for measuring solar absorptance utilizes 100 measurements between 250 and 2,800 nm for meeting reference 1. The solar absorptance calculation performed by the LPSR software uses reference 2. Air mass 0 is the extraterrestrial solar spectrum. From the LPSR 300 reflectance data, it is possible to determine solar absorptance for other air mass values.

Figure 2. AZ Technology LPSR.

One of the operator options is the Table200 dataset, which toggles the machine to make 200 measurements between 250 and 2,800 nm. The field inspection was performed with the 100-data point option; the laboratory measurements were with the 200-data point option to improve resolution. The need to minimize stray light during spectroreflectometer measurements must be strongly emphasized.

3. TRANSMISSION FROM REFLECTANCE MEASUREMENTS: LPSR 300 PROCEDURE

Two measurement runs were made for each sample—the first with a highly reflective backing and the second with a highly absorptive backing (fig. 3). Either a magnesium fluoride/aluminum mirror or a 3-by-3-in square of double-aluminized DuPont™ Kapton® was used for the reflective backing. The double-aluminized Kapton was preferred because of first surface reflection. Either a blackbody or a nonreflective 'velvet' made of 5% carbon fiber in elastomer (product of Energy Science Laboratories, Inc.) was used for the absorptive backing. Transmission is calculated using the formula:

$$\tau = \frac{1}{2}\left[-\rho_{\text{sample}} + \sqrt{\frac{4x - 4\rho_{\text{sample}} + \rho_{\text{mirror}}\rho^{2}_{\text{sample}}}{\rho_{\text{mirror}}}}\right] \tag{1}$$

where

τ = transmission
ρ_{sample} = reflectance of sample measured with blackbody backing
x = reflectance of sample measured with reflective backing
ρ_{mirror} = reflectance of reflective backing.

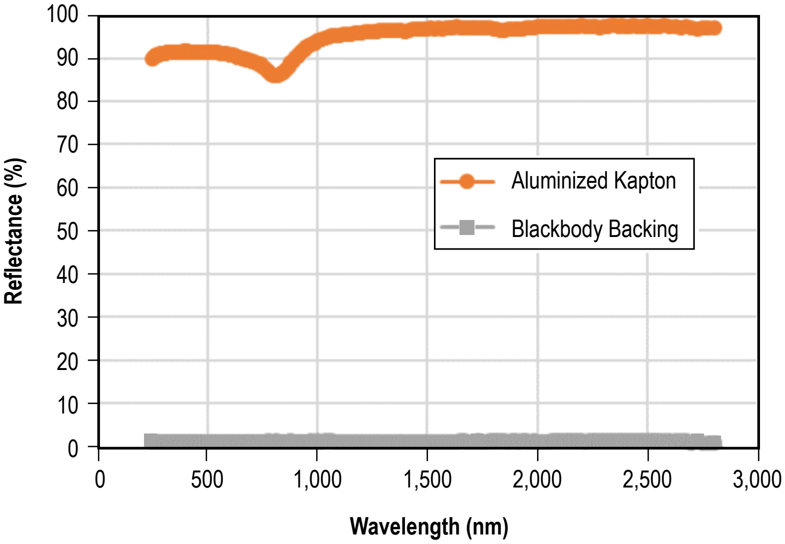

Figure 3. Typical backing material reflectance.

Note that the solar absorptance calculated by the LPSR 300 software from the measured total hemispherical spectral reflectance measurements assumes an opaque sample. Do not report this value if your sample is transparent. Instead, subtract this from 1 to determine the reflectance terms used in the transparency calculations. When determining the ratio of solar absorptance to thermal emittance, α_s/ε, use the integrated reflectance measurements from the LPSR 300 and the TEMP 2000A.

In the actual application, if the sample will be applied over another material, this approach should not be used; but rather, the sample should be measured with an appropriate backing. That is, the sample material should be applied over the substrate in the same manner as it will actually be utilized. For example, if the film were to be applied over an aluminum alloy, then the film should be measured with that backing and the absorptance reported as measured. For example:

LPSR 300 Test Data

(1) Measured total absorptance of sample, α_{sample}, with blackbody backing (not correct because of transparency): 0.9.

(2) Measured total absorptance of sample α_x with reflective backing: 0.05.

(3) Solar absorptance of reflective backing α_{mirror}: 0.015.

Note that the reflectance terms for the equation are determined as follows:

- Solar reflectance:

$$\begin{aligned}\rho_{\text{sample}} &= 1-\alpha_{\text{sample}} \\ &= 1-0.9 \\ &= 0.1.\end{aligned} \tag{2}$$

- Backed reflectance:

$$\begin{aligned}\mathrm{x} &= 1-\alpha_x \\ &= 1-0.050 \\ &= 0.950.\end{aligned} \tag{3}$$

- Reflectance of backing:

$$\begin{aligned}\rho_{\text{mirror}} &= 1-\alpha_{\text{mirror}} \\ &= 1-0.015 \\ &= 0.985.\end{aligned} \tag{4}$$

Calculate the solar transmittance, τ_s:

$$\tau_s = \frac{1}{2}\left[-\rho_{\text{sample}} + \sqrt{\frac{4x - 4\rho_{\text{sample}} + \rho_{\text{mirror}}\rho^2{}_{s}}{\rho_{\text{mirror}}}}\right] \tag{5}$$

$$\tau_s = \frac{1}{2}\left[-0.1 + \sqrt{\frac{(4)(0.95) - (4)(0.1) + (0.985)(0.1)^2}{0.985}}\right]$$

$$= 0.88029$$

Calculate the solar absorptance, α_s:

$$\alpha_s = 1 - \rho_{\text{sample}} - \tau_s \tag{6}$$

$$= 1 – 0.1 – 0.88$$

$$= 0.020.$$

4. COMPARISON OF METHODS

A variety of materials were measured using both PerkinElmer LAMBDA 1050 and AZ Technology LPSR 300 instruments. The measured data are direct measurements of transmission using the PerkinElmer spectrophotometer, and the calculated data uses the LPSR data reduced to transmission using equation (1). The results are presented in this section.

4.1 Narrow-Band Filter

This UV-bandpass filter (fig. 4) has an additional small peak of approximately 2% transmission around 710–730 nm that does get lost in the noise of the LPSR measurements. The difference of the main peak is approximately 3%.

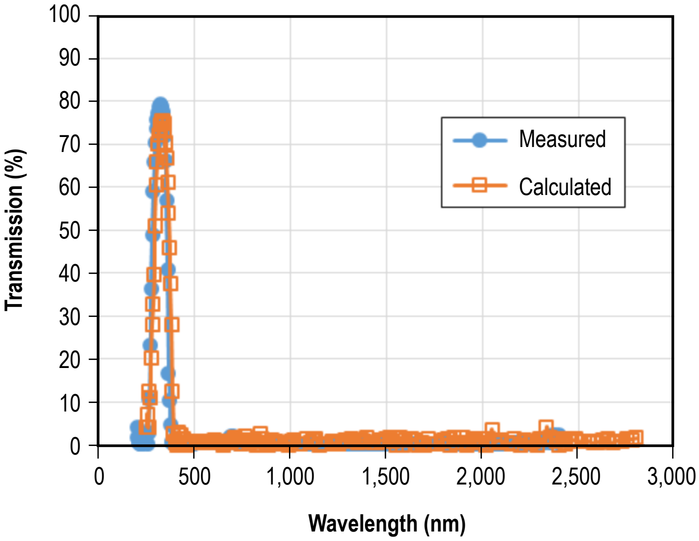

Figure 4. Narrow-bandpass filter.

4.2 Clear Polymer Films

Measurements were made on NeXolve Optinox® (fig. 5) and CORIN® (fig. 6) polymer films. The calculated transmission showed good agreement with the measured transmission.

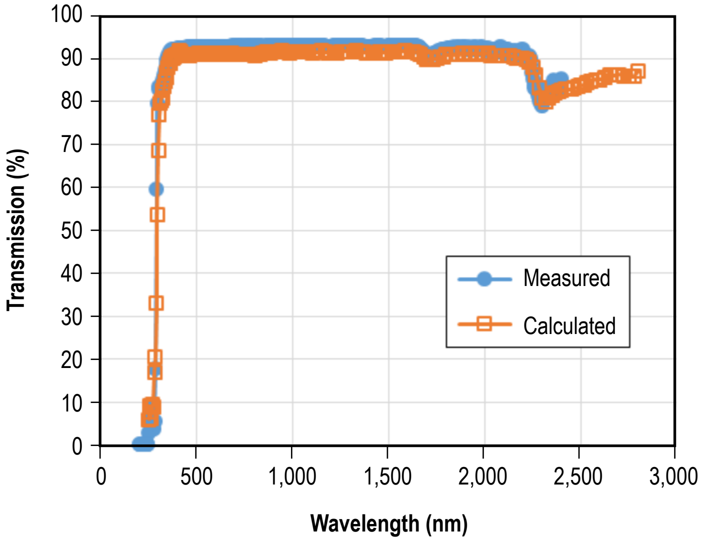

Figure 5. Optinox polymer film.

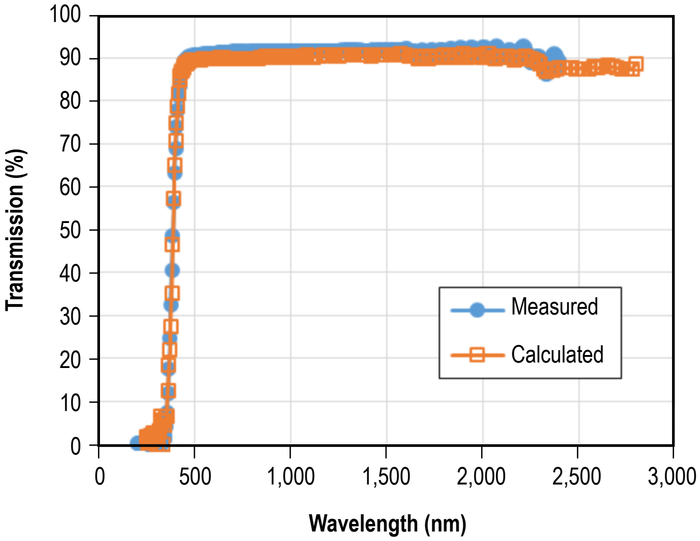

Figure 6. CORIN polymer.

4.3 Clear Polymer Films With Coatings

Measurements were made on NeXolve Optinox (fig. 7) and CORIN (fig. 8) polymer films coated with cerium oxide. The interference pattern seen in the coated CORIN is better defined by the directly measured transmission and demonstrates the difficulty in calculating transmission for multilayer materials.

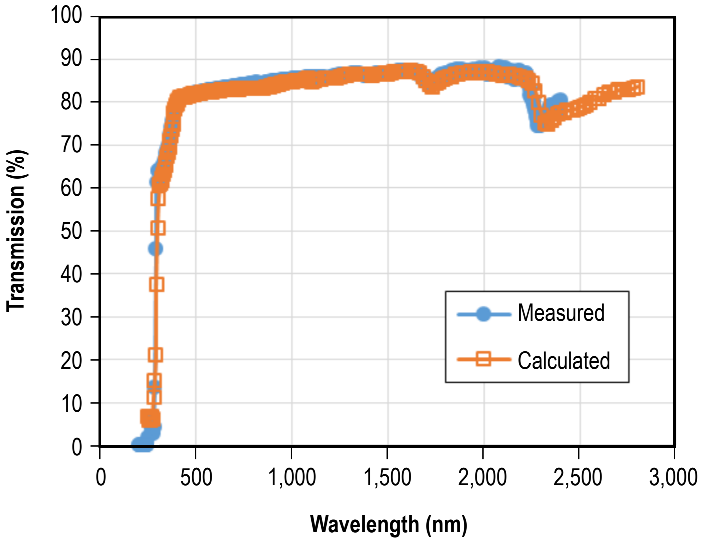

Figure 7. Optinox with cerium oxide coating.

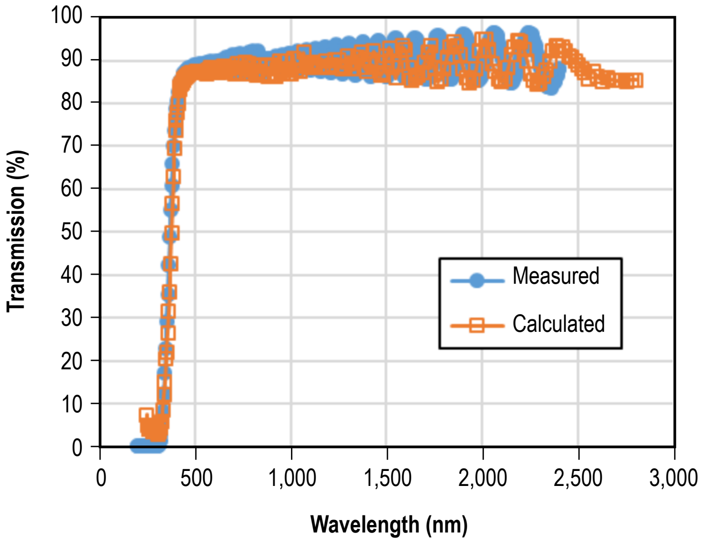

Figure 8. CORIN with cerium oxide coating.

4.4 Polymer Films Etched by Atomic Oxygen

The same films in the previous section were exposed to a fluence of 9.8×10^{20} atoms/cm^2 simulated AO in NASA Marshall Space Flight Center's Atomic Oxygen Beam Facility. The AO erosion resulted in a 'fogged' appearance of the samples and lower, flatter transmission curves (figs. 9, 10). Atomic oxygen increases surface texturing, which increases light scatter from the sample surface and reduces the light transmitted.

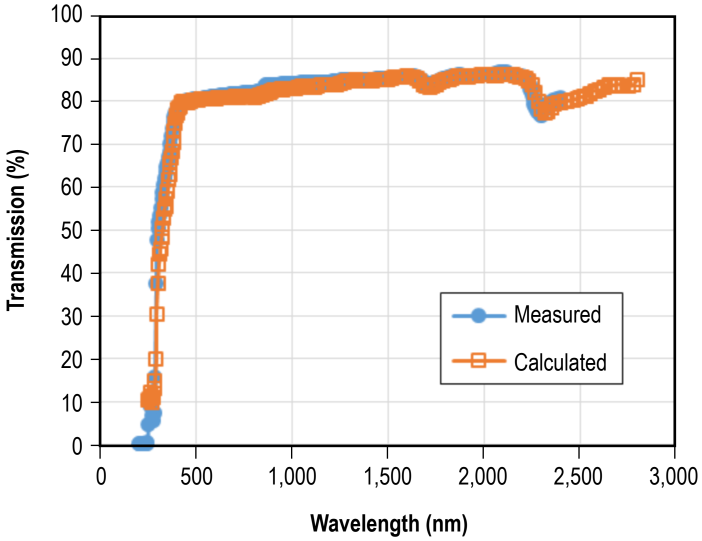

Figure 9. Optinox coated with cerium oxide and eroded by AO.

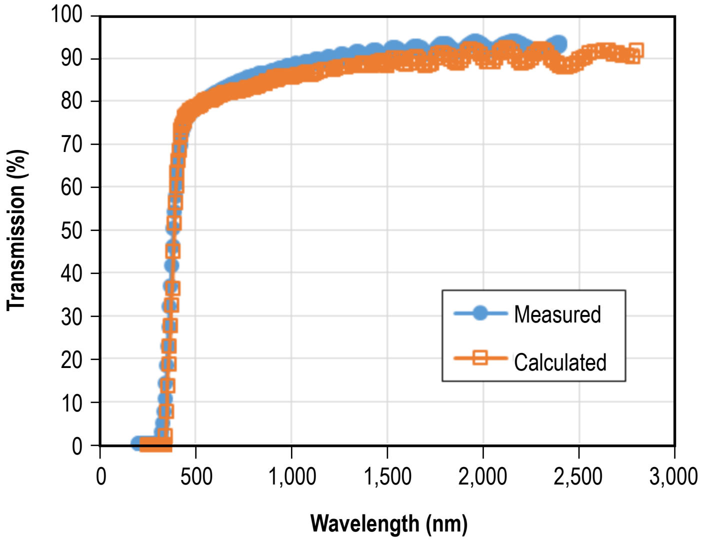

Figure 10. CORIN coated with cerium oxide and eroded by AO.

4.5 Windows

Figure 11 is a 0.1-in-thick window of poly (methyl methacrylate). The dip at approximately 1,900 nm is not as pronounced for the calculated transmission; more data points might have helped here. Figure 12 is a highly transmissive, 0.125-in-thick, UV-grade magnesium fluoride window. This is near the limit for both machines, and the curves are in good agreement.

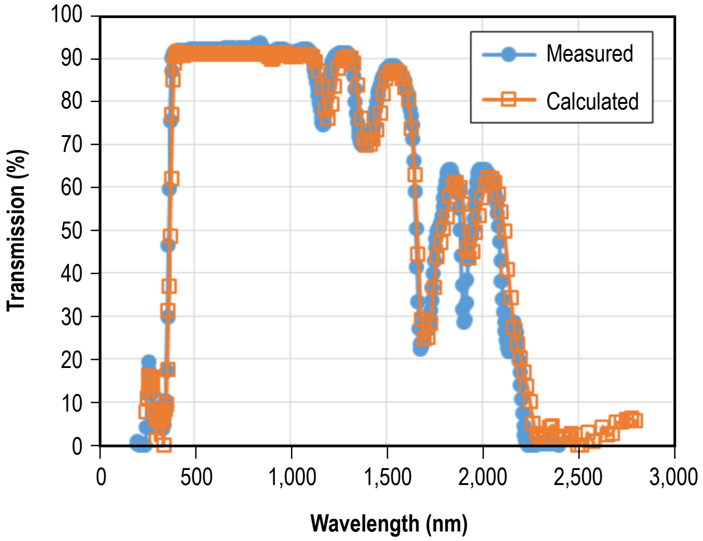

Figure 11. Poly (methyl methacrylate) window.

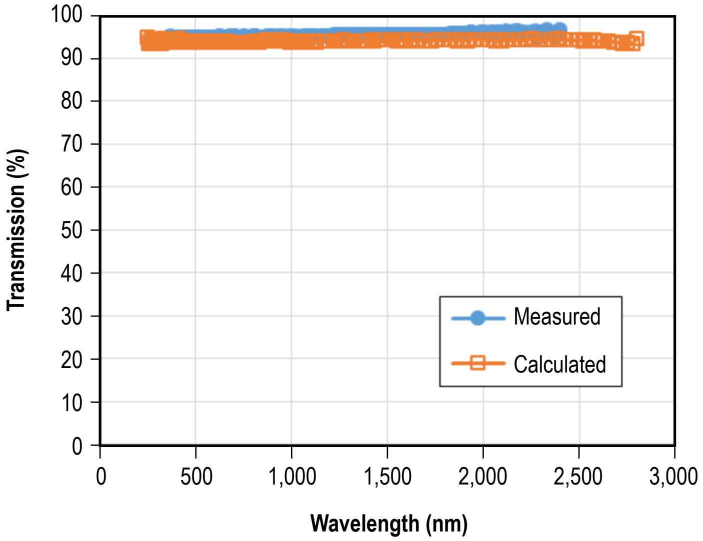

Figure 12. Magnesium fluoride window.

5. TRANSMISSION FROM INFRARED REFLECTANCE MEASUREMENTS: TEMP 2000/2000A PROCEDURE

The same method can be used to determine infrared transmission and to correct infrared emittance using an AZ Technology TEMP 2000A infrared reflectometer (fig. 13) per reference 3. One should note that the TEMP 2000A can only measure integrated values of infrared emittance and cannot resolve absorption bands. The TEMP 2000A includes a calibration puck with a gold side and a black side. If a blackbody nonreflecting cavity is available, it should be used instead of the black side of the calibration puck in the second measurement. This procedure can be used to approximate total transmittance for thin samples.

Figure 13. TEMP 2000A Infrared Reflectometer.

To see if a sample is partially transmitting, the gold and black pucks should be alternately placed on the sample as backing. If the sample is transmitting, the reflectance (or emittance) values will be different. To calculate the approximate total transmittance:

(1) Measure the sample using the gold backing: x.
(2) Measure the sample using the blackbody cavity or black backing: ρ_{sample}.
(3) Measure the gold that was used for the backing: ρ_{gold}.

Transmission of sample τ_{sample} may be calculated:

$$\tau_s = \frac{1}{2}\left[-\rho_{\text{sample}} + \sqrt{\frac{4x - 4\rho_{\text{sample}} + \rho_{\text{gold}}\rho_{\text{sample}}^2}{\rho_{\text{gold}}}}\right], \tag{7}$$

where

τ_s = transmittance of sample
ρ_{sample} = measured reflectance using black backing
x = measured reflectance using gold backing
ρ_{gold} = reflectance of gold puck.

Use the 0 to 1 full-scale values for ρ and x. Do not use percentages.

For reporting emittance or determining the value to use in the α_s/ε ratio, knowledge of the backing materials, if any, is necessary. If the view behind the film is known to be deep space, the absorptance above is essentially the emittance, although—in a rigorous sense—the emittance is, by definition, a surface property; and the absorptance calculated previously is a function of the material thickness. The passing of the Sun or other radiating bodies behind the material would obviously affect thermal energy balances, but the sample properties reported above could be used to estimate the impact.

The TEMP infrared reflectometer has two measurement modes: (1) absolute mode for near normal emittance and (2) relative mode for total hemispheric emittance. In general, the reference to thermal emittance means total hemispheric emittance at 300K.

For transparent samples measured using the TEMP infrared reflectance, report sample thickness, because the absorption that is determined from the TEMP manual equation is dependent on the sample thickness; i.e., the emittance for a 5-mil-thick sample will be different from a 2-mil-thick sample because of the difference in transmission.

Do not use the TEMP 2000A gold puck in lieu of the mirror or aluminum for LPSR measurements (i.e. UV and visible wavelength measurements), as the reflectance of the gold drops off in the blue visible to UV wavelengths.

6. CONCLUSIONS

When a bench spectrophotometer is not a viable option due to size or location of the sample, a portable spectroreflectometer used with adequate backing materials can be used to calculate transmission. In a similar manner, the portable infrared reflectometer can be used to calculate transmission in the infrared wavelengths. The analysis of the data taken with the portable LPSR 300 handheld instrument, compared to laboratory results from the PerkinElmer LAMBDA 1050, demonstrates the quality of data that can be obtained. For high spectral resolution, samples must be measured in the laboratory with large bench-top systems such as the LAMBDA 1050, but if lower spectral resolution is acceptable, then the LPSR 300 can provide measurements of transparent samples in the field with good accuracy.

APPENDIX—DERIVATION OF EQUATION ONE

The LPSR 300 focuses a beam onto the sample at a near-normal angle (15°) and measures the total hemispherical reflectance using a large integrating sphere. The interaction of the light with the sample can be decomposed into three components—proportion reflected by sample, ρ_{sample}, proportion absorbed by sample, α_{sample}, and proportion transmitted through the sample, τ_{sample} (assuming the sample is backed by a black body), where:

$$1 = \rho_{\text{sample}} + \alpha_{\text{sample}} + \tau_{\text{sample}} \ . \tag{8}$$

When the sample is backed by the mirror, only the proportion, τ_{sample} reaches the mirror. Of this, only the proportion $\tau_{\text{sample}}\rho_{\text{mirror}}$ is reflected back. A proportion, α_{sample}, of this reflected amount is absorbed going back through the sample. So, of the original beam, the proportion reflected back, x, is the amount reflected, ρ_{sample}, plus the amount that gets through to the mirror, reflects back and is not absorbed:

$$\tau_{\text{sample}}\rho_{\text{mirror}}\left(1-\alpha_{\text{sample}}\right) \ , \tag{9}$$

noting that

$$1-\alpha_{\text{sample}} = \tau_{\text{sample}} + \rho_{\text{sample}} \ , \tag{10}$$

yields the relationship:

$$x = \rho_{\text{sample}} + \tau_{\text{sample}}\rho_{\text{mirror}}\left(\tau_{\text{sample}} + \rho_{\text{sample}}\right) \ . \tag{11}$$

This implies the quadratic equation:

$$a\tau^2_{\text{sample}} + b\tau_{\text{sample}} + c = 0 \ , \tag{12}$$

where

$a = \rho_{\text{mirror}}$
$b = \rho_{\text{sample}}\rho_{\text{mirror}}$
$c = \rho_{\text{sample}} - x.$

Using the quadratic formula, yields:

$$\tau_{\text{sample}} = \frac{1}{2}\left(-b / a + \sqrt{\frac{b^2 - 4ac}{a^2}} \right) , \tag{13}$$

which implies equation (1). Equation (7) can be derived similarly.

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14. ABSTRACT

Normally, a spectrophotometer is used to directly measure transmission of material samples; however, a sample may be too large to fit into the spectrophotometer chamber, or a field inspection may be required. This Technical Memorandum describes the procedure for using measurements made with a portable spectroreflectometer to calculate transmission. A variety of materials were chosen for both direct transmission measurements and reflectance measurements. The as-measured and calculated transmission curves showed good agreement between the two instruments. The same method can be used for calculating infrared transmission using an infrared reflectometer.

15. SUBJECT TERMS

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