

DATA REDUCTION OF FTIR THERMAL EMISSION MEASUREMENTS UNDER COLD VACUUM CONDITIONS: PROCESSING OF INTERFEROGRAMS VS. SPECTRA. Y. Yang^{1,2}, R. E. Milliken², W. R. Patterson², M. S. Bramble², K. L. Donaldson Hanna³, and H. Zhang¹. ¹Planetary Science Institute, China University of Geosciences, Wuhan 430074, China; ²Department of Earth, Environmental, and Planetary Sciences, Brown University, Providence, RI, 02912, USA. ³Department of Physics, University of Oxford, Oxford, UK. Contact: yangyazhou1@gmail.com.

Introduction: The success of thermal infrared (TIR) instruments such as Diviner (on the Lunar Reconnaissance Orbiter) and the Thermal Emission Spectrometers (on the Mars Global Surveyor and Mars Exploration Rovers) have broadened our knowledge of the surface composition of the Moon and Mars [3-5], respectively, and TIR measurements by upcoming missions that target asteroids will provide new compositional information about primitive airless bodies [6,7]. However, lab studies have shown that TIR spectral features can be affected by strong thermal gradients when particulate materials are in a cold vacuum environment [1, 2, 8], as is the case for airless bodies.

To understand these effects, several laboratory instruments have been developed to measure emissivity spectra of materials under lunar and asteroid-like conditions (e.g., Asteroid and Lunar Environment Chamber (ALEC) instrument at Brown University [8], MoonBox at Oxford [10]). A Fourier Transform Infrared (FTIR) spectrometer is commonly used in these settings to measure emissivity spectra, but questions as to how best to radiometrically calibrate and reduce such data remain, particularly when samples are close to or lower than ambient temperature.

Background: The signal (FTIR output, V) obtained during laboratory emission measurements is a combination of energy (E) emitted from the sample, energy from the instrument, and energy emitted by the environment and then reflected (R) by the sample along the optical path, all of which are modulated by the instrument response, F [8-10]:

$$V_{measure}(T) = [E_{sample}(T) + R_{sample}E_{env}(T) - E_{instrument}(T)]F \quad (1)$$

It is common in commercial FTIRs to only report positive values for processed spectra (i.e., after applying the Fourier transform, FT, to the interferograms), which for Eq. 1 would imply that the energy coming into the system is always greater than the instrument energy if the spectrum is used as $V_{measure}$. However, when the sample is colder or only slightly warmer than ambient temperature, the energy emitted by the sample may be less than that of the instrument. Moreover, the ratio of sample energy to instrument energy will vary with wavenumber and can have values <1 and >1 for a given measurement. Because a standard FTIR spectrum only reports positive values, it becomes difficult to separate $E_{instrument}$ from the ob-

served FTIR output, $V_{measure}$, in this scenario when using only processed spectra.

Here we present results for different data processing methods to derive emissivity spectra from measurements made under vacuum and varied temperature conditions with the ALEC. Data are reduced two ways, using the spectra that are output by the FTIR software (arbitrary units vs. wavenumber) and using the original interferograms (IFG) [11].

Methods: ALEC was cooled to $\sim 85K$ with LN_2 and each sample cup was surrounded by a black shroud to minimize E_{env} , making it negligible in Eq. (1) such that:

$$V_{measure}(T) = [E_{sample}(T) - E_{instrument}(T)]F = V_{sample}(T) - V_{instrument}(T) \quad (2)$$

The $V_{instrument}$ was determined by measuring the signal while looking at a cold ($\sim 85K$) well coated with Nextel black paint for which E_{sample} is negligible over the measured wavelength range, reducing Eq. (1) to:

$$V_{instrument}(T) = E_{instrument}(T) \cdot F \quad (3)$$

The response function F was calculated by measuring a blackbody at a certain temperature and employing the Planck function to calculate the blackbody radiance at the same temperature [13]. The sample emissivity spectrum can be obtained by:

$$\mathcal{E}_{sample} = \frac{E_{sample}(T)}{E_{planck}(T)} = \frac{[V_{measure}(T) + V_{instrument}(T)]/F}{E_{planck}(T)} \quad (4)$$

Note that Eq. (4) is appropriate only when $E_{sample} > E_{instrument}$ over the full wavenumber range if spectra are used for the V terms. Another necessary condition is that the IFG of energy originating from the instrument and sample have the same phase error.

The IFG, which is a function of optic path differences x , should be symmetric around the zero path difference (ZPD). However, a frequency dependent phase error $\phi(\nu)$ commonly affects the symmetry of the measured IFG [12]. The relation between IFG and power spectra $S(\nu)$ can be described as [12]:

$$IFG(x) = \int_{-\infty}^{+\infty} S(\nu) \cdot \cos(2\pi\nu x) d\nu \Leftrightarrow \int_{-\infty}^{+\infty} S(\nu) e^{-i2\pi\nu x} d\nu \quad (5)$$

here for negative frequency $S(-\nu) = S(\nu)$. When phase error is considered, this becomes [12]:

$$IFG(x) = \int_{-\infty}^{+\infty} S(\nu) \cdot \cos[2\pi\nu x + \phi(\nu)] d\nu \Leftrightarrow \int_{-\infty}^{+\infty} S(\nu) e^{-i\phi(\nu)} e^{-i2\pi\nu x} d\nu \quad (6)$$

Therefore, after applying the FT on the measured IFG, the power spectrum is $S(\nu) e^{-i\phi(\nu)}$ which contains the phase error. To obtain the real power spectrum $S(\nu)$, a phase correction is needed, which can be done either

before FT on the original IFG or after FT on the resulting power spectra [12]. For the IFG of the instrument contribution (Fig. 1), which may be largely from the detector itself [6], there is an additional phase shift of π :

$$IFG_d(x) = \int_{-\infty}^{+\infty} S_d(\nu) \cdot \cos[2\pi\nu x + \theta(\nu) + \pi] d\nu \Leftrightarrow -\int_{-\infty}^{+\infty} S_d(\nu) e^{-i\theta(\nu)} e^{-i2\pi\nu x} d\nu \quad (7)$$

In contrast to using spectra for the V terms in (1)-(4), which assumes E_{sample} is always larger than $E_{instrument}$, the measured (IFG_m) is always the sum of sample's IFG_s and detector's IFG_d , no matter which energy is greater. As such, if IFG_d is measured directly, then IFG_s can be easily separated from the measured IFG_m :

$$IFG_s(x) = IFG_m(x) - IFG_d(x) \quad (8)$$

IFG_s can then be converted to power spectra (V_{sample}) and emissivity can be obtained by:

$$\mathcal{E}_{sample} = [V_{sample}(T) / F] / E_{plank}(T) \quad (9)$$

The importance of preserving phase information by processing interferograms rather than power spectra was noted by [11]. If the phase errors within IFG_d and IFG_s are the same ($\varphi(\nu) = \theta(\nu)$), then the measured IFG_m will have the same phase error:

$$IFG_m(x) = IFG_s(x) + IFG_d(x) = \int_{-\infty}^{+\infty} [S_s(\nu) - S_d(\nu)] \cdot \cos[2\pi\nu x + \varphi(\nu)] d\nu \Leftrightarrow \int_{-\infty}^{+\infty} S_m(\nu) e^{-i\varphi(\nu)} e^{-i2\pi\nu x} d\nu \quad (10)$$

and the phase correction can be applied before or after the FT. However, the energy from the detector passes through the beam splitter in an inverse path compared to the energy from the sample [6, 11]. Therefore, it is possible that some differences exist between the phase errors of IFG_d and IFG_s .

Results: Fig. 1 shows the IFG of the instrument and an in-house built blackbody (see [13] for more information about this blackbody) measured at temperatures from 275K to 500K. At 300K, the blackbody IFG is flat, implying E_{sample} is close to $E_{instrument}$. The IFG of the instrument and blackbody are out of phase when the temperature is high (340K, 500K) and in phase at lower temperature (275K). Therefore, the signal measured at high temperature is as described in Eq. (2), but at low temperature the measured signal is:

$$V_{measure}(T) = [E_{instrument}(T) - E_{sample}(T)] F \quad (11)$$

At temperatures close to ambient (300K) it will be difficult to know which one is larger, and deriving emissivity data from spectra produced by the FTIR software instead of the raw IFG can lead to errors.

Fig. 2 shows the power spectra of the in-house blackbody and a labradorite (LAB) powder (particle size < 45 μ m) after processing of IFG (Eq. 8) and original FTIR output (spectra) (Eq. 2). Results from the two methods are similar for the blackbody, whereas differences for LAB are much larger and reach ~31%. The latter indicates a strong thermal gradient exists in the sample and that some of the volume of sample measured is much colder than the 353K setpoint, as expected for cold vacuum conditions.

Conclusions: When using IFG data, sample signal can be easily separated from that of the FTIR instrument and effects of phase error can be properly corrected. The same is not always true when using spectra as the starting point for deriving emissivity, particularly when samples are close to or colder than ambient conditions. It is recommended that lab data acquired under cold vacuum conditions be processed using IFG to avoid these complications, especially when true sample temperature is unknown or poorly constrained.

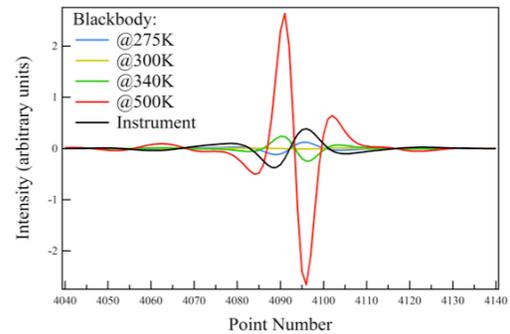


Fig. 1. Interferograms of instrument (Nextel paint cold well) and in-house built blackbody [13] energy measured at different temperatures centered around the ZPD.

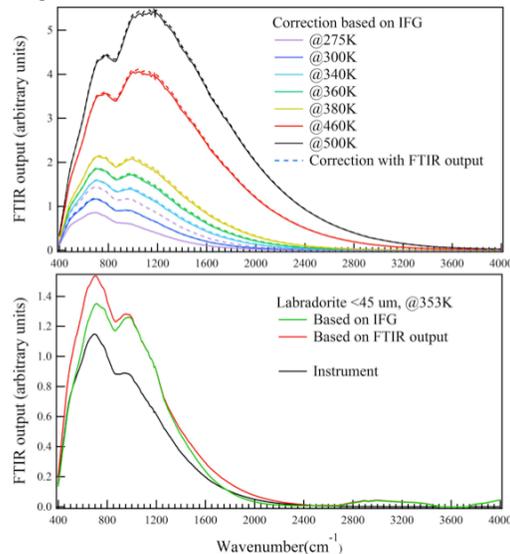


Fig. 2. Power spectra of samples separated from the measured signal based on FTIR output and IFG data reduction. Top: in-house built blackbody [12]; Bottom: powdered LAB.

References: [1] Logan L. M. et al. (1973) *JGR*, 78, 4983-5003. [2] Salisbury J. W. and Walter L. S. (1989) *JGR*, 94, 9192-9202. [3] Christensen P. R. et al. (2001) *JGR*, 106, 23823-23871. [4] Ruff S. W. et al. (2006) *JGR*, 111, E12S18. [5] Greenhagen B. T. et al. (2010) *Science*, 329, 1507-1509. [6] Christensen P. R. et al. (2017) arXiv: 1704.02930. [7] Levison H. F. et al. (2017) 48th LPSC Abstract#2025. [8] Donaldson Hanna K. L. et al. (2017) *Icarus*, 283, 326-342. [9] Ruff S. W. et al. (1997) *JGR*, 102, 14899-14913. [10] Thomas I. R. et al. (2012) *Rev. Sci. Instrum.*, 83, 124502. [11] Brown R. J. and Young B. G. (1975) *Appl. Opt.*, 14, 2927-2934. [12] Forman M. L. et al. (1966) *JOSA*, 56, 59-63. [13] Bramble M. S. et al., (2018) 49th LPSC, #1598.