DATA PROCESSING IN NEMS-FTIR SPECTROSCOPY

Converting EMILIE$^{\mathrm{TM}}$ spectra to absorbance units and extracting sample mass

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This guide provides an introduction to converting EMILIE™ spectra into absorbance units (AU) and establishing a correlation with sample mass. The theoretical framework presented here is based on the approach by N. Dudani & S. Takahama [1], developed for analyzing spectral data from electrostatically precipitated nanoparticles on a zinc selenide crystal in ATR-FTIR spectroscopy.

This guide outlines the steps from the raw signal to the final absorbance spectrum of the sample and a sample mass calculation, using a sampled chip, which is pre-loaded with 9 ng of polystyrene particles as an example.

1 ACQUISITION OF A NEMS-FTIR SPECTRUM

The following section describes how to acquire a NEMS-FTIR spectrum with EMILIE™ . More details on optimal FTIR spectrometer and PHILL™ settings can be found in the manual for EMILIE™ & PHILL™ .

The following data processing steps are required to obtain a blank-corrected NEMS-FTIR sample spectrum.

Step 1 - Record a reference NEMS-FTIR spectrum of the spectrometer light source with an EMILIE™ LIGHT chip: The reference, or background, spectrum of the spectrometer's light source is recorded using an EMILIE™ LIGHT chip. Figure 1 shows the NEMS-FTIR reference spectrum of a Bruker Vertex 70 equipped with a globar and a KBr Broadband beamsplitter.

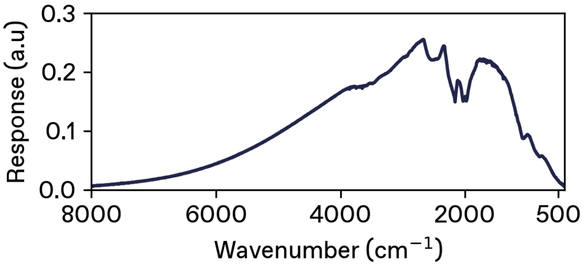

Figure 1: NEMS-FTIR reference spectrum of the globar of a VERTEX 70 equipped with a KBr beamsplitter recorded with an EMILIE™ LIGHT chip.

Step 2 - Record a NEMS-FTIR spectrum of your sample & divide it by the reference spectrum (step 1) to obtain your sample spectrum: The sample spectrum is recorded with a sampled EMILIE™ chip (i.e. an EMILIE™ chip on which a sample has been deposited). Figure 2 shows the NEMS-FTIR spectrum of a chip on which 9 ng of polystyrene has been deposited before, and after division by the globar reference spectrum recorded in step 1.

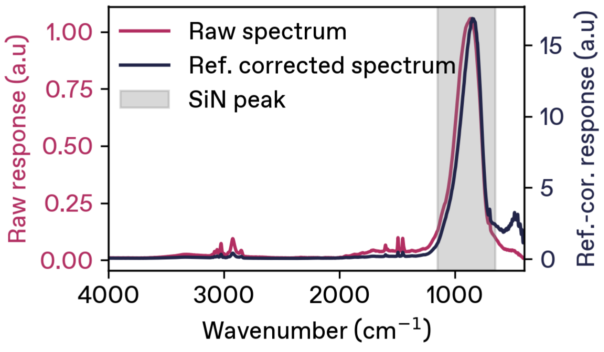

Figure 2: NEMS-FTIR spectrum of a chip sampled with polystyrene before, and after correction with the globar reference spectrum.

Step 3 - Record the NEMS-FTIR spectrum of a blank EMILIE™ chip & divide it by the reference spectrum

(step 1) to obtain your blank spectrum: A blank spectrum can be recorded to remove spectral interferences from concomitant species. The blank chip should be sampled with everything in your sample (for example, your sample solvent) but the analyte.

Step 4 - Signal normalization: To account for the use of different output ranges in PHILLharmonics, we recommend using the silicon nitride (SiN) peak of the EMILIE™ chip material as an internal standard for normalization of the spectral data. The broad SiN peak is located between 1000 cm^{-1} and 700 cm^{-1} with the maximum at 835 cm^{-1}. Normalize the sample and blank spectra from step 2 and step 3 by multiplying the signal by a factor such that in both cases, the SiN peak height at 835 cm^{-1} is equal to 1 as shown in Figure 3.

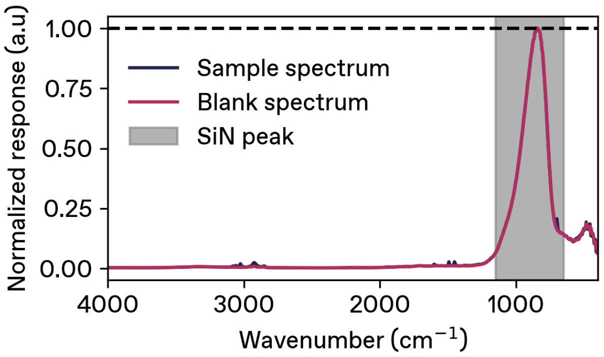

Figure 3: Background corrected and normalized NEMS-FTIR spectra of the polystyrene sample and blank. Normalization of the two spectra was achieved by adjusting height of the silicon nitride peak to 1.

Step 5 - Blank correction: After background correction and normalization, the NEMS-FTIR spectrum of the blank can be subtracted from the NEMS-FTIR spectrum of the polystyrene sample to obtain the final blank corrected sample spectrum. Figure 4 shows the post-processed NEMS-FTIR spectrum of polystyrene after subtraction of the blank spectrum. Subtraction of the blank removes the broad SiN peak, revealing all the characteristic peaks expected for polystyrene.

2 CONVERSION OF THE NEMS-FTIR SIGNAL TO ABSORBANCE

In the context of NEMS-FTIR spectroscopy — a photothermal technique — sample scattering is assumed to be negligible for both particulate and uniform samples. The absorbance for a non-scattering sample at a specific wavenumber $\tilde{\nu}$ is given by

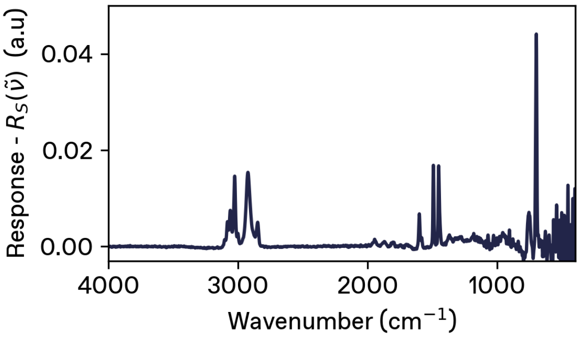

Figure 4: NEMS-FTIR spectrum of polystyrene after reference correction, normalization, and subtraction of the blank chip spectrum.

$$A(\tilde{\nu}) = -\log_{10}(T(\tilde{\nu})) = -\log_{10}(1-\alpha(\tilde{\nu})) \quad (1)$$

where $T(\tilde{\nu})$ is transmittance and $\alpha(\tilde{\nu})$ absorptance.

2.1 Calibration using the known silicon nitride absorptance

The NEMS-FTIR signal can be calibrated using the chips' intrinsic SiN standard. This has been done by recording the spectrum of 12 clean, unloaded EMILIE™ chips by transmission FTIR spectroscopy with the internal detector, the results shown in Figure 5. The absorptance of SiN can be directly calculated from its measured transmittance $\alpha(\tilde{\nu}) = 1 - T(\tilde{\nu})$, resulting in an absorptance of $\alpha_{SiN}(835cm^{-1}) = 0.24 \pm 0.01$. The high precision of the 50 nm thick SiN thin film is reflected in the small associated standard deviation. This absorptance value for SiN can be used to convert the sample spectrum to absorptance.

The NEMS-FTIR signal (see Section 1) can now be related to absorptance using the absorptance value for SiN determined above, through the calibration factor β

$$\beta = \frac{\alpha_{SiN}(835cm^{-1})}{R_{SiN}(835cm^{-1})}\left[1 - \frac{\Sigma_P}{\Sigma_{IR}}\right]\gamma_{IR} \quad (2)$$

with the area of the perforation Σ_P, the area of the IR spot on the EMILIE chip Σ_{IR}, and the relative responsivity factor γ_{IR}. The latter relates the NEMS-FTIR signal response to the IR beam spot, as shown in Fig-

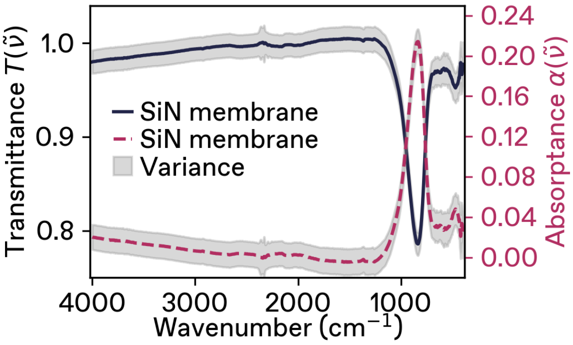

Figure 5: Average transmittance of 12 individual clean, unloaded EMILIE™ chips made of 50 nm low-stress silicon nitride. The minimum transmittance, or maximum absorptance, is located at approximately $\tilde{\nu} = 835\, cm^{-1}$.

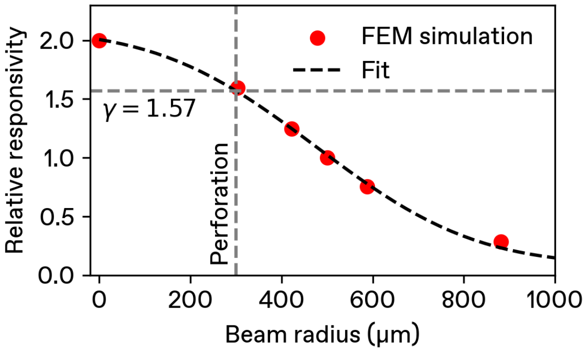

Figure 6: Plot of relative photothermal responsivity factor γ for a 50 nm thick and 1×1 mm^2 large EMILIE™ chip as a function of incident beam size.

ure 6. The IR spot size can be controlled through the aperture used in the FTIR spectrometer. The beam diameter on the chip is then given by $d_{\text{beam}} = f_{\text{EMILIE}} \cdot f_{\text{spectrometer}} \cdot d_{\text{aperture}}$, where $f_{\text{EMILIE}} \approx 0.167$ accounts for the focusing ratio of EMILIE™ , and $f_{\text{spectrometer}}$ for the spectrometer-specific beam broadening beyond the nominal aperture. This factor is 1.8 for the Vertex series and 1.64 for the Invenio series from Bruker Optics. For example, with a 6 mm aperture on a Vertex system, this results in a beam diameter of approximately $d_{\text{beam}} = 0.167 \cdot 1.8 \cdot 6$ mm ≈ 1.8 mm on the EMILIE™ chip. Therefore, the area of the incident infrared beam is greater than the membrane and, consequently, Σ_{IR} can be set equal to the membrane area 1 mm^2. For the desired situation that the IR beam illuminates the entire EMILIE™ membrane $\gamma_{IR} = 1$ and the perforated area of approximately $\Sigma_P = 0.108$ mm^2, the following term takes the specific value $\left[1 - \frac{\Sigma_P}{\Sigma_{IR}}\right] \gamma_{IR} = 0.89$.

2.2 Conversion to absorbance

The assumption of a uniform sample film does not apply to an EMILIE™ chip where the sample is typically located on the central perforated area. Having a diameter of 600 µm, this results in a sample area $\Sigma_S = \pi\, 0.3^2$ mm^2 $- \Sigma_P \approx 0.175$ mm^2. In this case, the sample is distributed over an area Σ_S that is smaller than the incident infrared beam's area Σ_{IR}. The area ratio of the sample and the infrared beam, therefore, needs to be considered for the accurate scaling of the NEMS-FTIR signal R_S of the sample.

In comparison to conventional spectroscopy, the photothermal response of the nanomechanical membrane is not uniform over the entire membrane. The response of the EMILIE™ chip is higher for a sample concentrated in its center as opposed to an evenly distributed sample. To account for both effects, the area ratio $\Sigma_S/(\Sigma_{IR} - \Sigma_P)$ and a correction factor γ_S to account for the relative photothermal responsivity are included:

$$R_S(\tilde{\nu}) = \frac{\Sigma_S}{\Sigma_{IR} - \Sigma_P} \frac{1}{\beta} \alpha_S(\tilde{\nu})\, \gamma_S\,, \tag{3}$$

where $\alpha_S(\tilde{\nu})$ is the sample absorptance. Solving (3) for the sample absorptance yields

$$\alpha_S(\tilde{\nu}) = \beta R_S(\tilde{\nu}) \frac{\Sigma_{IR} - \Sigma_P}{\Sigma_S} \frac{1}{\gamma_S}, \tag{4}$$

with which it is now possible to calculate the absorbance (1). For an aperture set to ensure full illumination of the membrane, for an EMILIE™ chip, this results in a ratio of $(\Sigma_{IR} - \Sigma_P)/\Sigma_S = (1$ mm^2 $-$ 0.108 mm$^2)/(\pi\, 0.3^2$ mm^2 $- 0.108$ mm$^2) \approx 5.1$. For the case of sample covering also the perforation thereby contributing to the response, $\Sigma_P \pi\, 0.3^2$ mm^2. An approximation of the responsivity distribution as a function of the incident beam spot radius [2] can be used to estimate the photothermal responsivity correction factor of $\gamma_S = 1.57$, as shown in Figure 6. In other words, a sample located in the very center of the membrane would result in a response approximately 1.57 times higher than that for the same sample distributed over the entire membrane.

3 CONVERSION OF ABSORBANCE TO SAMPLE MASS

The absorbance of the sample can be related to its decadic attenuation coefficient $\mu_{10}(\tilde{\nu})$ to obtain the corresponding sample mass. According to Beer-Lambert law, the absorbance of a uniform sample (particulates or uniform film) scales linearly with effective film thickness h_{eff}

$$A_S(\tilde{\nu}) = \mu_{10}(\tilde{\nu}) h_{eff} = \mu_{10}(\tilde{\nu}) \frac{m_S}{\rho_S \Sigma_S}. \tag{5}$$

The effective film thickness h_{eff} can be written as a function of the sample mass m_S, sample mass density ρ_S, and the sample area Σ_S that is illuminated by the IR light. Since the sample area is smaller than the IR light beam, Σ_S corresponds to the area occupied by an even sample film.

It is assumed that only small absorptance values are possible due to maximum sample masses limited to a few nanograms $(\alpha_S(\tilde{\nu}) \ll 1)$. In that case, the absorbance (1) can be linearized using a first-order Taylor series approximation $A_S(\tilde{\nu}) \approx \alpha_S(\tilde{\nu}) / \ln(10)$. Combining, (1) and (5) and solving for the sample mass gives

$$m_S = \frac{\alpha_S(\tilde{\nu})}{\ln(10)} \frac{\rho_S \Sigma_S}{\mu_{10}(\tilde{\nu})}. \tag{6}$$

Inserting the sample absorptance (4) allows for calculation of the sample mass from the NEMS-FTIR signal:

$$m_S = \frac{\Sigma_{IR} - \Sigma_P}{\gamma_S} \frac{\rho_S}{\ln(10)} \beta R_S(\tilde{\nu}) \frac{1}{\mu_{10}(\tilde{\nu})} \tag{7}$$

where $\tilde{\nu}$ is selected for specific vibrational modes of the sample. If the raw signal is normalized to the intrinsic absorption of silicon nitride, as described in step 4, $R_{SiN}(835\,cm^{-1})$ = 1. This approach offers the advantage of being independent of the sample area Σ_S, relying only on the incident beam area, sample density, and its decadic attenuation coefficient $\mu_{10}(\tilde{\nu})$. The sample-specific $\mu_{10}(\tilde{\nu})$ can be retrieved from the literature. Alternatively, it can be derived from refractive index data.

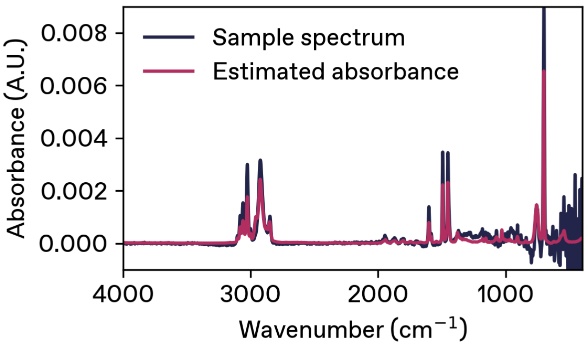

Figure 7: Absorbance-corrected NEMS-FTIR spectrum of a sampled chip loaded with 9 ng polystyrene compared to the estimated absorbance as calculated by (5). The refractive index of bulk polystyrene is taken from [4].

3.1 Comparison to the absorbance estimated from refractive index data

For particulate samples, the decadic linear attenuation coefficient can be derived based on a sparse particle film model, which results in [3]

$$\mu_{10}(\tilde{\nu}) = \frac{6\pi\tilde{\nu}}{\ln(10)} \mathrm{Im} \left\{ \frac{\tilde{n}^2(\tilde{\nu}) - 1}{\tilde{n}^2(\tilde{\nu}) + 2} \right\} \tag{8}$$

with the wavenumber $\tilde{\nu}$ and complex refractive index $\tilde{n}$ of the sample material.

This enables the estimation of the absorbance of a target substance, such as polystyrene nanoparticles, from its complex refractive index, defined as $\tilde{n} = n + ik$, where n and k represent the real and imaginary parts, respectively. A comparison of a NEMS-FTIR spectrum in absorbance units to a refractive index reference spectrum calculated from (8) is shown in Figure 7.

REFERENCES

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[3] C. F. Bohren and D. R. Huffman. Absorption and Scattering of Light by Small Particles. John Wiley & Sons, Ltd, 1998.

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