Chapter 7 Recommended Tests

Different parameters specify the performance of spectral sensors, and some of them are dependent on external factors e.g. the SNR depends on the optical power level coupled into the spectral sensor.

In this chapter, certain tests that allow the characterization of the performance of NeoSpectra modules are explained. These tests are the ones that were used to define the specifications of NeoSpectra modules.

1. Spectral range

1.1. Definition

The spectral range, is the total useful wavenumber (***v***) or wavelength (***λ***) range for the module [4]**.** The upper and lower wavelength limits ($\boldsymbol{\lambda_U}$ and $\boldsymbol{\lambda_L}$ respectively) are determined by the wavelength points where the Power Spectral Density (PSD) (also known as single beam spectra) reaches one tenth of maximum measured energy over the range [5]. (see illustration in Figure 7.1)

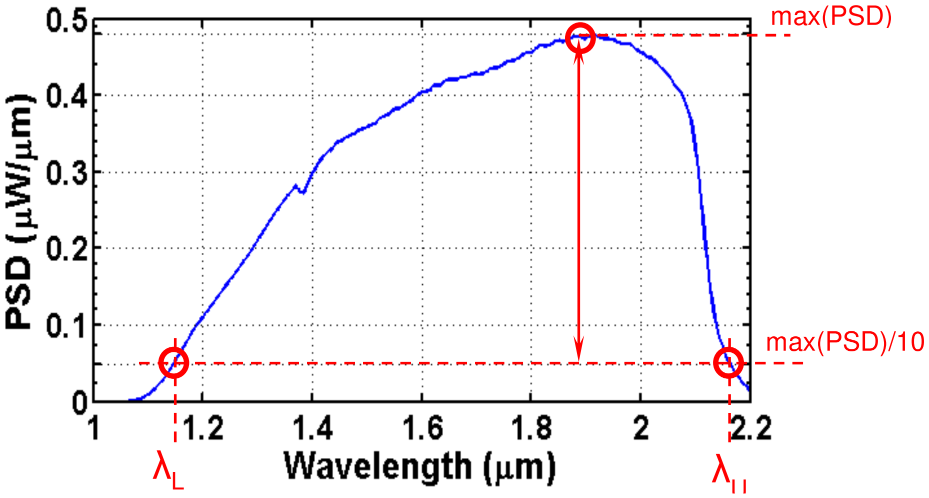

Figure 7.1: Determination of the upper and lower limits of the spectral range

1.2. Characterization method

The PSD is obtained by applying a Fourier Transform on the light source’s measured interferogram with no sample in the light path. It can be directly obtained from the “Interferogram & PSD” tab in SpectroMOST (see Chapter 4 - Section2). The data are reported by using external processing for the calculation of the upper and lower wavelength limits for 100 consecutive measurements, and plotting the calculated values in a plot similar to the one shown in Figure 7.2 [5]. Variation in the wavelength limits in the plot can be interpreted as unstable performance of the system.

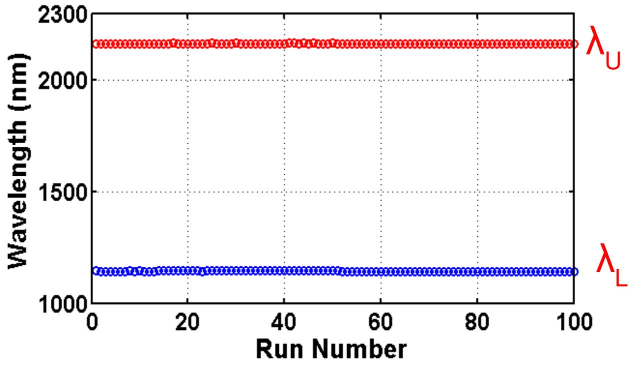

Figure 7.2: Plotting upper and lower wavelengths for the characterization of the spectral range

2. Signal-to-Noise Ratio (SNR)

2.1. Definition

Noise is defined as the variation in the signal response for repeated measurements. The Signal to Noise Ratio (SNR) measures the module's ability to reproduce a spectrum under the same conditions (e.g. temperature) and the same instrumental configurations (e.g. resolution, and integration time) over a certain period of time [1].

2.2. Characterization method

The SNR can be visually evaluated by measuring the 100% line. The 100% line is obtained by dividing two single-beam spectra (***$S_1(v)$*** & ***$S_2(v)$*** with no sample in the beam path) acquired under identical conditions of resolution and measurement time and taken immediately one right after the other.

$$T_{100\%line}(\upsilon) = \frac{S_2(\upsilon)}{S_1(\upsilon)} \times 100$$

Ideally, the 100% line should be a flat line across the wavelength range. Practically, due to system non-idealities and noise, the 100% line looks like the plots shown in Figure 7.3.

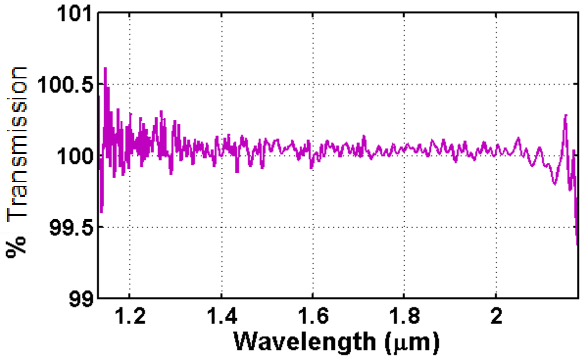

Figure 7.3: Example of 100% line

At a certain wavelength ***Λ_o*** , the ***SNR*** is calculated from Root Mean Square Noise (***N_{rms}***), which is the standard deviation of the baseline value in 100 consecutive 100% lines. The relationship between ***SNR*** and ***N_{rms}*** is given by

$$SNR = \frac{100}{N_{rms}}$$

To visualize the variation of the SNR across the spectral range, the SNR is calculated at each wavenumber as described above. The values of the SNR are then plotted against the wavelength / wavenumber.

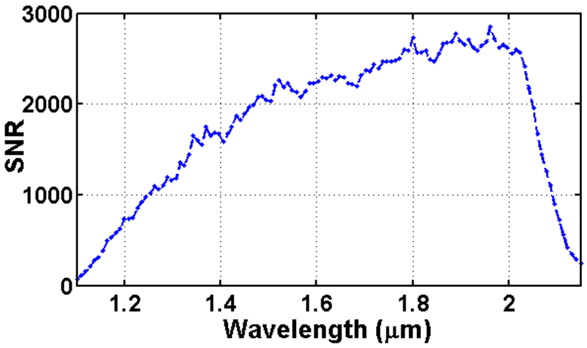

Figure 7.4: Example of the variation of the SNR across the spectral range

2.3. Effect of scan time on SNR

The noise consists of random and repetitive components. The repetitive components cannot be eliminated from the signal. However, the contribution of the random components can be reduced by averaging a bigger number of scans (***N***N_{scan}) i.e. increasing the integration time (t_{scan}). The value of the measured SNR of a certain instrument is proportional to the square root of the number of averaged scans i.e. the square root of the integration time: $SNR \propto \sqrt{N_{scan}} \propto \sqrt{t_{scan}}$ [1].

You can test this behavior by adjusting the scan time from the software, and calculate the SNR at certain wavelengths using the method explained in section 2.2. Plotting SNR versus the square root of the scan time should result in a linear function (see Figure 7.5).

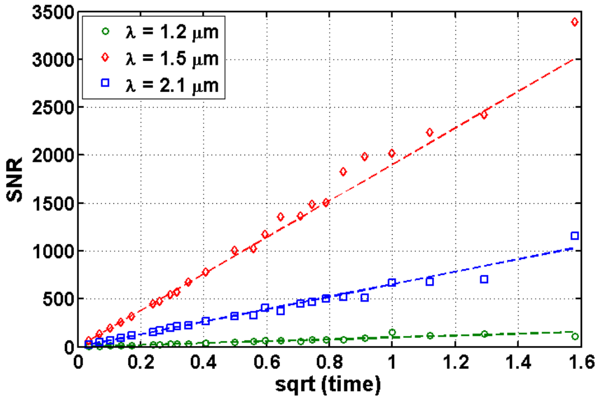

Figure 7.5: Example plot that shows the effect of increasing the scan time on the SNR

3. Resolution

3.1. Definition

Resolution is the minimum spacing between two consecutive wavelength / wavenumber points that can be fully resolved by the module. Similar to any FT-IR instrument, the resolution of SWS62221 is limited by the maximum Optical Path Difference (OPD) between the interfering beams in the Michelson interferometer i.e. the maximum travel range of the moving mirror.

The resolution in wavenumber (**Δv**) is constant across the spectral range. The relationship between resolution in wavelength (**$\Delta\lambda$**) at certain wavelength **λ** (in nm), and **Δv** (in cm^{-1}) is governed by **$\Delta\lambda = 10^7 \Delta v \lambda^2$** plotted in Figure 7.6

In NeoSpectra, the resolution can be adjusted by selecting one of the following pre-set values:

- $\Delta\lambda$ = 8 nm at λ=1,550 nm ➔ Δv = 33.3 cm^{-1}
- $\Delta\lambda$ = 16 nm at λ=1,550 nm ➔ Δv = 66.6 cm^{-1}

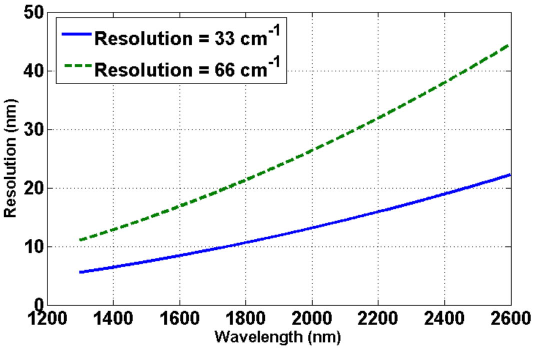

Figure 7.6: Variation of resolution in wavelength across the spectral range

3.2. Characterization method

Resolution (**Δv** in wavenumber, and **$\Delta\lambda$** in wavelength) may be evaluated in several ways. The *nominal* resolution (in cm^{-1}) is given by the reciprocal of the maximum optical path difference (OPD, in cm). Resolution may also be evaluated by calculating the full width at half maximum (FWHM) of the instrument line shape function obtained taking both the maximum OPD and apodization function into account (see Figure 7.7). The resolution is characterized by measuring the absorption spectrum of a reference sample with several very sharp absorption bands (such as methylene chloride) or a narrow band-pass optical filter [5].
The FWHM of the bands in these spectra when measured at high resolution should be significantly narrower than the resolution to be measured.

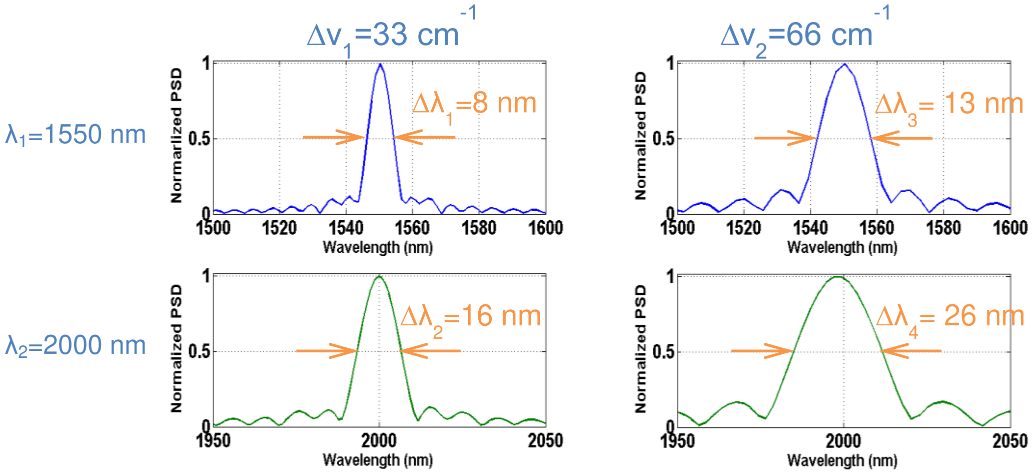

Figure 7.7: Wavelength resolution of Δv=33 cm^{-1} and Δv=66 cm^{-1} measured at λ=1550 nm and λ=2000 nm

4. Wavelength errors

4.1. Definitions

There are two different types of wavelength errors that can be qualified separately:

- **Wavelength Accuracy:** this factor quantifies the discrepancy between the actual measured value of a certain wavelength and the true standard value. It is defined as the difference between the measured wavelength of a wavelength standard, and the nominal wavelength reported for that wavelength standard under the same conditions of resolution and apodization function.
- **Wavelength Repeatability:** this factor quantifies the module's ability to reproduce absorptions at the same wavelength for the same sample. It is quantified by calculating the standard deviation of wavelength error for different measured spectra for the same standard sample.

4.2. Characterization method

There are several materials with unique spectra that enable their use for the characterization of wavelength errors (see examples in Table 7.1).

Table 7.1: Example of materials used for characterization of wavelength errors and their corresponding absorption peaks

Materials	Pathlength (mm)	Absorption peaks used for characterization of wavelength errors (nm) [††]
Methylene Chloride	1	1155, 1417, 1690, 2245
TS5	10	1446.6, 1652.3, 1693.1, 1948, 2060.1, 2111, 2248.2, 2353.3, 2373.4, 2385.4, 2537.5

The wavelength errors are calculated by taking several consecutive spectra measurements of reference materials and calculating the errors according to the definitions described in section 4.1.

[††] See details of measurement conditions in [3]

4.3. Photometric linearity

4.3.1. Definition

Photometric linearity is an important parameter that gives an indication about the conformation of the spectrometer's spectral response to Beer-Lambert's law at different concentration levels and/or thicknesses of the sample.

4.3.2. Characterization method

Below, we describe two possible methods for the characterization of the photometric linearity of a NeoSpectra module.

Characterization by changing sample concentration:

Characterization can be done by plotting the measured absorbance levels (A_{meas}) against the calibrated values of the standard materials with known absorbance values (A_{Calib}) at certain wavelengths for different concentration levels. The values of the slope and the intercept of the regression line of this plot are used as indicators of the performance of the spectrometer (see Figure 7.8). Ideally, the regression line of this plot should be a line with a slope 1 and intercept 0.

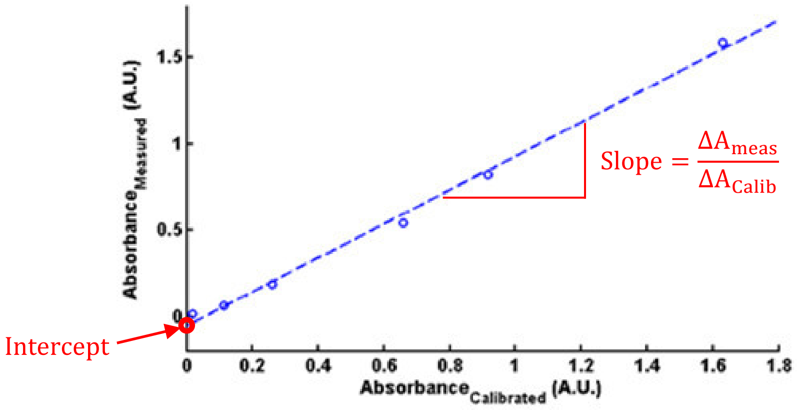

Figure 7.8: Plot for the characterization of the photometric linearity by changing the concentration levels of the sample

The samples to be used for the characterization, the number of datapoints, the concentration levels, the wavelengths at which the measurements are to be performed, and the acceptable values of slope and intercept usually depend on the requirements of the target application. For instance, the pharmacopoeia guidelines, stipulate that a minimum set of four standards with reflectances varying between 10% and 90% should be acquired at wavelengths 1200 nm, 1600 nm, and 2000 nm. Standards having lower reflectances (eg 2%, 5%) should be added to the set if the instrument is being employed for the measurement of low reflectance (less than 10% reflectance). The value of the slope should be in the range of 1.0±0.05, and the value of the intercept should be in the range of 0.0±0.05 [6].

Characterization by changing sample thickness:

A simpler but less accurate method is to plot the measured absorbance levels (A_{meas}) at a certain wavelength against the thickness of sheets of a polymer (e.g. acrylic (see Figure 7.9)) that is used as a sample. The values of the intercept and the norm of residuals of the regression line are used as indicators of the performance of the spectrometer (see Figure 7.10).

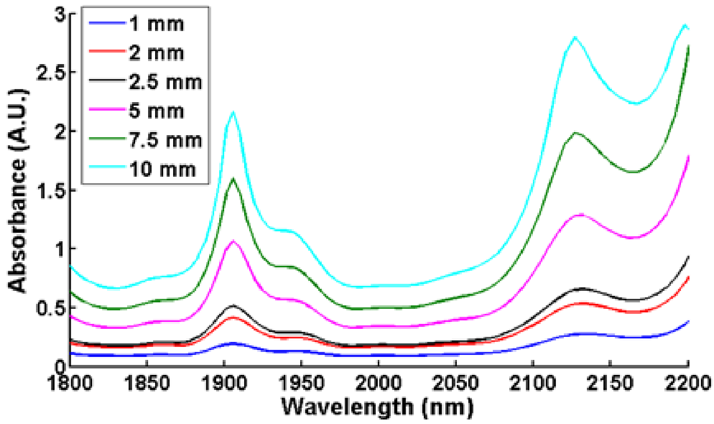

Figure 7.9: NIR spectral response of acrylic sheets at different thicknesses

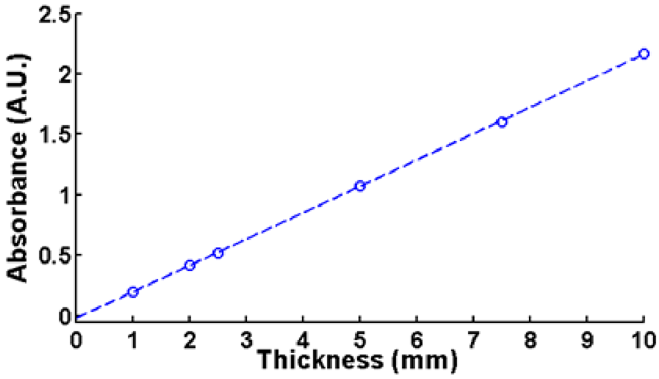

Figure 7.10: Typical plot for variation of absorbance values at different thicknesses of an acrylic sample