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Fusion Strategies of Spectral Data Generated by MEMS-FPI NIR Spectral Detectors

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Introduction

Spectroscopic methods are used in physics and chemistry to determine the properties of samples or radiation sources based on a measured spectrum. One branch of spectroscopy is near-infrared spectroscopy (NIR spectroscopy), in which the sample to be analyzed is irradiated by an NIR radiation source and the transmitted or reflected radiation is recorded. The NIR radiation (750 nm to 2,500 nm) is plotted over the wavelength as an intensity distribution and evaluated using various methods. Usually statistical but nowadays also machine learning methods are used.
Due to the simplified and partly unnecessary sample preparation, NIR spectroscopy has a decisive advantage over other analytical methods. For this reason, NIR spectroscopy has increasingly been applied, especially in recent years, in agriculture, feed and food production as well as in process chains such as recycling plants.
For consumers as well as process applications, there is a demand for more compact and simpler measurement principles. Thus, MEMS sensors consisting of MEMS devices are increasingly used. MEMS components (microelectromechanical systems) are characterized by a particularly small size and miniaturization of the individual components, so that they have dimensions of only a few micrometers. These days, NIR spectral detectors are also being marketed which are implemented as MEMS components [1].
MEMS-FPI NIR spectral detectors (Figure 1) are technically based on a Fabry-Perot interferometer (FPI). Incident radiation is filtered by an optical bandpass and then reflected between two semi-transparent mirrors. The distance between these mirrors can be varied. Thus, constructive interference occurs for exactly one wavelength and is transmitted through the second mirror; the other spectral regions are cancelled out by destructive interference. The intensity of the filtered wavelength is converted into a proportional current by a photosensor. By continuously varying the distance between the two semi-transparent mirrors, a quasi-continuous spectrum can be generated.

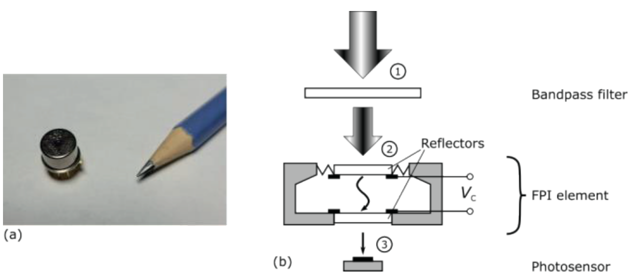

Fig. 1: MEMS-FPI NIR spectral detector (a) and the internal structure (b).

MEMS-FPI NIR spectral detectors have the disadvantage of a reduced spectral range. Typically, these types of detectors only record a partial range of the spectrum of about 300 nm (see table 1). Therefore, several detectors are needed to record the complete NIR spectrum.

Tab. 1: Specifications of MEMS-FPI NIR detectors [2].

Name	Spectral response range	Spectral resolution
C14272	1350 to 1650 nm	18 nm
C13272-03	1550 to 1850 nm	20 nm
C14273	1750 to 2150 nm	22 nm

Problem

In this paper, different fusion approaches of several spectral ranges (partial spectra) to a coherent spectrum shall be investigated. For this purpose, three MEMS-FPI NIR spectral detectors are used to measure different samples and to generate different but coherent spectra. The partial spectra are then combined into a quasi-continuous spectrum using different approaches and finally evaluated.

Experimental Setup

In order to investigate the partial spectra of various MEMS-FPI NIR spectral detectors, sensor electronics were developed and constructed using these detectors. Three spectral detectors from the manufacturer Hamamatsu Photonics K.K. [2] were used. The sensor electronics were designed according to the manufacturer's specifications and controlled using software developed in-house. Figure 2 shows the schematic of the experimental setup.
The detectors were used to measure different types of plastic (polypropylene, polystyrene, PET and polyurethane) with the reflection method. A spectral resolution of 5 nm was set. Each spectral point was measured ten times in succession and then averaged. Four spectra were measured from these already averaged values, which were then also averaged.

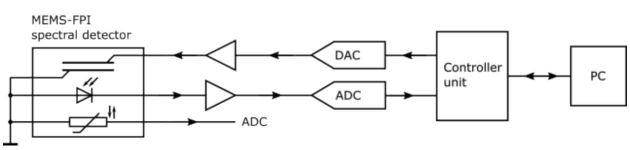

Fig. 2: Schematic experimental setup illustrated for one spectral detector.

By recording dark s_d and reference measurements s_r at the beginning of the measurement series, the absorption spectra A of the respective NIR detectors were determined from the raw values s_m of the intensities according to equation 1.

$$A(i) = \frac{s_m(i) - s_d(i)}{s_r(i) - s_d(i)} \quad (1)$$

As can be seen in Figure 3 (top), three partial spectra are obtained which have overlapping regions. It can be observed that the partial spectra in the overlapping areas show an approximately continuous course, although an offset can be seen at this point. The overlapping areas can be treated by different methods. On the one hand, a separate and distinct observation as well as a fusion of the partial spectra with subsequent evaluation is conceivable.

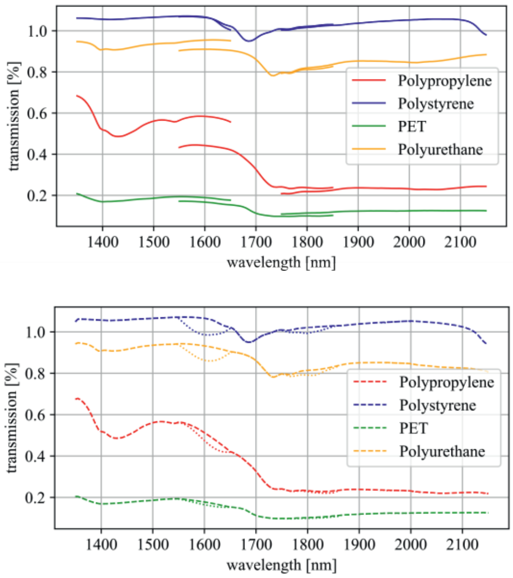

Fig. 3: Separate (top) and merged (bottom) spectra using linear (dotted) and sinusoidal (dashed) interpolation.

Figure 3 (bottom) shows the fusion of the three partial spectra in which the overlapping regions were approximated by a regression in which the regions were merged by a linear function. Also shown in Figure 3 (bottom) is the interpolation of the spectra using a sinusoidal function corresponding to equation 2 in the region of overlapping. A_l and A_r, respectively, describe the spectra converging to the left and right into the superposition region.

$$A(i) = \frac{1}{4} A_l(i) \left(\sin\left(i - \frac{\pi}{2}\right) + 1 \right) + \frac{1}{4} A_r(i) \left(\sin\left(i + \frac{\pi}{2}\right) + 1 \right) \quad (2)$$

In the fusion approaches mentioned above, the normalization and the offset of the partial spectra were not taken into account. However, both play a decisive role in the evaluation of NIR spectra. One possibility of fusion is the normalization to one of the partial spectra and the subsequent interpolation. Such a fitting was performed with the middle partial spectrum (1550 nm to 1850 nm).

In addition to the possibilities already mentioned, various methods of interpolation or regression can be used to fuse the partial spectra and obtain a quasi-continuous spectrum. For these, also so-called routing problems, different methods are used. Among others, a classical spline method can be applied.

Results

In order to evaluate the fusion of the partial spectra into a quasi-continuous spectrum, a multivariate data analysis was performed. Here, the spectra were first smoothed according to Savitzky-Golay and then a baseline correction was performed. A Principal Component Analysis (PCA) was chosen as the evaluation method for the general estimation of the separation and determination of the scores.

Figure 4 shows the PCA scores plot for the sinusoidal interpolation test series. In the scores plot it can be seen that the different plastics can be well separated from each other. Using only two latent variables PC-1 and PC-2, it is already possible to separate the different plastics.

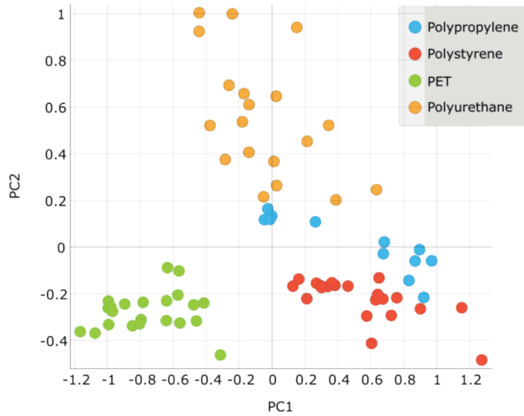

Fig. 4: PCA results of the test series using a sinusoidal interpolation.

The evaluation was performed with all fusion algorithms and the spectra were subsequently classified. Different classification methods were used to separate the plastic types as clearly as possible. Table 2 shows the results according to the different fusion approaches. The results of the two methods Random Forest and Logistic Regression are shown. Random Forest is a classification and regression method, which consists of several uncorrelated decision trees, which are concatenated one after the other. Logistic Regression is a statistical method of regression analysis of mostly multiple variables.

The AUC score (Area Under Curve) indicates the normalized area under an ROC curve, which corresponds to the relative frequency distribution of the sensitivity and false positive rate. Thus, a statement can be made about the hit probability of the classification. The CA score (Classification Accuracy), on the other hand, describes the ratio of correctly classified versus all classifications. The value can be interpreted as a percentage value. The metrics were determined separately for each case and then averaged.

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Tab. 2: Results of classification analysis.

Fusion methods	Model	AUC	CA
Partial spectra	Random Forest	0.992	0.950
	Logistic Regression	0.951	0.932
Linear interpolation	Random Forest	0.983	0.966
	Logistic Regression	0.913	0.892
Sinus interpolation	Random Forest	0.996	0.981
	Logistic Regression	0.995	0.952
Spline	Random Forest	0.852	0.844
	Logistic Regression	0.790	0.756

From table 2 it can be seen that the sinusoidal interpolation, apart from the separate consideration, provides the best results over all classification models. This is followed by linear interpolation. The spline method gives the worst results.
With the sinusoidal interpolation a weighted regression between the partial spectra takes place whereby a smooth transition between the overlapping area or the regression area and the rest of the spectrum takes place. According to the analysis results, this ensures a good fusion of the partial spectra to a coherent spectrum without losing essential information. With the spline method, on the other hand, the actual spectrum is too strongly influenced by the interpolation, which negatively affects the spectral information at these points and makes analysis more difficult.
Current investigations determine the influence of the fusion of the partial spectra regarding the quantitative analysis of more complex samples. Among other things, the significance is investigated by means of various methods such as Partial Least Squares (PLS).

Conclusion

In this paper, different approaches for the fusion of partial spectra generated by MEMS-FPI NIR spectral detectors were presented. For this purpose, MEMS-FPI NIR spectral detectors were used to measure different samples for different spectral ranges and the resulting partial spectra were displayed together. The partial spectra have overlapping ranges which were smoothed and regressed by different methods. Subsequently, the resulting spectra were evaluated by chemometric methods and compared with the original partial spectra. It could be proven that the fusion of the spectra by means of a sine function does not negatively influence the interpretability of the spectra.

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