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Differentiation and Identification of Polymers using LIBS in Combination with Multivariate Analysis Techniques

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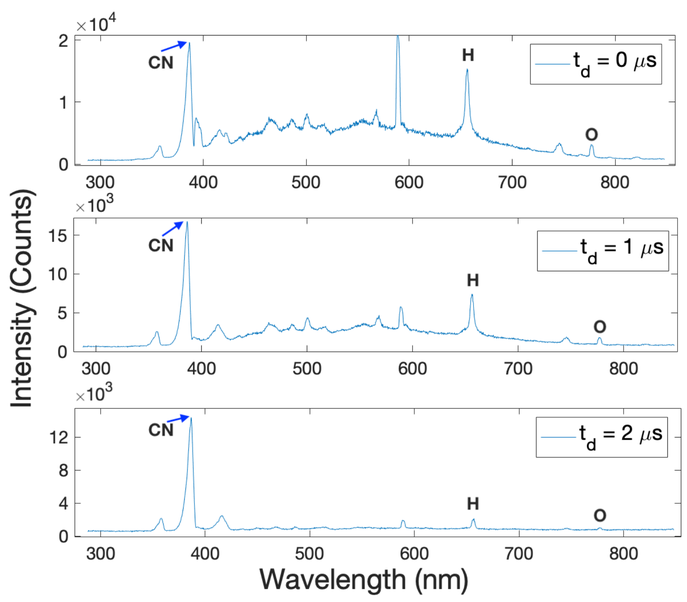
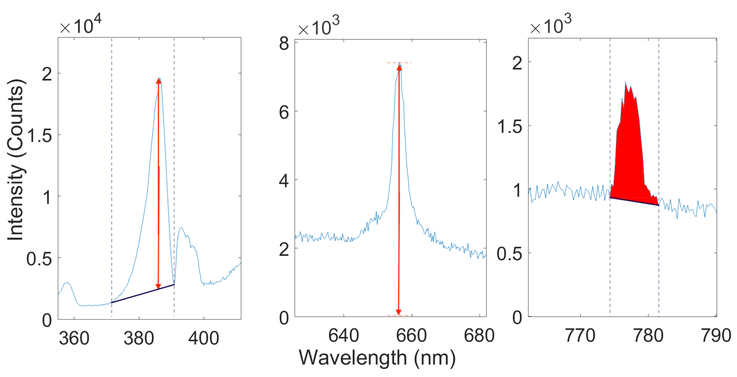
1. Introduction

Every year, hundreds of millions of tonnes of polymer waste are being produced. This has made it necessary for new methods of polymer sorting to be developed. Laser-induced breakdown spectroscopy (LIBS) has received a lot of recognition for its potential applications in polymer identification, since it allows for fast analysis without sample preparation. The proposed method aims to differentiate and identify seven different polymers using LIBS in combination with Principal Component Analysis (PCA) and k-means algorithms.

2. Acquisition and spectral analysis

During LIBS, a pulsed laser creates a plasma by ablating and exciting a portion of the sample material. During this process, a background continuum and spectral lines are emitted. The continuum decays faster, allowing the spectral lines to be analyzed. For this reason, a delay time t_d between the initiation of the laser pulse and the recording of the signal is set. The atoms and ions of an optically thin plasma will emit line radiation, resulting in a complex spectrum containing information about the elemental composition of the ablated material. Like this, it is possible to distinguish different materials.

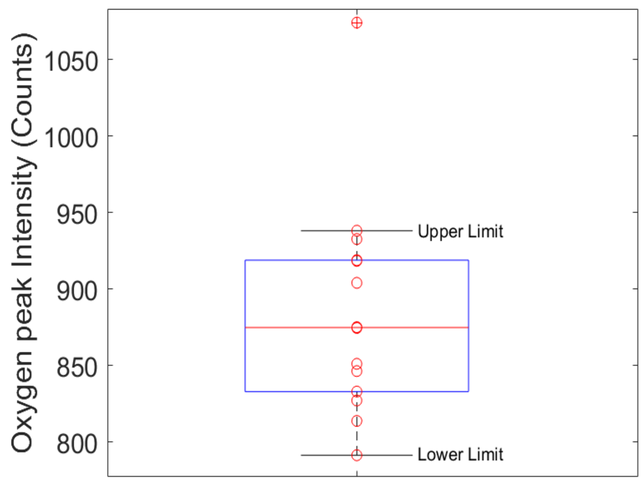


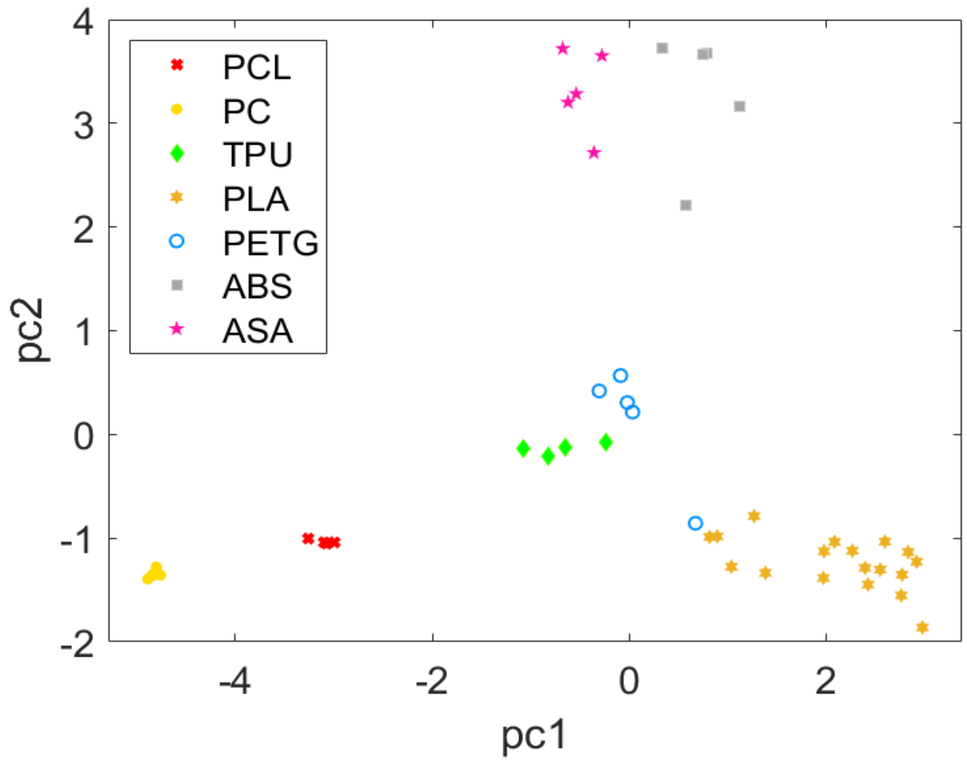


The raw spectra need to be processed so that the relevant chemical information needed to identify each polymer can be extracted. For that, the information was obtained in the form of spectral descriptors. These represent properties of specific regions of each spectrum, such as peak intensities or areas, selected in regions that differ from polymer to polymer. In this study, the chosen regions were the ones comprising the cyanide (-CN), hydrogen (H) and oxygen (O) peaks. As these descriptors were calculated for the three peaks, a total of nine descriptors were used.
To process the information from these descriptors, the k-means clustering algorithm was used, clustering the data into groups based on their similarities. PCA was then employed to reduce the dimensionality of this problem.
The Adjusted Rand Index (ARI) and cluster variability were then used to evaluate the quality of the results. ARI was used as a measure for cluster purity, while cluster variability was used as a measure for how spread the data within each cluster was.

3. Results

With the optimized setup settings, 1 μs delay time and a laser power of 130 mW, the differentiation of seven polymer types was possible. In order to achieve a higher accuracy, an outlier removal process was carried out by means of the Interquartile Range (IQR) rule.





PLA samples with nine different colors were used to verify that color additives would not have a strong impact on the clustering process. All the PLA samples are contained in the same cluster, indicating that the methodology applied is not strongly influenced by the sample colors. However, repeatability was limited, as cluster positions change for different measuring sessions. This drawback might be caused by changing experimental conditions, such as small misalignments in the focusing of plasma light on the optical fiber or changes in atmospheric conditions.

4. Conclusions

LIBS has proven to be a reliable method for the differentiation and classification of polymers when coupled with multivariate analysis techniques. In addition, with the methodology used, the influence of color additives in the differentiation process was successfully surpassed. Although repeatability was found to be limited, the methodology used for the differentiation of the polymers shows promise, as this work was carried out under non-controlled experimental conditions.

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