Investigating Complex LIBS Samples Through the Integration of Raman Spectroscopy and Advanced Machine Learning Methods

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Laser-induced breakdown spectroscopy (LIBS) which is an optical spectroscopy technique relies on data visualizations to interpret experimental results of spectra data. Dendrograms are most commonly used for this task, however, there are a number of algorithmic issues that arise with this method. Thus, to limit the practical issues that arise within hierarchical clustering methods, this paper explores additional advanced machine learning methods to more effectively visualize and analyze LIBS spectra data. These additional methods include refinements to the already commonly used clustering approach, as well as the addition of K-Means methods in conjunction with Raman spectroscopy data for faster and more reliable sample identification, classification, and pattern recognition. To best illustrate the proposed methodology, we used spectra data that was obtained from a laboratory LIBS set up as well as a handheld LIBS unit. The data constituted of spectra obtained from various complex samples consisting of Lead (Pb), Chromium (Cr), Tin (Sn), Gold (Au), Tantalum (Ta), Niobium (Nb). To perform the physical analysis, the open-source statistical programming language R was used in combination with various packages that will be described in detail in the presentation. In summary, by using this newly refined approach we aim to improve spectra visualization to allow for more efficient and effective interpretation.