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Application of Graph Theory to Unsupervised Classification of Materials by Laser-Induced Breakdown Spectroscopy

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Abstract

In this paper we present a new approach for unsupervised classification of materials from the spectra obtained using the Laser-Induced Breakdown Spectroscopy technique. The method is based on the calculation of the correlation matrix between the LIBS spectra, which is interpreted as an Adjacency matrix in the framework of Graph theory. A threshold is applied on the edge values, which is determined through maximization of the Modularity of the Graph. The classification of the spectra is done automatically after the calculation of the Modularity parameter. An example of the application of the proposed method is given, based on the study of six bronze standards of known composition. The advantages of the proposed approach with respect to Principal Component Analysis are also discussed.

Keywords: Laser-Induced Breakdown Spectroscopy; Unsupervised Classification; Graph Theory; Principal Component Analysis; Visual Analytics.

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