Quantitative Elemental Analysis Using Laser-Induced Breakdown Spectroscopy and 1D Convolutional Neural Networks

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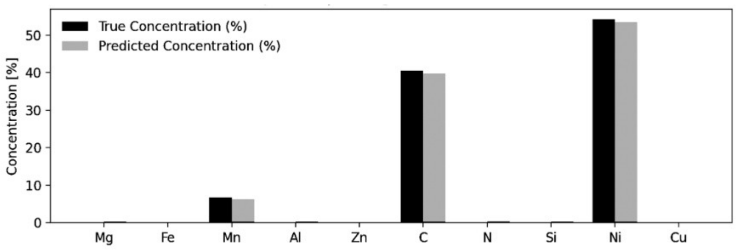
Laser-Induced Breakdown Spectroscopy (LIBS) is a powerful analytical technique for elemental analysis, however the manual interpretation of complex spectral datasets remains a significant challenge [1]. This work presents a machine learning-based framework designed to automate and enhance the prediction of elemental composition directly from LIBS spectra. To overcome the scarcity of large, annotated experimental datasets, training data was generated synthetically using NIST Atomic Spectra Database.

Rather than limiting the task to binary element detection, we address the more demanding problem of concentration estimation across a broad spectral window (200–1000 nm). We propose a customized 1-Dimensional Convolutional Neural Network (1D CNN) that efficiently captures spectral features characteristic of atomic emission. To manage problem complexity and stabilize the training process, the model is initially evaluated on a representative subset of 10 elements.

The figure below presents the results of the proposed model for a representative LIBS spectrum. The comparison between true and predicted concentrations shows that the model accurately reproduces the elemental composition of the sample.



The result of the proposed model on a spectrum of a sample consisting of carbon (C), manganese (Mn) and nickel (Ni).

[1] P. Dehbozorgi et al. (2026) Analysis and Sensing, 6, e202500106.

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