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A novel baseline correction method using convex optimization framework in laser-induced breakdown spectroscopy quantitative analysis

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Abstract: For laser-induced breakdown spectroscopy (LIBS) quantitative analysis technique, baseline correction is an essential part for the LIBS data preprocessing. As the widely existing cases, the phenomenon of baseline drift is generated by the fluctuation of laser energy, inhomogeneity of sample surfaces and the background noise, which has aroused the interest of many researchers. Most of the prevalent algorithms usually need to preset some key parameters, such as the suitable spline function and the fitting order, thus do not have adaptability. Based on the characteristics of LIBS, such as the sparsity of spectral peaks and the low-pass filtered feature of baseline, a novel baseline correction and spectral data denoising method is studied in this paper. The improved technology utilizes convex optimization scheme to form a non-parametric baseline correction model. Meanwhile, asymmetric punish function is conducted to enhance signal-noise ratio (SNR) of the LIBS signal and improve reconstruction precision. Furthermore, an efficient iterative algorithm is applied to the optimization process, so as to ensure the convergence of this algorithm. To validate the proposed method, the concentration analysis of Chromium (Cr) ,Manganese (Mn) and Nickel (Ni) contained in 23 certified high alloy steel samples is assessed by using quantitative models with Partial Least Squares (PLS) and Support Vector Machine (SVM). Because there is no prior knowledge of sample composition and mathematical hypothesis, compared with other methods, the method proposed in this paper has better accuracy in quantitative analysis, and fully reflects its adaptive ability.

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