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Statistical evaluation of spectral interferences in LIBS

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ABSTRACT: Line broadening due to plasma processes or the instrument degrade spectral resolution leading to uncertainty in the elemental profile obtained by optical emission spectroscopy. A novel approach to quantify spectral interferences in laser-induced breakdown spectroscopy (LIBS) is introduced. This algorithm establishes a statistical interference factor (SIF) to quantify spectral interferences for individual line assignment in LIBS while using the full information provided by a spectrum. This factor combines fundamentals of plasma emission with a Bayesian analysis of the experimental spectrum using eventual prior knowledge about the sample and/or the conditions of analysis. Two types of prior knowledge were used to interpret spectra from a pure silicon sample as well as a NIST SRM 610 glass sample and alumina with a controlled Ni contamination at different concentrations. Knowledge of the elemental composition confirmed the existence of spectral lines with high sensitivity to interference while other lines are more appropriate for analysis by having their attribution stable despite having knowledge of the composition.

Laser induced breakdown spectroscopy (LIBS) itself is a technique of atomic emission spectroscopy which provides qualitative and quantitative elemental analysis of samples under investigation. There are many advantages of using LIBS including little to no sample preparation[1], minimal loss of sample[2], real time analysis[3], and analysis of materials in any state of matter[4]. LIBS has been applied to many environmental[5,6,7], biomedical[8,9], forensics[10,11,12], and industrial[13,14] application fields, to name a few.

The elemental analysis starts with the assignment of spectral lines. The reference for spectral line assignment is a database such as the National Institute of Standards and Technology Atomic Spectra Database (NIST)[15], Atomic Line List Harvard-Smithsonian Center for Astrophysics (Kurucz)[16], or Massachusetts Institute of Technology Wavelength tables (MIT)[17]. Each database contains information on the experimental or calculated emission lines of atoms and ions by their emission wavelength, probability of emission, and energy level involved in the transition.

The spectral line assignment can be tainted by spectral interferences. While high spectral resolution is a first step for confidence in spectral line assignment, it cannot prevent all spectral interferences that occur: spectral line coincidence[19], overlap with a broadened line wing[20], spectrometer stray light[21], and background continuum[22]. These interferences create uncertainty in the line assignment for elemental analysis.

Quantifying the spectral interference is needed for a more accurate analysis[23] and validation of method[24]. Such quantification being included in the calculation of error rates can lead to reduction