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Tesis: **"SEMI-AUTOMATIC ELEMENTAL IDENTIFICATION AND QUANTIFICATION BY LASER-INDUCED BREAKDOWN SPECTROSCOPY"**

Resumen:

Chemical analysis has deep effects in our everyday lives, it is not only used as a tool for quality control, but also for designing better materials to meet everyday needs. One of the optical techniques used in recent times for chemical analysis has been the Laser-Induced Breakdown Spectroscopy (LIBS); an atomic emission spectroscopy technique with many advantages being its low cost, lack of sample preparation and reduced acquisition times among the most important. LIBS makes use of a strong focused electromagnetic field to produce a plasma, whose spectral emission is a signature that uniquely identifies every chemical element contained in the sample. Automatic elemental identification is a task that has not been resolved completely since human intervention is still required. In this work, a new procedure for semi-automatic identification of emission species in LIBS spectra was developed, where major elements are identified automatically. Although minor emission elements and traces still need human intervention, it is enough to relax the search conditions in the proposed procedure to obtain a high precision identification. LIBS is not only used to determine sample's elemental content but also to perform quantitative analysis. Since its origins, LIBS qualitative analysis has relied on external standards; i.e. materials with known composition, which are used to obtain calibration curves. Although this method is still the most precise in terms of quantification limits, there are situations where standards are very expensive or nearly impossible to obtain. An alternative route is provided by the so called standarless quantification procedures, such as Calibration-Free (CF), that relieves the requirement of an external standard at expenses of elaborated calculations. One of the most complicated computation procedures required by the CF method is the spectral deconvolution, due to the high number of spectral emission lines measured in a LIBS spectrum. A novel automatic deconvolution procedure was proposed in this work, which is aimed to overcome some weakness of the traditional methods used for deconvolution, as the Levenberg–Marquardt algorithm. The original work of CF states that, in order to make a proper quantification, every element present in the sample must be measured. However, it is shown in this work that the cited requirement is not necessary, because the concentration ratio for two distinct elements, measured by means of a LIBS spectrum, is independent of the other emission species.