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激光诱导击穿光谱定量分析钢铁和铝合金中的元素

张宁1,李嘉铭1*,张庆茂1,郭亮1

1华南师范大学,信息光电子科技学院,51006

* jmli@m.scnu.edu.cn

钢铁和铝合金在国民经济和国防工业上都是非常重要的金属,广泛应用于航空、航天及汽车等领域。在冶炼、加工制造及分类回收等过程中实时在线进行元素成分的定量分析显得尤为重要。然而,传统的方法,如 AAS、ICP-MS、ICP-AES 和 XRF等通常受限于复杂的预处理,仪器价格昂贵等条件,难以做到实时在线监测。激光诱导击穿光谱是一种可以对样品中的元素进行定性及定量分析的原子发射光谱技术。目前,常用的定量分析方法包括标准曲线法和免定标法。标准曲线法是通过一系列的标准样品建立以横坐标为浓度纵坐标为光谱相对强度的线性曲线。标准曲线法通常对应较好的定量分析的准确度,平均相对误差基本低于10%。然而,标准曲线法需要标准样品,无法分析基体元素,易受基体效应影响,限制了此法在人体生物组织,矿产等领域的应用。结合机器学习的方法可以有效提高分析的精密度和准确度。免定标激光诱导击穿光谱通过数学模型描述等离子物理状态,无需标准样品,不受基体效应的影响,定量分析准确度较低的限制可以通过自吸收校正及一点定标法进行补偿。总的来说,免定标法在元素定量分析的层面上有很大的应用前景。

关键词:钢铁;铝合金;激光诱导击穿光谱;定量分析;准确度



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Both sheets of steel and aluminum alloys are vital essential metals in the national economy and defense industry, and they widely used in the fields of aeronautics, astronautics, and cars. The quantitative elemental composition analysis is particularly important in real-time online during the smelting, processing, manufacturing, sorting, and recovery processes. However, traditional methods such as AAS, ICP-MS, ICP-AES, and XRF are often limited to conditions of complex pre-processing, and expensive instruments, which make real-time online monitoring difficult. Laser-induced breakdown spectroscopy is an atomic spectroscopy that enables the qualitative and quantitative analysis of elements in samples. Currently, the commonly used methods for quantitative analysis are the calibration curve method and the calibration-free method. The calibration curve method involves the construction of a curve from a series of referenced samples with the elemental concentration as a horizontal coordinate and the relative intensity of the spectrum as a vertical coordinate. The calibration curve method usually corresponds to better accuracy of quantitative analysis, with an average relative error of generally less than 10%. However, the calibration curve method requires referenced samples, suffering from matrix effects easily, and can not analyze matrix elements, limiting the application of this method to biological tissue, minerals, and other areas. An approach that combines machine learning can effectively improve the precision and accuracy of the analysis. Calibration-free laser-induced breakdown spectroscopy describes the physical state of the plasma utilizing a mathematical model, without the need for referenced samples, independent of matrix effects, and the limitations of the lower accuracy of quantitative analysis can be compensated by the methods of one-point calibration and self-absorption correction. Overall, the calibration-free method has great potential for application in the background of quantitative elemental analysis.

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- *第一作者(报告人)联系方式: 张宁、13710591544、2020022434@m.scnu.edu.cn