

1. Record Nr.	UNINA9910623989403321
Autore	Palleschi Vincenzo
Titolo	Chemometrics and Numerical Methods in LIBS
Pubbl/distr/stampa	Newark : , : John Wiley & Sons, Incorporated, , 2022 ©2022
ISBN	1-119-75961-7 1-119-75957-9 1-119-75956-0
Descrizione fisica	1 online resource (381 pages)
Disciplina	543.52
Soggetti	Electronic books.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Cover -- Title Page -- Copyright Page -- Contents -- List of Contributors -- Preface -- Introduction and Brief Summary of the LIBS Development -- Part I Introduction to LIBS -- Chapter 1 LIBS Fundamentals -- 1.1 Interaction of Laser Beam with Matter -- 1.2 Basics of Laser-Matter Interaction -- 1.3 Processes in Laser-Produced Plasma -- 1.4 Factors Affecting Laser Ablation and Laser-Induced Plasma Formation -- 1.4.1 Influence of Laser Parameters on the Laser-Induced Plasmas -- 1.4.2 Laser Wavelength () -- 1.4.3 Laser Pulse Duration () -- 1.4.4 Laser Energy (E) -- 1.4.5 Influence of Ambient Gas -- 1.5 Plasma Properties and Plasma Emission Spectra -- References -- Chapter 2 LIBS Instrumentations -- 2.1 Basics of LIBS instrumentations -- 2.2 Lasers in LIBS Systems -- 2.3 Desirable Requirements for Atomic Emission Spectrometers/Detectors -- 2.4 Spectrometers -- 2.4.1 Czerny-Turner Optical Configuration -- 2.4.2 Paschen-Runge Design -- 2.4.3 Echelle Spectrometer Configuration -- 2.5 Detectors -- 2.5.1 Photomultiplier Detectors -- 2.5.2 Solid-State Detectors -- 2.5.3 The Interline CCD Detectors -- 2.5.3.1 The Image Intensifier -- References -- Chapter 3 Applications of LIBS -- 3.1 Industrial Applications -- 3.1.1 Metal Industry -- 3.1.2 Energy Production -- 3.2 Biomedical Applications -- 3.3 Geological and Environmental Applications -- 3.4 Cultural Heritage and Archaeology

Applications -- 3.5 Other Applications -- References -- Part II
Simplifications of LIBS Information -- Chapter 4 LIBS Spectral Treatment
-- 4.1 Introduction -- 4.2 Baseline Correction -- 4.2.1 Polynomial
Algorithm -- 4.2.2 Model-free Algorithm -- 4.2.3 Wavelet Transform
Model -- 4.3 Noise Filtering -- 4.3.1 Wavelet Threshold De-noising
(WTD) -- 4.3.2 Baseline Correction and Noise Filtering -- 4.4
Overlapping Peak Resolution.
4.4.1 Curve Fitting Method -- 4.4.2 The Wavelet Transform -- 4.5
Features Selection -- 4.5.1 Principal Component Analysis -- 4.5.2
Genetic Algorithm (GA) -- 4.5.3 Wavelet Transformation (WT) --
References -- Chapter 5 Principal Component Analysis -- 5.1
Introduction -- 5.1.1 Laser-Induced Breakdown Spectroscopy (LIBS) --
5.2 The Principal Component Analysis (PCA) -- 5.3 PCA in Some LIBS
Applications -- 5.3.1 Geochemical Applications -- 5.3.2 Food and
Feed Applications -- 5.3.3 Microbiological Applications -- 5.3.4
Forensic Applications -- 5.4 Conclusion -- References -- Chapter 6
Time-Dependent Spectral Analysis -- 6.1 Introduction -- 6.2 Time-
Dependent LIBS Spectral Analysis -- 6.2.1 Independent Component
Analysis -- 6.2.2 3D Boltzmann Plot -- 6.2.2.1 Principles of the
Method -- 6.3 Applications -- 6.3.1 3D Boltzmann Plot Coupled with
Independent Component Analysis -- 6.3.2 Analysis of a Carbon Plasma
by 3D Boltzmann Plot Method -- 6.3.3 Assessment of the LTE
Condition Through the 3D Boltzmann Plot Method -- 6.3.4 Evaluation
of Self-Absorption -- 6.3.5 Determination of Transition Probabilities
-- 6.3.6 3D Boltzmann Plot and Calibration-free Laser-induced
Breakdown Spectroscopy -- 6.4 Conclusion -- References -- Part III
Classification by LIBS -- Chapter 7 Distance-based Method -- 7.1
Cluster Analysis -- 7.1.1 Introduction -- 7.1.2 Theory -- 7.1.2.1 K-
means Clustering -- 7.1.2.2 Hierarchical Clustering -- 7.1.3
Application -- 7.2 Independent Components Analysis -- 7.2.1
Introduction -- 7.2.2 Theory -- 7.2.3 Application -- 7.3 K-Nearest
Neighbor -- 7.3.1 Introduction -- 7.3.2 Theory -- 7.3.3 Application
-- 7.4 Linear Discriminant Analysis -- 7.4.1 Introduction -- 7.4.2
Theory -- 7.4.2.1 The Calculation Process of LDA (Two Categories) --
7.4.3 Application.
7.5 Partial Least Squares Discriminant Analysis -- 7.5.1 Introduction
-- 7.5.2 Theory -- 7.5.3 Application -- 7.6 Principal Component
Analysis -- 7.6.1 Introduction -- 7.6.2 Theory -- 7.6.3 Application
-- 7.7 Soft Independent Modeling of Class Analogy -- 7.7.1
Introduction -- 7.7.2 Theory -- 7.7.3 Application -- 7.8 Conclusion
and Expectation -- References -- Chapter 8 Blind Source Separation in
LIBS -- 8.1 Introduction -- 8.2 Data Model -- 8.3 Analyzing LIBS Data
via Blind Source Separation -- 8.3.1 Second-order BSS -- 8.3.2
Maximum Noise Fraction -- 8.3.3 Independent Component Analysis --
8.3.4 ICA for Noisy Data -- 8.4 Numerical Examples -- 8.5 Final
Remarks -- References -- Chapter 9 Artificial Neural Networks for
Classification -- 9.1 Introduction and Scope -- 9.2 Artificial Neural
Networks (ANNs) -- 9.3 Cost Functions and Training -- 9.4
Backpropagation -- 9.5 Convolutional Neural Networks -- 9.6
Evaluation and Tuning of ANNs -- 9.7 Regularization -- 9.8 State-of-
the-art LIBS Classification Using ANNs -- 9.9 Summary --
Acknowledgments -- References -- Chapter 10 Data Fusion: LIBS +
Raman -- 10.1 Introduction -- 10.2 Data Fusion Background -- 10.3
Data Treatment -- 10.4 Working with Images -- 10.4.1 Vectors
Concatenation -- 10.4.2 Vectors Co-addition -- 10.4.3 Vectors Outer
Sum -- 10.4.4 Vectors Outer Product -- 10.4.5 Data Analysis -- 10.5
Applications -- 10.6 Conclusion -- References -- Part IV Quantitative
Analysis -- Chapter 11 Univariate Linear Methods -- 11.1 Standards

-- 11.2 Matrix Effect -- 11.3 Normalization -- 11.4 Linear vs Nonlinear Calibration Curves -- 11.5 Figures of Merit of a Calibration Curve -- 11.5.1 Coefficient of Determination -- 11.5.2 Root Mean Squared Error of Calibration -- 11.5.3 Limit of Detection -- 11.6 Inverse Calibration -- 11.7 Conclusion -- References.

Chapter 12 Partial Least Squares -- 12.1 Overview -- 12.2 Partial Least Squares Regression Algorithms -- 12.2.1 Nonlinear Iterative PLS -- 12.2.2 SIMPLS Algorithm -- 12.2.3 Kernel Partial Least Squares -- 12.2.4 Locally Weighted Partial Least Squares -- 12.2.5 Dominant Factor-based Partial Least Squares -- 12.3 Partial Least Squares Discriminant Analysis -- 12.4 Results of Partial Least Squares in LIBS -- 12.4.1 Coal Analysis -- 12.4.2 Metal Analysis -- 12.4.3 Rocks, Soils, and Minerals Analysis -- 12.4.4 Organics Analysis -- 12.5 Conclusion -- References -- Chapter 13 Nonlinear Methods -- 13.1 Introduction -- 13.2 Multivariate Nonlinear Algorithms -- 13.2.1 Artificial Neural Networks -- 13.2.1.1 Conventional Artificial Neural Networks -- 13.2.1.2 Convolutional Neural Networks -- 13.2.2 Other Nonlinear Multivariate Approaches -- 13.2.2.1 The Franzini-Leoni Method -- 13.2.2.2 The Kalman Filter Approach -- 13.2.2.3 Calibration-Free Methods -- 13.3 Conclusion -- References -- Chapter 14 Laser Ablation-based Techniques - Data Fusion -- 14.1 Introduction -- 14.2 Data Fusion of Multiple Analytical Techniques -- 14.2.1 Low-level Fusion -- 14.2.2 Mid-level Fusion -- 14.2.3 High-level Fusion -- 14.3 Data Fusion of Laser Ablation-Based Techniques -- 14.3.1 Introduction -- 14.3.2 Classification of Edible Salts -- 14.3.2.1 LIBS and LA-ICP-MS Measurements of the Salt Samples -- 14.3.2.2 Mid-Level Data Fusion of LIBS and LA-ICP-MS of Salt Samples -- 14.3.2.3 PLS-DA Classification Model for Salt Samples -- 14.3.3 Coal Discrimination Analysis -- 14.3.3.1 LIBS and LA-ICP-TOF-MS Measurements of the Coal Samples -- 14.3.3.2 Mid-Level Data Fusion of LIBS and LA-ICP-TOF-MS of Coal Samples -- 14.3.3.3 PCA Combined with K-means Cluster Analysis for Coal Samples -- 14.3.3.4 PLS-DA and SVM for Coal Samples Analysis.

14.4 Comments and Future Developments -- Acknowledgments -- References -- Part V Conclusions -- Chapter 15 Conclusion -- Index -- EULA.
