Multi-Instrument LIBS Harmonization for Rare-Earth Element Imaging

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Motivation

Rare-earth elements (REEs) present a demanding analytical challenge in LIBS due to their dense emission spectra, extensive line overlap, and strong matrix effects[1]. These factors complicate both elemental identification and quantification, while variations in instrumental configuration, optical alignment, or acquisition parameters further compromise spectral consistency across laboratories. This study presents an interlaboratory evaluation of LIBS applied to REE-bearing minerals, carried out between laboratories in Portugal and the Czech Republic.

Key Ideas

Using shared samples, the work assesses the consistency of spectral features and imaging results across different LIBS setups. Machine-learning models are applied to process and classify spectra, promoting data interoperability and adherence to FAIR principles. This standardized, data-driven processing framework enables cross-laboratory comparison, calibration transfer, and data reuse, even in the presence of strong matrix effects and spectral complexity typical of REE element analysis.

Methodology

Findable	Unique/persistent identifier (PID), rich metadata, searchable data.	Fixed sample ID, provence information
Accessible	Trusted repositories, data collections, access agreements and licenses.	Cloud, Zenodo, Wikidata
Interoperable	Common file formats and structures, standardised spectral descriptors.	.h5 file format, wl, step intensity, nx, ny, energy
Reusable	Usage licenses, files with instructions to interpret data.	Data reader scripts, README files

System	LIBS PT	LIBS CZ
Energy (mJ)	51	8
WL Range (nm)	180 to 920	190 to 860
Spectrometer	Avantes (8 channels)	Lightigo (5 channels)
Laser	Nd:YAG Quantel (1064 nm)	Lightigo (1064 nm)

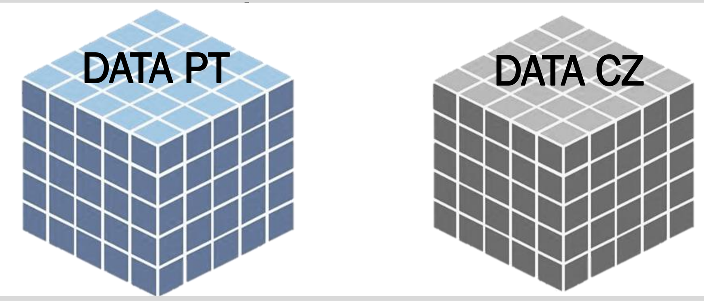
Table 1. Main characteristics of the LIBS systems used in this work.

Sample Description

Figure 1. Sample from Khibiny Mountains, Murmansk Oblast, Russia, with 48 x 38 mm, entirely mapped by the Portuguese LIBS instrument and partially mapped by the Czech Republic LIBS instrument, due to system high sample limitations.

Pipeline

1. Import RAW Data



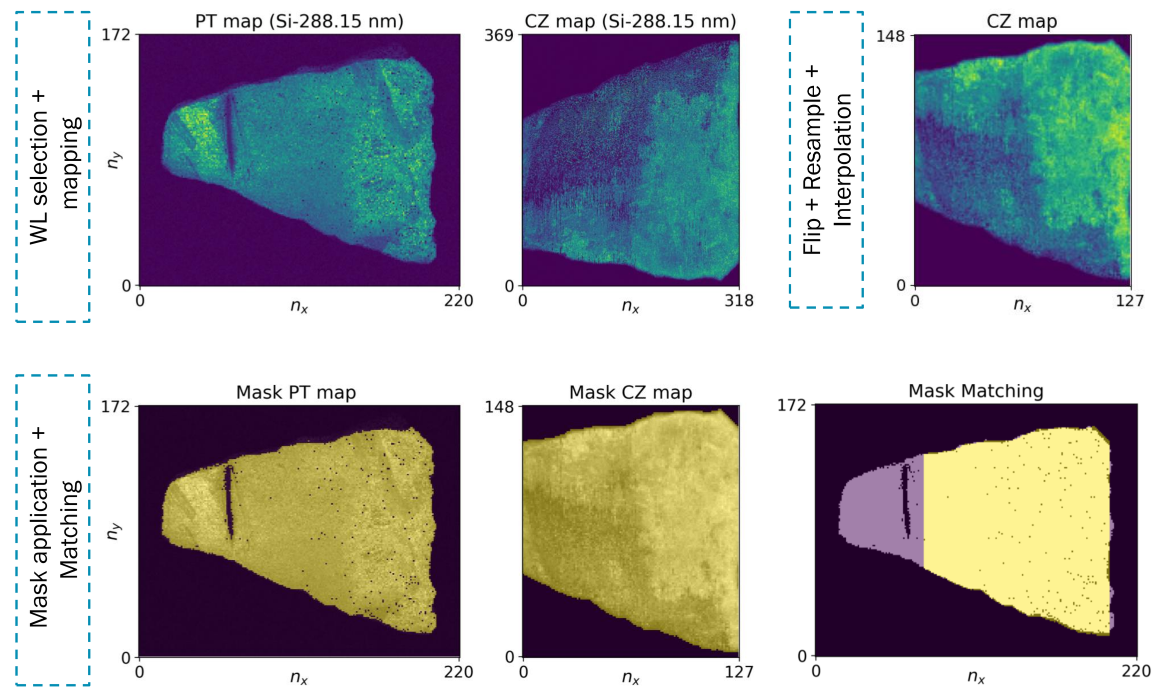
2. Pre-Processing

Baseline Removal

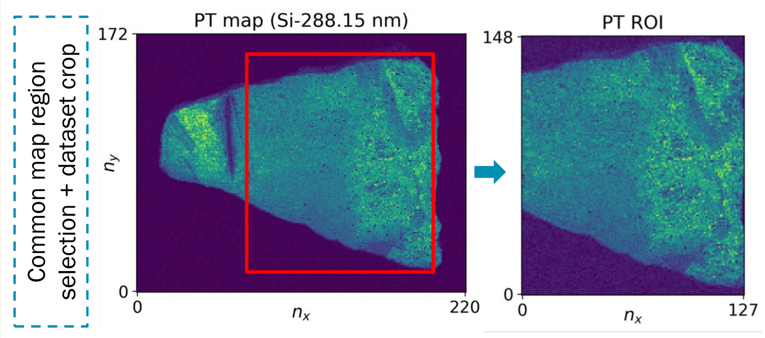
- Assymetric Least Squares Smoothing

3. Dataset Registration and Matching

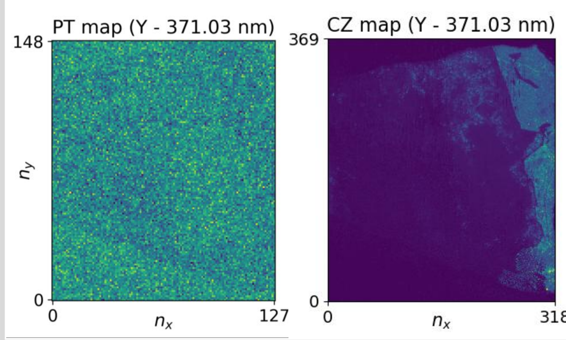
1. Wavelength selection
   - mapping alignment
2. Flip
3. Resample
4. Interpolation
5. Mask
   - Percentile threshold
6. Template matching



4. Region of Interest (ROI)



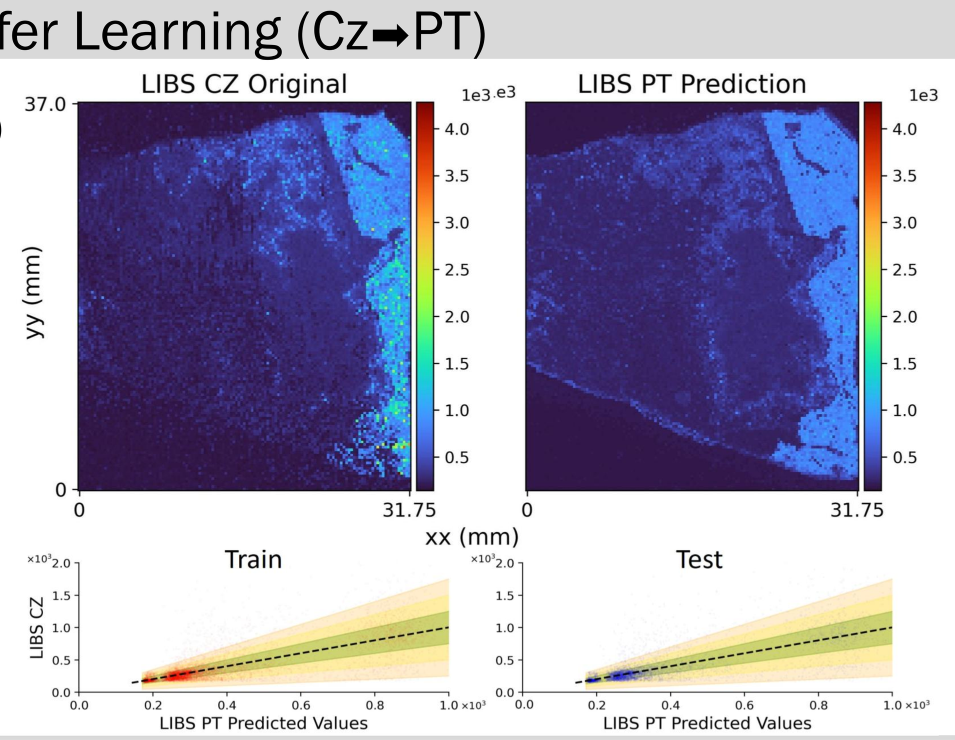
5. Rare Earth Analysis: Yttrium



- PT map without information for the 371.03 nm;
- CZ map shows the Y distribution.
- Transfer knowledge from CZ to PT.

6. Transfer Learning (Cz➡PT)

1. Spectra_CZ ➡ Target Selection(Tr)
   - Y (371.03 nm) map
2. Goal:
   - F[Spectra_PT] = Tr
3. Prevent Overfit:
   - Mutual Information between: Tr and Spectra PT
3. Model:
   - K-Nearest Neighbors (KNN)
   - K=25



Conclusions

The results identify key factors influencing data variability and propose best-practice guidelines for LIBS spectral imaging, **contributing to the development of reliable, reproducible, and instrument-agnostic methodologies** for REE analysis in geochemical and mineralogical studies. The application of the **transfer learning using a KNN method to the Portuguese data enabled the detection of Y with 371.03 nm line**, a map that before has only noise and good performance on the Czech Republic spectral data. This outcome was only possible due to the access to comprehensive metadata describing the analytical conditions and acquisition parameters, thereby enabling cross-laboratory knowledge transfer.

[1] Gaft, M., et al. "Imaging rare-earth elements in minerals by laser-induced plasma spectroscopy: Molecular emission and plasma-induced luminescence." *Spectrochimica Acta Part B: Atomic Spectroscopy* 151 (2019): 12-19.

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