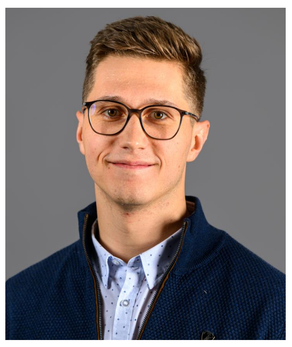
Three-Dimensional Chemical Imaging: Integrating Computed Tomography and Laser-Induced Breakdown Spectroscopy for Multi-Scale Analysis



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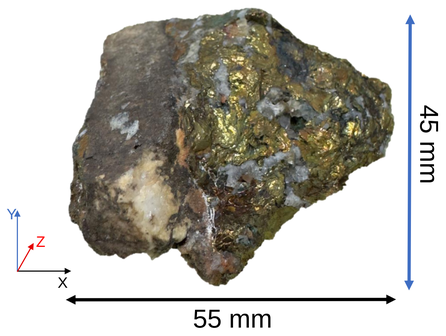
Introduction

Computed Tomography (CT) and Laser-Induced Breakdown Spectroscopy (LIBS) are widely used techniques for material characterization, each offering unique advantages. CT provides high-resolution three-dimensional (3D) morphological information and insights into the internal structures of an object in a non-destructive manner. This distinctive imaging technique has evolved into a versatile tool in various scientific and industrial fields. However, it has limitations in terms of non-visual material characterization, as it lacks the ability to determine the chemical composition. In contrast, LIBS provides high-sensitivity elemental composition analysis but is inherently a surface-based and two-dimensional (2D) method. Additionally, LIBS generally require almost a flat sample surface for reliable measurements, limiting its application for complex geometries and internal chemical analysis. The main goal of this methodology is to combine the strengths of both techniques to achieve three-dimensional material characterization.

Workflow of 3D Localized Chemical Imaging

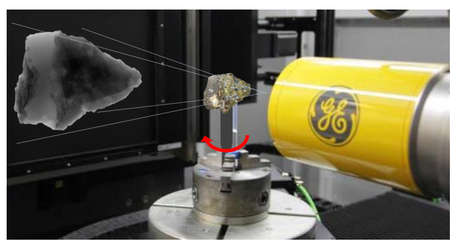
Geological sample

- Chalcopyrite (Morocco)



MicroCT measurement

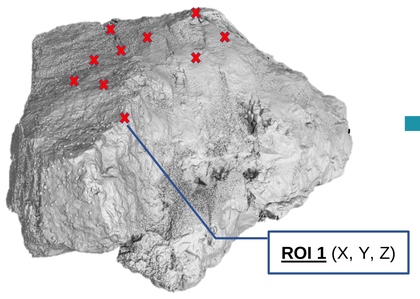
- GE Phoenix v|tome|x L240



- High-resolution 3D imaging without sample destruction
- Reveals internal structures and density variations
- Detailed morphological information

3D model

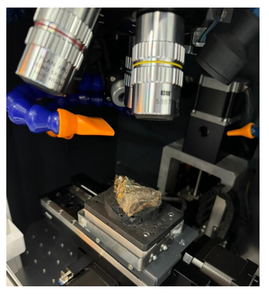
- Volume Graphics - VG Studio Max



- Volume reconstructed from CT measurement
- Definition of coordinates system (compatibility with LIBS)
- Precise selection of regions of interest

LIBS measurement

- Lightigo FireFly

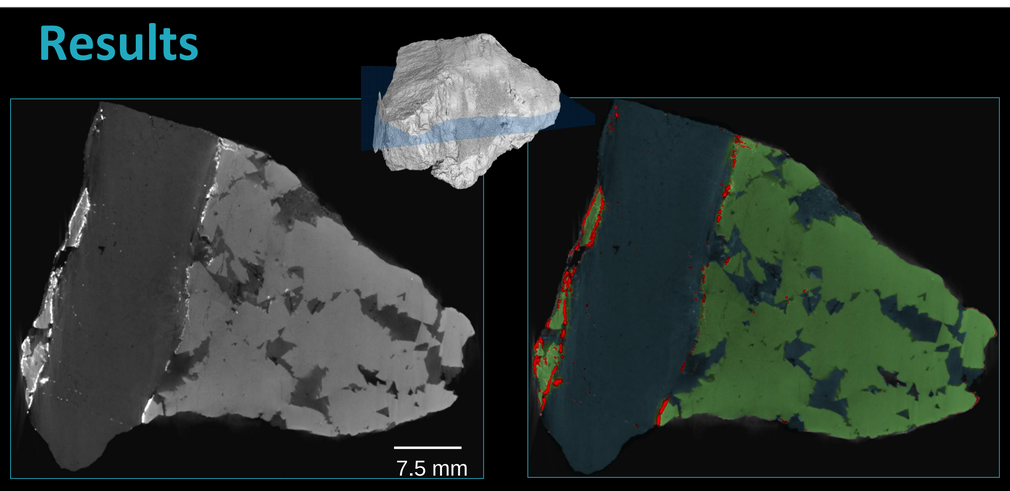


- Localization of the regions of interest
- Chemical analysis of selected regions
- Evaluation of material composition

Key contributions:

- Non-destructive sample preparation and measurements
- Fast analysis of chemical composition in three dimensions
- Preserves the integrity of the original surface

Results



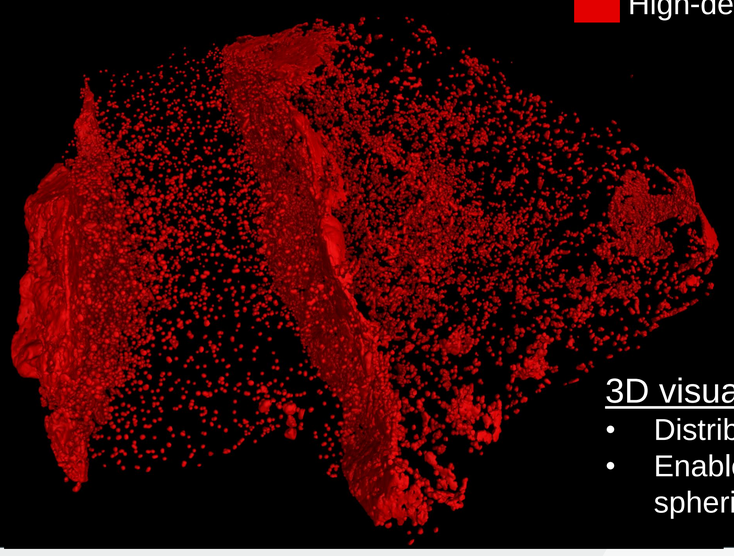
Low-density material

Mid-density material

High-density material

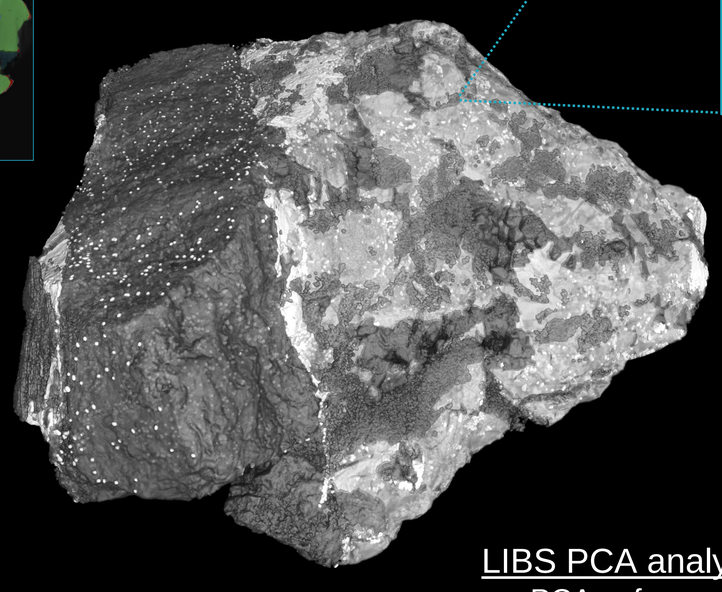
Segmentation

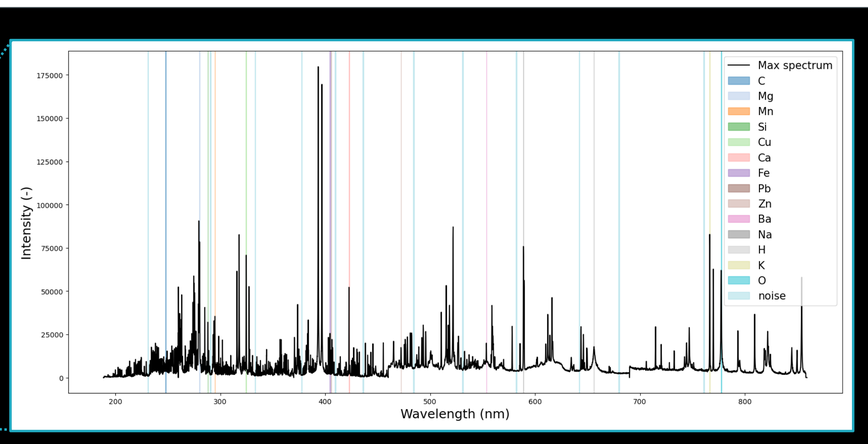
- The combination of thresholding and neural network workflow



3D visualization

- Distribution of high-density particles
- Enables to evaluate size, morphology, sphericity, etc.



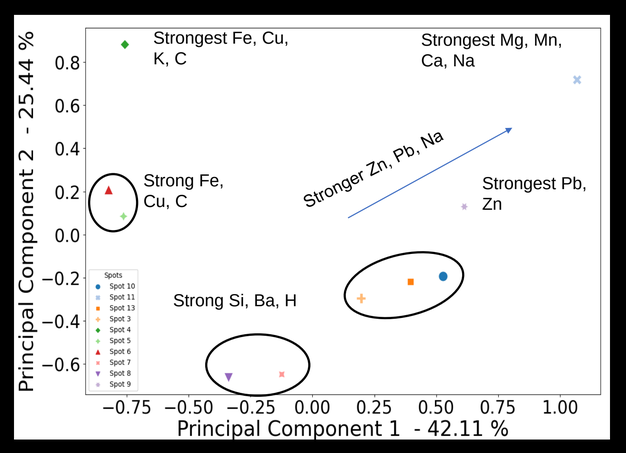


Spectral analysis

- Selected spectral lines based on the maximum intensity across all measurements
- Calculated the spectral line area and SNR, then normalized (0-1) to minimize the impact of stronger lines
- Identified spectral lines of 14 chemical elements

LIBS PCA analysis

- PCA of spectral line SNR revealed three distinct matrix types in the score plot



Limitations and conclusions

We developed hybrid methodology integrating CT and LIBS for multi-scale imaging. This approach enables the precise selection of regions of interest (ROIs) based on CT morphology, followed by targeted LIBS measurements to obtain elemental composition data. By correlating structural and chemical information, we achieve a more comprehensive understanding of heterogeneous geological sample. ROIs must be visible in both CT and LIBS measurements. In complex or highly structured samples, some regions may be shadowed or inaccessible for LIBS. Despite these constraints, the integration of CT and LIBS provides a powerful tool for advanced 3D chemical imaging, with potential applications in materials science, archaeology, and biomedical research.

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