Semi-quantification of elemental concentrations in Ca-Mg-Fe carbonate minerals using a portable Raman spectrometer

Yonghwi Kim*†[1], Marie-Camille Caumon*[1], and Jean Cauzid*[1]

[1]GeoRessources – Univesité de Lorraine, CNRS : UMR7359, Université de Lorraine, CRAN, UMR 7039 – France

Résumé

Semi-quantitative elemental analysis of carbonate minerals, particularly complex Ca–Mg–Fe solid solutions, is essential for accurate geological characterization yet remains challenging using non-destructive field techniques. This study introduces a portable Raman spectroscopy-based matrix model for rapid, non-destructive quantification of elemental concentrations (Ca, Mg, Fe) in carbonate minerals, using five end-members (calcite, ankerite, dolomite, siderite, and magnesite) as reference standards. This model utilizes Raman intensity ratios at specific wavenumbers correlated with the volume fractions of carbonate phases, converting these into mass fractions via mineral densities and reference compositions.
The performance of the Raman matrix model was corroborated by comparing atomic absorption spectroscopy (AAS)-calibrated portable X-ray fluorescence (pXRF) data. The results demonstrated high correlation coefficients for Mg# estimations between Raman-derived compositions and reference chemical analyses. This method was further attested using the external RRUFF Raman database, striking an optimal balance between analytical flexibility and compositional accuracy. We confirmed that spectral overlaps arising from accessory phases were successfully resolved through advanced spectral decomposition, ensuring reliable discrimination of mineral constituents. Synthetic binary carbonate mixtures further confirmed a robust linear correlation between Raman intensity ratios and mineral proportions, highlighting their reliability for quantifying carbonate compositions. Moreover, the Raman-derived compositions closely matched their bulk elemental Ca-Mg-Fe composition in the synthetic carbonate mixtures.

In conclusion, this capability is critical for interpreting natural carbonate assemblages, where intermediate compositions prevail and pure end-member phases are uncommon. Collectively, the portable Raman matrix method constitutes a significant advancement for future in situ adaptation in field environments, equipping geoscientists with a rapid, non-destructive tool for compositional characterization and refined geological interpretation.
This work has been funded by the European Union in the frame of the DeepBEAT project (GA no. 101177617) under its Horizon Europe programme. Views and opinions expressed are, however, those of the author(s) only and do not necessarily reflect those of the European Union or HaDEA. Neither the European Union nor the granting authority can be held responsible for them.

*Intervenant
†Auteur correspondant: yonghwi.kim@univ-lorraine.fr

Mots-Clés: Portable Raman, Semiquantitative analysis, Elemental concentration, Carbonate minerals, Carbonate mixtures