Goldschmidt 2026 Abstract
https://doi.org/10.46427/gold2026.37368

Fast, non-destructive mineral and orientation mapping using mid-infrared spectroscopy

PENELOPE L. KING[1], YILE LIU[1], M. CATHERINE WILSBACHER[1], ASIKA M.K . DHARMARATHNA[1,2], TIMOTHY SCARR[1], KATHRYN S. HAYWARD[1], JULIA BRAND[3], CARSTEN LAUKAMP[4], SHANE MULE[4], JESSICA STROMBERG[4], AARON J. CAVOSIE[5] AND JANELLE STEVENSON[2]

[1]Research School of Earth Sciences, Australian National University
[2]School of Culture, History & Language, Australian National University
[3]Centre for Creative & Cultural Research, University of Canberra
[4]CSIRO - Mineral Resources
[5]Space Science and Technology Centre (SSTC), School of Earth and Planetary Sciences, Curtin University

Micron- or sub-micron scale mineral mapping using scanning electron microscopy (SEM) provides mineral composition, abundance and textures, whereas electron backscatter difraction (EBSD) is required to determine crystallographic orientation. These methods can be challenging for minerals with abundant light elements (e.g., phyllosilicates, borosilicates), and are not generally amenable to fragile 3D surface coatings or vugs. Raman spectral mapping is useful for some samples; however, fluorescence of Fe-rich materials may limit its application. We are introducing a new, non-destructive approach to map minerals in 3D and 2D.

Specular reflectance mid-infrared (IR) spectra record the composition, structure and crystal orientation of a mineral. The method is sensitive to vibrational bonds including those containing Si-O, H-O, P-O, B-O, C-O, Al-O, C-N, C-H, N-O, and S-O. Commercial software on IR microscopes measure the features of specific spectral bands but do not employ the full hyperspectral range using mineral libraries.

We are preparing a physical mineral collection, open database of reference spectra, and open software. Hand-picked, pure grains were placed in random orientations, mounted in epoxy, and polished to 0.3 μm. Micro-IR specular reflectance spectra (5600 – 650 cm^{-1}) were collected with a Bruker INVEVIO-X with Hyperion II microscope and MCT-A detector. We used an unpolarized beam, 4 cm^{-1} resolution, and 64 scans to maximize signal and speed. Thus far, the mineral database includes 70 mineral mounts each with spectra of 200+ randomly oriented grains (with known x-y position). For quality control of the mineral database, python codes have been developed to detect contaminants and find the spectral endmembers in each mount.

We are applying machine learning to identify minerals using IR spectra. Our preliminary tests of basalts measured with SEM-based methods show good agreement, even though our spectral library was small. Importantly, reflected IR spectra identify alteration minerals and crystal orientation, needed for measuring H in minerals. The method can be used on fragile 3D minerals without sample preparation. Future work includes using EBSD for crystaographic orientation, theoretical models for spectral bands, developing deconvolution methods for very fine-grained material, and upscaling the approach to validate core scanning (e.g., HyLogger) and field investigations (e.g., Agilent Exoscan).