183-14 - USING X-RAY DIFFRACTION AND RAMAN SPECTROMETRY TO HELP STUDENTS BETTER UNDERSTAND UNIT CELLS AND SOLID SOLUTIONS. AN ENGAGEMENT COMBINING NSF GEOPATH AND NSF MRI FUNDING

Tuesday, October 12, 2021

5:00 PM - 5:15 PM

Oregon Convention Center - B113/B114 (Hybrid Room)

Abstract

Unit cells and solid solutions can be difficult concepts to demonstrate to students due to their intangibility. Additionally, unit cells within mineral groups will change size depending on the ionic radius of the major cation involved in the solid solution, as well as the coordination of the major cation. To facilitate the students' understanding of unit cells and solid solutions, we utilized powder X-ray diffraction (PXRD), single crystal X-ray diffraction (SCXRD), and Raman spectrometry of carbonate minerals as part of a two-week NSF sponsored GEOPATH summer research engagement. The SCXRD was acquired through the NSF Major Research Instrumentation Program (*CHE #1919785*).

The 2θ of the highest intensity peak of carbonate minerals in PXRD patterns will shift to higher values as the unit cell of the carbonate decreases. This shift is the result of the *d* spacing of the 104 hkl plane decreasing and directly related to the size of the cation in the carbonate. SCXRD is very powerful in unit cell determinations. It will easily give the size of the unit cell, as well as many other crystallographic information. Our measured SCXRD c axis for calcite was 17.02 Å, while it was 15.65 Å for rhodochrosite. This is the direct result of Ca in calcite having a larger ionic radius than Mn in rhodochrosite. The bond length between the Ca and O in calcite is 2.36 Å. The bond length between Mn and O in rhodochrosite is 2.19 Å. This difference in bond length can be seen through Raman shifts for rhodochrosite increasing in value, as compared to calcite, as the bond lengths between the divalent cation and oxygen become shorter.

Assessment of the GEOPATH students' attitude towards conducting research suggests that utilizing the PXRD, SCXRD, and Raman were impactful. The students expressed confidence in their ability to conduct research, understand scientific data, desire to conduct more research, and identified more as scientists as a result of this experience. Pre- and post-testing creative exercise assessment demonstrated a greater understanding of instrumentation in mineral research, and how PXRD, SCXRD, and Raman data related to unit cells, bond distances, and cations within carbonate minerals.

Geological Society of America Abstracts with Programs. Vol 53, No. 6, 2021
doi: 10.1130/abs/2021AM-364302

Author

M

James MacDonald
Florida Gulf Coast University

Authors

B

Alli Barbosa
Florida Gulf Coast University

M

Gregory J. McManus
Florida Gulf Coast University

Ask a question or comment on this session (not intended for technical support questions).

Have a question or comment? Enter it here.

Presentation File(s)

MacDonald et al unit cell.pdf View Download

0:00 / 15:48