Laser induced breakdown spectroscopy as a basis for enhanced provenance studies

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Provenance studies using the compositions of minerals in modern and ancient sediments have enriched our interpretation of Earth's history. Tourmaline, one of the three most significant refractory heavy minerals, is an exceptional provenance indicator in (meta)clastic rocks, in part because its chemistry provides a record of its geological history. Tourmaline forms in an exceptionally wide range of temperature (~150 - 950°C), pressure (1 MPa – 7 GPa) and chemical environments (geo/hydrothermal, metamorphic, igneous) and retains these environmental signatures through weathering processes. To enhance tourmaline's utility as a lithologic provenance indicator, 164 tourmalines from world-wide localities representing 5 known petrogeneic associations were analyzed with Laser Induced Breakdown Spectroscopy (LIBS) and modeled using multivariate statistics.

LIBS captures attributes of the entire chemical spectrum. Each spectrum contains 13,600 - 40,000 variables, depending on the spectrometer's resolution. Multivariate analyses of the spectra uses a series of Partial Least Squares Regression models. In each model, one petrogenetic association is investigated; samples are modeled as either belonging to that association or belonging to the group of all other associations. Each investigated association is eliminated from subsequent models. Spectra from half of the locations for each petrogenetic association are used to train the models; the remaining half of the spectra are used to validate the models and calculate success rates.

Our data indicate that tourmaline provenance can be easily discriminated and binned into the five categories. The first model recognizes calcareous metamorphic tourmalines (92% success). Next, tourmalines from pelitic metamorphic rocks are recognized (96% success) followed by tourmalines from hydrothermal systems (94% success). Finally, silicic igneous tourmalines are distinguished from those in Li-rich pegmatites (92% success). Overall, 74 of the 79 samples in the validation set were correctly identified (93.7% success rate). Such a robust approach provides a new data-rich technique to establish source areas and to constrain tectonic and sedimentary processes.