EGU21-16170
https://doi.org/10.5194/egusphere-egu21-16170
EGU General Assembly 2021

Multi-Element Correlation Analysis of Cu-bearing Tourmaline using LA-ICP-Time-Of-Flight-MS

Hao A.O. Wang[1], Michael S. Krzemnicki[1,2], Susanne Büche[1], Sarah Degen[1,2], Leander Franz[2], and Rainer Schultz-Guttler[3]

[1]Swiss Gemmological Institute SSEF, Basel, Switzerland (hao.wang@ssef.ch)

[2]Department of Environmental Sciences, Mineralogy and Petrology, University Basel, Basel, Switzerland

[3]Geological Institute, Sao Paulo State University, Brazil

Major, minor and trace element analysis using laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) has been applied to a broad range of mineral samples for characterization, mineral resources prospection, tracing and provenance determination, radiometric dating and studies on mineral formation conditions. In this study, we present a state-of-the-art LA-ICP-Time-Of-Flight-MS (LA-ICP-TOF-MS) technique for multi-element analysis of gem-quality Cu-bearing tourmaline from Brazil, Mozambique and Nigeria, with a special focus on elemental correlation among and within various provenances.

A TOF-MS obtains a full mass spectrum from $^{7}Li^{+}$ to $^{238}U^{+}$ simultaneously with an improved mass resolving power. These advantages over other conventional ICP-MS setups allow the TOF users to apply a novel concept of “first measure, then determine” which elements are of interest for the analysis of geological samples. Since the TOF-MS technique requires no/limited a priori knowledge about the sample before measurement, this technique can be beneficial for studying elements which occur infrequently in the minerals and for analysing full elemental composition in unidentified inclusions.

Multi-element composition of more than 400 Cu-bearing tourmaline samples (majority elbaite, Na-rich) was analysed using LA-ICP-TOF-MS that cover various colors, qualities and provenances available in the gem and jewellery trade. In order to investigate the elemental correlation, a non-linear unsupervised dimension reduction was performed on the high dimensional multi-element dataset using t-distributed stochastic neighbor embedding (t-SNE) algorithm. An unsupervised calculation works solely with the elemental concentrations and without labels of data points, for example color or provenance. The clusters in the geochemical data visualization indicates elemental similarity of various samples. We found that t-SNE algorithm is better than principle component analysis (PCA) algorithm in maintaining intrinsic elemental correlation from the original high dimensional space and embedding such information onto low dimensional datasets for visualization. Therefore, the t-SNE method excels in distinguishing within-group elemental similarities from between-group similarities. The separation of subgroups achieved with t-SNE is in agreement with the confirmed geographic provenances.

Additionally, a unique type of Cu-bearing liddicoatite (Ca and REE-rich) was recently discovered near Maraca in Mozambique (Nampula area). Since they have been reported so far only from this occurrence, this type of tourmaline is especially interesting to study how elements correlated during tourmaline formation. Applying t-SNE calculation on these samples, we have found two groups (or four subgroups) of these tourmaline samples. When multi-element concentration was plotted, it can be seen that light-REEs (La to Nd) have an apparent correlation with Ca concentration, however a negative correlation was observed between mid-REEs (Sm to Ho) and Ca. A correlation of Na to Bi and Th was also observed.

In a rare four-color (pink, purple, blue, green) Cu-bearing tourmaline sample from Quintos mine in the state of Rio Grande do Norte, Brazil, multi-element analysis was conducted along a profile across the entire color variation, from the core of the crystal (pink) to the rim of the crystal (green) to monitor elemental variations and correlations throughout the crystal growth process of this tourmaline within the pegmatite.