Trace Element Analysis for Gemstones using Laser Ablation Inductively Coupled Plasma Time Of Flight Mass Spectrometry (LA-ICP-TOF-MS) and Its Application in Origin Determination using Machine Learning

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The main driving force for trace element analysis of gemstones is the demand from the trade for laboratories to deliver a scientifically based opinion about the geographic origin of gemstones. This demand is essentially caused by the monetary impact such an origin "label" (e.g. Kashmir sapphire), but also by the growing need for traceability of gems due to political (trade bans) or ethical (fair trade) reasons.

In this work, we first demonstrate analytical capabilities of trace element analysis using Laser Ablation Inductively Coupled Plasma Time Of Flight Mass Spectrometry (LA-ICP-TOF-MS). We take the benefit of simultaneous multi-element (from $7Li^+$ to $238U^+$) detection of the TOF-MS setup, so that users can measure gemstones with little or no knowledge about the matrix. This feature is desired when collecting unexpected/rarely appearing trace elements in gemstones or analyzing unknown inclusions. In addition, high mass resolving power and low limit of detection of nearly all elements in the periodic table allows improved precision and accuracy in elemental quantification.

In a case study, we present how trace element analysis of gemstones may provide gemmologists complementary information in origin determination using machine learning (ML) based data visualization. This novel technique is compared with conventional statistical methods, such as principle component analysis (PCA). We illustrate that, by applying machine learning algorithm on multi-element chemical data, a more obvious and clearer separation can be seen among gemstones from different origins than that using PCA. Thus machine learning has great potential to be a highly versatile tool to visualize trace element data of gemstones and assist gemmologists in origin determination.