Apatite trace element composition as an indicator of ore deposit types: A machine learning approach

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Abstract

The diverse suite of trace elements incorporated into apatite in ore-forming systems has important applications in petrogenesis studies of mineral deposits. Trace element variations in apatite can be used to distinguish between fertile and barren environments, and thus have potential as mineral exploration tools. Such classification approaches commonly employ two-variable scatterplots of apatite trace element compositional data. While such diagrams offer accessible visualization of compositional trends, they often struggle to effectively distinguish ore deposit types because they do not employ all the high-dimensional (i.e., multi-element) information accessible from high-quality apatite trace element analysis. To address this issue, we use a supervised machine-learning-based approach (eXtreme Gradient Boosting, XGBoost) to correlate apatite compositions with ore deposit type, utilizing such high-dimensional information. We evaluated 8629 apatite trace element data from five ore deposit types (porphyry, skarn, orogenic Au, iron oxide copper gold, and iron oxide-apatite) along with unmineralized magmatic and metamorphic apatite to identify discriminating parameters for the individual deposit types, as well as for mineralized systems. According to feature selection, eight elements (Th, U, Sr, Eu, Dy, Y, Nd, and La) improve the model performance. We show that the XGBoost classifier efficiently and accurately classifies high-dimensional apatite trace element data according to the ore deposit type (overall accuracy: 94% and F1 score: 89%). Interpretation of the model using the SHAPley Additive exPlanations (SHAP) tool shows that Th, U, Eu, and Nd are the most indicative elements for classifying deposit types using apatite trace element chemistry. Our approach has broad implications for the better understanding of the sources, chemistry, and evolution of melts and hydrothermal fluids resulting in ore deposit formation.

Keywords: Machine learning, apatite, trace elements, ore deposit fertility, XGBoost, LA-ICP-MS

Introduction

To develop a quantitative, process-based model for ore-forming systems, a characterization of melt and hydrothermal fluid source, composition and evolution is required (e.g., Andersson et al. 2019). Various minerals in ore-forming systems can constrain the conditions of mineralization based on variations in their mineral chemistry, thus recording the evolution of melts and hydrothermal fluids and yielding constraints on the metatrogenic processes (Clark and Williams-Jones 2003; Pisiak et al. 2017; Chapman et al. 2021; Qiu et al. 2021). As a common accessory mineral in igneous, metamorphic, and clastic sedimentary rocks, apatite has a broad range of applications in the geosciences, including thermochronology studies to investigate tectonic unroofing (Fitzgerald et al. 1991), fault slip rates (Birchau et al. 2006), landscape evolution (Braun et al. 2006), petroleum system maturation (Burtn et al. 1994), and the record of volatile budgets and volcanic eruption triggering (Stock et al. 2016). The structure of apatite also facilitates the substitution of more than half the stable members of the periodic table as trace elements (Hughes 2015), including the rare earth elements and Sr, Y, Th, and U (Sh and Chappell 1999; Chew et al. 2011; Zhou et al. 2022a). Apatite trace element chemistry thus has important applications in igneous and metamorphic petrogenesis studies and in improving the understanding of ore deposit formation (Chu et al. 2009; O’Sullivan et al. 2020; Yu et al. 2021, 2022).

Previous studies that have employed apatite trace element chemistry to classify protolith rock type or fertility have typically employed binary or ternary discrimination diagrams with the variables being apatite trace element abundances or elemental ratios. Belousova et al. (2002) analyzed trace elements in apatite...