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Machine-learning oxybarometer developed using zircon trace-element chemistry and its applications

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Abstract

Magmatic oxygen fugacity (f_{O_2}) is a fundamental property to understanding the long-term evolution of the Earth's atmosphere and the formation of magmatic-hydrothermal mineral deposits. Classically, the magmatic f_{O_2} is estimated using mineral chemistry, such as Fe-Ti oxides, zircon, and hornblende. These methods, however, are only valid within certain limits and/or require a significant amount of a priori knowledge. In this contribution, a new oxybarometer, constructed by data-driven machine learning algorithms using trace elements in zircon and their corresponding independent f_{O_2} constraints, is provided. Seven different algorithms are initially trained and then validated on a data set that was never utilized in the training processes. Results suggest that the oxybarometer constructed by the extremely randomized trees model has the best performance, with the largest R^2 value (0.91 ± 0.01), smallest RMSE (0.45 ± 0.03), and low propagated analytical error (~0.10 log units). Feature importance analysis demonstrates that U, Ti, Th, Ce, and Eu in zircon are the key trace elements that preserve f_{O_2} information. This newly developed oxybarometer has been applied in diverse systems, including arc magmas and mid-ocean ridge basalts, fertile and barren porphyry systems, and global S-type detrital zircon, which provide f_{O_2} constraints that are consistent with other independent methods, suggesting that it has wide applicability. To improve accessibility, the oxybarometer was developed into a software application aimed at enabling more consistent and reliable f_{O_2} determinations in magmatic systems, promoting further research.

Keywords: Machine learning, zircon, trace elements, magmatic oxygen fugacity, oxybarometer