American Mineralogist, Volume 109, pages 315–324, 2024

Identifying serpentine minerals by their chemical compositions with machine learning

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Abstract

The three main serpentine minerals, chrysotile, lizardite, and antigorite, form in various geological settings and have different chemical compositions and rheological properties. The accurate identification of serpentine minerals is thus of fundamental importance to understanding global geochemical cycles and the tectonic evolution of serpentine-bearing rocks. However, it is challenging to distinguish specific serpentine species solely based on geochemical data obtained by traditional analytical techniques. Here, we apply machine learning approaches to classify serpentine minerals based on their chemical compositions alone. Using the Extreme Gradient Boosting (XGBoost) algorithm, we trained a classifier model (overall accuracy of 87.2%) that is capable of distinguishing between low-temperature (chrysotile and lizardite) and high-temperature (antigorite) serpentines mainly based on their SiO_2, NiO, and Al_2O_3 contents. We also utilized a *k*-means model to demonstrate that the tectonic environment in which serpentine minerals form correlates with their chemical compositions. Our results obtained by combining these classification and clustering models imply the increase of Al_2O_3 and SiO_2 contents and the decrease of NiO content during the transformation from low- to high-temperature serpentine (i.e., lizardite and chrysotile to antigorite) under greenschist–blueschist conditions. These correlations can be used to constrain mass transfer and the surrounding environments during the subduction of hydrated oceanic crust.

Keywords: Serpentine, machine learning, XGBoost, classifications, *k*-means, clustering