American Mineralogist, Volume 110, pages 217–231, 2025

Unraveling clay-mineral genesis and climate change on Earth and Mars using machine learning-based VNIR spectral modeling

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Abstract

Clay minerals are common in martian geological units and are globally widespread on Earth. Understanding the origin, formation, and alteration of clay minerals is crucial for unraveling past environmental conditions on Earth and Mars, in which the composition and crystallinity of clay minerals serve as important surrogate indicators for addressing these issues. Here, 621 soil and sediment samples from five chronosequences representing different climatic zones of China were investigated using visible to near-infrared reflectance (VNIR) in combination with X-ray diffraction (XRD) analysis. The crystallinity of clay minerals (i.e., illite crystallinity, illite chemistry index, kaolinite crystallinity) and clay mineral alteration index (CMAI) were analyzed with conventional methods and then predicted through a spectral modeling approach. Our results show that kaolinite with a pedogenic or sedimentary origin is characterized by a broad crystallinity range and a poorly ordered structure, especially when generated in an intense weathering environment. Predictive models were constructed with data-mining methods, including partial least-squares regression (PLSR), random forest (RF), and Cubist algorithms. The predictive performance of the crystallinity and CMAI proxies is robust, with an overall accuracy of 78% and a residual prediction deviation (RPD) of 2.57. We also found that the model's accuracy in predicting clay-mineral-related proxies increased by 45% using random forest (RF) and Cubist compared to the PLSR models. We suggest that VNIR spectroscopy combined with RF and Cubist methods has the potential to be an alternative and broadly applicable tool for analyzing typical clay-mineral proxies, substituting for a series of common mineralogic analyses. Spectral modeling can reveal genetic and climatic information at both field and regional scales, which has profound implications for Mars missions and other space exploration programs.

Keywords: Crystallinity, illite, kaolinite, chemical weathering, XRD analysis, South China