What spinel composition in rocks tells us: a combined approach from data-driven and physics-based modelling

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Diversity within the geochemical data of crustal and mantle rocks is proved to be intrinsically linked with the distinct modes of differentiation within the different depths of the mantle and crust that took place throughout the planet's geological history. Thus, the preparation and use of numerous (tectonic) discrimination diagrams based on the geochemical signatures associated with the different (tectonic) processes became a very common practice. Despite being a quick tool to recognize the "thought to be" tectonic framework, it possesses several significant demerits. For instance, one cannot apply the method for sure to the data set obtained for older rocks which might be the products of fundamentally different tectonic or compositional or genetic regimes, since the discrimination approach must rely on the rocks from well-observed modern tectonic settings as training data. In the last few decades, increasing data availability allowed the scientific community to adapt unsupervised machine learning techniques in the large (often global and unbiased) geochemical dataset to reveal the hidden structure within it. This provides more scientific insight about the underlying geodynamic processes what traditional discrimination methods often fails to deliver. Here we focussed on one such commonly used discrimination method, characterized by mineral chemistry of Chrome spinel [having $(Mg,Fe^{2+})(Cr,Al,Fe^{3+})_2O_4$ formula with minor Ti, Mn, Ni etc.] from peridotitic rocks. Cr# (Cr/Cr+Al) and Mg# ($Mg/Mg+Fe^{2+}$) parameters of spinel are long been recognized as a key petrogenetic indictor owing to its sensitivity towards progressive degree of mantle melting in different geotectonic environments. However, a recent study has challenged the assumption of spinel being resistant to post-formation modification (e.g., fluid-rock interaction, metasomatism, serpentinization, regional metamorphism etc) and questioned the effectiveness of chrome spinel chemistry as a mantle melting indicator, rather proposed to be a tracer for metasomatic processes. This conflicting observation basically motivated us to apply multivariate statistical method to identify the key processes that leads to the geochemical diversity within the spinel compositional spectrum. We first made a comprehensive and unbiased spinel composition (major elements) database based on the previously available compilation and addition of relevant data from literature spanning all tectonic framework and diverse peridotite lithology. The frequency of the dataset is 4639 for the Ti-Al-Cr-$Fe3^{+}$-Fe^{2+}-Mg-Mn-Ni system though that significantly increased (more than 6500) in the reduced Al-Cr-$Fe3^{+}$-Fe^{2+}-Mg system. However, for our preliminary analysis we have used the larger element-system dataset to get broader picture of the elemental behaviour. To avoid constant-sum constraint (represented by percent) we have performed centered logratio transformation of the data. Non-gaussian distribution of the element concentration allows us to systematically apply independent component analysis, ICA. Finally, the IC vectors demonstrating most orthogonal relationship are thought to be the potential geochemical processes responsible for the variation in spinel chemistry. In order to find the implication of IC vectors, we then performed plausible forward models to acquire the data direction of the progressive geological processes like melting, metamorphism and melt-rock interaction. Comparison with the forward models and IC vectors clearly suggest the interaction of different geological processes leading to a complex geochemical data structure in spinel chemistry that was not previously demonstrated vividly and laid the foundation for future studies.

Keywords: Chrome-spinel, Unsupervised machine learning, Independent component analysis, Tectonic discrimination

