

Progressive evolution of the whole rock composition during metamorphism revealed by machine learning technique

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Geochemical evolutions with respect to the major components of the metamorphic rocks during the subduction-related metamorphism are documented on the basis of multivariate statistical analyses applied for mapped metamorphic rocks collected from the Sanbagawa metamorphic belt in central Shikoku, whose metamorphic conditions range from the pumpellyite-actinolite to epidote-amphibolite facies. Recent progress of computational and information science provides a number of algorithms revealing a hidden structure of large datasets. This contribution applied *k*-means cluster analysis (KCA) and non-negative matrix factorization (NMF) to a series of metapelites, which is the main lithotype of the Sanbagawa metamorphic belt. The analyzed dataset contains 235 sample with 14 elements accumulated from the literature. As a result, we obtain five clusters in KCA and four endmembers for NMF which successfully explains compositional variations of the studied dataset.

The result of KCA clearly shows that the chemical compositions of the metapelites are different between the western part (Besshi area) and eastern part (Asemigawa area) of the studied dataset. In the western part of the studied dataset, clusters show a good correspondence with the metamorphic grade. In the higher metamorphic grade part, a monotonous decrease in SiO₂ and Na₂O and an increase in other components are detected. On the other hand, the compositional change with the metamorphic degree is less obvious in the eastern part. Endmember decomposition using NMF revealed that the evolutionary change of the whole rock composition correlated with the metamorphic grade is approximated to a stoichiometric increase of garnet-like component in the whole rock composition. This phenomenon could be related to the precipitation of garnet and effusion of other components during progressive dehydration. Thermodynamic modeling considering the evolutionary change of the whole rock composition predicted followings: (1) the lower-grade whole rock composition prefers the crystallization of garnet at the conditions of the garnet zone while biotite becomes stable together with garnet in higher-grade whole rock compositions at the same PT conditions, (2) the higher-grade whole rock composition can retain more H₂O than the lower-grade one. These results indicated the mechanism suppressing the dehydration at the high-pressure metamorphic conditions. Perhaps such kind of mechanism should be considered in the forward modelling in treating the fluid cycle in subduction zones, though quantitative model has not been established yet.

Keywords: machine learning technique, Sanbagawa metamorphic belt, subduction zone, pseudosection analysis, material cycle