

Application of principal component analysis to seafloor basalt and its quantitative interpretation

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Bulk chemical compositional data of rocks consist of tens of elements, and analysis of high dimensional data is needed for interpretation of such data sets. In the traditional studies, a certain pairs of elements were empirically chosen to represent specific processes such as degree of melting and effect of crystal differentiation. To elucidate hidden processes without using empirical knowledge, principal component analysis (PCA) has been utilized for the interpretation of the compositional variations of sediments and igneous rocks (Kuwatani et al., 2014; Ueki, 2014). For example, application of PCA to compositions of arc basalt has revealed that principal components differ among volcano, and distinguishes processes such as mixing and crystal differentiation (Ueki, 2014). To further develop the application of PCA to the interpretations of bulk rock compositions, a quantitative evaluation of contribution rates and factor loadings are needed. In this study, to establish a quantitative interpretation of factor loadings, bulk compositions of seafloor basalt are chosen for PCA, and the results were quantitatively compared with theoretical fractionation processes.

Sample data sets were from seafloor basalt collected from Cocos plate by IODP expedition 334. The samples were collected from the depth of 99-164 meter below seafloor (mbsf). As these samples were collected from narrow region, it is expected that the processes controlling the compositions of these basalt are relatively simple. Empirical factors such as Nb/Zr and Cr/Zr ratios suggest that the compositional variations of the samples originate from different degree of melting and crystal differentiations (Uno et al., in prep.).

Principal component analysis was applied to the compositions of 43 basalt samples for 10 major elements (Si, Ti, Al, Fe, Mg, Mn, Ca, Na, K, P), and 33 minor elements (Li, Sc, V, Cr, Co, Ni, Cu, Sr, Rb, Y, Zr, Nb, Cs, Ba, La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Hf, Ta, Pb, Th, U).

The first three principal components account for 80% of the data variance: the contribution factor of PC1 is 52%. The factor loading is high for Middle REE (MREE) and low for incompatible elements (i.e., elements that partition preferentially to silicate melt compared to rock) such as Rb and Ba. The PC2 has contribution factor of 19%, and factor loadings are high for Ni, Co and heavy REE (HREE), whereas those are low for incompatible elements such as Rb, Ba and Th. As the factor loadings of PC2 change continuously from high values for compatible elements to low values for incompatible elements, the PC2 suggest fractionation of melt. The PC3 contributes 8% of the data variance, and factor loadings are high for Cs, Li, U, and loss on ignition (i.e., bulk water content). As solubility for aqueous fluids are high for these elements, the PC3 suggests chemical alteration by aqueous fluids.

The depth profiles of PC1-3 are consistent with the empirical factor of Nb/Zr, Cr/Zr ratios and the amount of altered minerals, respectively. These results suggest that the bulk compositions of seafloor basalt of the Cocos plate are controlled by crystal differentiation, degree of melting and hydrothermal alteration.

For the quantitative interpretations of the PCA, the factor loadings of each PCA were compared with the various kinds of partition coefficients. For PC2, the patterns of factor loadings can be quantitatively explained by the partition coefficients of basaltic melt/peridotite. On the other hand, PC1 cannot be explained by simple melt/mineral partitioning, but can be explained quantitatively by olivine/pyroxene partitioning. These quantitative relations between factor loadings and partition coefficients show the effectiveness of PCA for elucidating fractionation processes.

In this presentation, the cause of quantitative relation between the factor loadings and fractionation processes will be discussed.

Keywords: principal component analysis, seafloor basalt, elemental differentiation, Costa Rica