

Analysis of zonal structure of phenocryst minerals considering element diffusion: Approach based on Bayesian statistics

*Fumitoshi Morisato¹, Kazuhito Ozawa¹

1. Department of Earth and Planetary Science, Graduate School of Science, The University of Tokyo

From the zonation structure found in the phenocrysts in the volcanic rocks, when the equilibrium with the melt is guaranteed, sequence data on melt composition with high degree of freedom and short time scale of homogenization can be obtained by using partitioning coefficients. Then, it is expected that constraints on physical processes related to the differentiation process inside the crust and on primary magma will be possible. However, due to the diffusion of elements in the crystal, analysis using partitioning coefficients is often insufficient. On the other hand, if the influence of diffusion can be estimated from the compositional zoning structure affected by element diffusion, time information can be obtained. However, when the zonal structure becomes complicated, such as when formed in multiple crystal growth stages, the number of parameters to be considered in analysis increases and the dependence among the parameters becomes complicated.

In this study, we developed a method to elucidate the physical processes experienced by magma system through restored information on temporal change of melt composition by evaluating the influence of element diffusion quantitatively from the zonation structure of the phenocryst mineral that experienced the multistage crystallization process.

In this study, we have constructed a forward model for the formation of zonal structure by crystal growth and subsequent element diffusion, and estimated the parameters characterizing the model by Parallel tempering Markov Chain Monte Carlo (PT-MCMC) method. We conducted validation test for our method by using numerically generated zonal structure which is added noise. In our crystal growth model, the zonal structure is formed by several stages where the element diffusion progresses after crystal growth. Classification of the crystal growth stage was constrained based on a profile with a low diffusion rate such as Cr_2O_3 in the case of orthopyroxene.

In our model on crystal growth, the melt composition as the starting point of calculation is the whole rock composition of the most primitive natural lava. The melt composition change is calculated by fractionation or addition of small amount of olivine, orthopyroxene, and spinel repeatedly. Each solid phase is spherically symmetric and the spherical shell with the composition that is local equilibrium with melt grows for each calculation step. Calculation was made with assuming that the partition coefficients are always constant. It is assumed that olivine and orthopyroxene affect trace elements and major components MgO , FeO and SiO_2 , and spinel affects a trace element only.

In our model on element diffusion, based on the method of Ozawa (2004), nondimensionalized was calculated. The diffusion coefficient considered only temperature dependence. In the calculation scheme, the second order center difference is adopted in the spatial direction, and the backward difference was adopted in the time direction.

Using the simulated zonal structure by the forward model and the analyzed zonal structure, eight series of Markov chains expanded with parameters expressing pseudo temperature were generated, and parameter estimation was performed by parallel tempering Markov Chain Monte Carlo method (Hukushima & Nemoto, 1996). After a given sampling times, the optimum value of the parameter was determined from

the average value or the mode value while checking the histogram shape of the obtained sample.

Sampled parameters are following five types in each zoning section: initial Mg#, final Mg#, modal fraction of orthopyroxene, and modal fraction of spinel in the crystal growth stage; logarithm of maximum compression time in element diffusion stage.

Keywords: Volcanic rocks, Crystal growth, Element diffusion