Data driven construction of thermodynamic model of hydrous melt using machine learning technique

*Kenta Ueki[1], Tatsu Kuwatani[1], Hikaru Iwamori[1]

1.Japan Agency for Marine-Earth Science and Technology, Department of Solid Earth Geochemistry

H_2O in silicate melt drastically changes the phase relation of magma. Phase relations and physico-chemical properties of hydrous magma have been determined based on various experiments. However, each experiment was carried out under independent P-T condition and melt composition. To model the phase relation of hydrous magmas in continuous P–T–composition space of a natural melting zone, numerical model must be developed.
In order to conduct a numerical modeling, we need to develop a consistent set of a thermodynamic equation and its parameter values. Generally, thermodynamic equation is constructed based on a priori information such as theoretical predictions or observations using natural samples. However, little is known about the microstructure and physico-chemical properties of hydrous melt. It means that modeling of hydrous melt lacks a pripri information. In this situation, we have to construct both the non-linear model equation and parameter values based on small size of experimental data set. In addition, silicate melt exhibits a multi-component system. The degree of freedom in terms of composition, pressure and temperature ranges are large. In this case, previous methods used in earth science field such as analytical or empirical methods are not effective for the modeling.
In order to obtain the optimal thermodynamic parameter values based on experimental results obtained within discrete and limited P-T-compositional conditions, we use cross-validation technique. In the cross-validation, we divide the dataset (experimental results) into two groups. We optimize parameter values to make the best fit of the first group (the training data). The external validity (generalization ability) of the parameter set is obtained using the second group (the test data).
For the selection of the model equation, we test all possible combinations of coefficients of the thermodynamic equation. For the each combination of coefficients, we use leave-one-out cross-validation, in which the one experimental result is used for the test data, and the rest is used for the training data. All the possible ways to divide the original data are tested, and the average residual is regarded as the validity of the model equation. The combination of coefficients to minimize average residue is regarded as the model equation and the optimized parameter is regarded as the optimal thermodynamic parameter set.
We develop a thermodynamic model to calculate phase equilibrium between hydrous melt and olivine as a model system. We use experimentally determined melt composition, H_2O concentration, pressure, temperature and olivine composition during the melting of hydrous and anhydrous mantle peridotite (e.g., Hirose and Kushiro, 1993; Hirose and Kawamoto, 1995) as a dataset. Specific heat of melt and non-ideality model for the olivine solid solution are taken from previous studies. We assume the regular solution for the basic equation of the non-ideality of melt, in which non-ideal free energy is described as linear functions of concentrations of end-member components. Especially for the H_2O, polynomial of degree 2 is considered because a strong non-linear relationship between H_2O concentration and phase relation has been reported.
The optimal model uses the first-degree term against all end-member components. However, the second-degree term of the H_2O component is not selected for the optimal model equation. Forward calculations conducted using the optimized model equation and parameter set reproduce the experimentally determined genetic conditions of hydrous magmas. The method presented in this study, data driven method for construction of the thermodynamic model can be applicable to various systems

such as modeling of rock forming minerals and multi-phase systems.

Keywords: Machine learning, Thermodynamics, Hydrous melt, Phase equilibrium

