Optimization of non-ideal parameters of amphibole solid solution using exchange Monte Carlo Method

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Minerals in rocks possess huge information on dynamics of the Earth's interiors within their chemical compositions and textures. Recent progress of analytical instruments and computation abilities enable us to open new approaches to extract information from rocks by machine-learning techniques. In this study, we show the results of petrological optimizing problem by using exchange Monte Carlo method (Hukushima and Nemoto, 1996; Okamoto et al., 2015).
Estimates of P-T paths of metamorphic rocks are of special importance for understanding dynamic behaviors of subduction zones and crusts. Based on Gibbs' phase rule, when the number of compositional variables of a mineral is larger than the degree of thermodynamic freedom of the system, we can obtain pressure and temperature solely from chemical composition of the mineral; this approach is called as Gibbs' method (Spear 1993). Amphibole is one of the most suitable minerals for this analyses, because (1) amphibole is common in various metamorphic rocks, and (2) it has the complex compositions which compositional variables can compensate the degree of freedom, and (3) it commonly show a growth zoning, which is useful for drawing continuous P-T path during its growth. Okamoto and Toriumi (2001; 2004) applied this method to mineral assemblage of amphibole –plagioclase –epidote –chlorite - water in eight component system, in which thermodynamic freedom, f, is four. By using amphibole compositions, which is written as solid solution of six or seven components, they succeeded in decompression P-T paths from zoning of amphiboles in the Sanbagawa belt.
One of large problems on this thermodynamic analysis using amphibole is the lack of accurate activity model of amphibole due to its complex compositions. Even when we assume simple regular solution model (symmetrical), 21 non-ideal parameters (Margules parameters) are required for mixing of seven endmembers. In binary solution, the Margules parameter is the critical temperature of the solvus, but it is difficult to obtain solvus temperature accurately from complex solid solution like amphibole. Alternatively, Okamoto and Toriumi (2004) proposed the other approach for determining the Margules parameters by using the framework of Gibbs' method as follows. Since the system described above (thermodynamic freedom = 4, independent amphibole component = 5; one amphibole composition is excess), we can estimate one compositional variable of amphibole itself as well as P, T and the composition of other minerals. Accordingly, we can compare the calculated and observed compositions. Using various amphibole compositions from natural metamorphic rocks, we can optimize the Margules parameters from numerous natural data. However, this optimization problem on such many parameters (21 W's) would have several local minimums or broad minimum, and the results would be sensitive to the analytical errors of amphibole compositions. To overcome this hardly-relaxing problem, in this study, we construct the optimization scheme by using the exchange Monte Carlo Method (Hukushima and Nemoto, 1996). We succeeded the performance of the algorithm by using the synthetic data. We will discuss the applications to natural system and seek appropriate ways to obtain the realistic P-T paths from zoned minerals.

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