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Thermodynamic equilibrium at heterogeneous pressure

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Recent advances in metamorphic petrology point out the importance of grain-scale pressure variations in high-temperature metamorphic rocks. Pressures derived from chemical zonation using unconventional geobarometry based on equal chemical potentials fit mechanically feasible pressure variations. Here a thermodynamic equilibrium method is presented that predicts chemical zoning as a result of pressure variations by Gibbs energy minimization.

Equilibrium thermodynamic prediction of the chemical zoning in the case of pressure heterogeneity is done by constraint Gibbs minimization using linear programming techniques. Compositions of phases considered in the calculation are discretized into ‘pseudo-compounds’ spanning the entire compositional space. Gibbs energies of these discrete compounds are generated for a given range and resolution of pressures for example derived by barometry or from mechanical model predictions. Gibbs energy minimization is subsequently performed considering all compounds of different composition and pressure. In addition to constraining the system composition a certain proportion of the system is constraint at a specified pressure. Input pressure variations need to be discretized and each discrete pressure defines an additional constraint for the minimization. The proportion of the system at each different pressure is equally distributed over the number of input pressures. For example if two input pressures P_1 and P_2 are specified, two constraints are added: 50 percent of the system is constraint at P_1 while the remaining 50 percent is constraint at P_2.

The method has been tested for a set of 10 input pressures obtained by Tajčmanová et al. (2014) using their unconventional geobarometry method in a plagioclase rim around kyanite. Each input pressure is added as constraint to the minimization (1/10 percent of the system for each discrete pressure). Constraining the system composition to the average composition of the plagioclase rim successfully predicts the observed chemical zoning.

In conclusion, Gibbs minimization provides identical results to the geobarometry approach based on chemical potentials thus validating the inferred pressure gradient. The thermodynamic consistency of the calculation is supported by the similar result obtained from two different approaches.

Reference:

Tajčmanová, L., Podladchikov, Y., Powell, R., Moulas, E., Vrijmoed, J. C. & Connolly, J. A. D. (2014). Grain scale pressure variations and chemical equilibrium in high–grade metamorphic rocks. *Journal of Metamorphic Geology*, (in press).