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Computation of thermodynamic equilibrium in systems under stress

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Metamorphic reactions may be partly controlled by the local stress distribution as suggested by observations of phase assemblages around garnet inclusions related to an amphibolite shear zone in granulite of the Bergen Arcs in Norway. A particular example presented in fig. 14 of Mukai et al. [1] is discussed here. A garnet crystal embedded in a plagioclase matrix is replaced on the left side by a high pressure intergrowth of kyanite and quartz and on the right side by chlorite-amphibole. This texture apparently represents disequilibrium. In this case, the minerals adapt to the low pressure ambient conditions only where fluids were present. Alternatively, here we compute that this particular low pressure and high pressure assemblage around a stressed rigid inclusion such as garnet can coexist in equilibrium.

To do the computations we developed the Thermolab software package. The core of the software package consists of Matlab functions that generate Gibbs energy of minerals and melts from the Holland and Powell database [2] and aqueous species from the SUPCRT92 database [3]. Most up to date solid solutions are included in a general formulation. The user provides a Matlab script to do the desired calculations using the core functions. Gibbs energy of all minerals, solutions and species are benchmarked versus THERMOCALC, Perple_X [4] and SUPCRT92 and are reproduced within round off computer error. Multi-component phase diagrams have been calculated using Gibbs minimization to benchmark with THERMOCALC and Perple_X. The Matlab script to compute equilibrium in a stressed system needs only two modifications of the standard phase diagram script. Firstly, Gibbs energy of phases considered in the calculation is generated for multiple values of thermodynamic pressure. Secondly, for the Gibbs minimization the proportion of the system at each particular thermodynamic pressure needs to be constrained. The user decides which part of the stress tensor is input as thermodynamic pressure.

To compute a case of high and low pressure around a stressed inclusion we first did a Finite Element Method calculation of a rigid inclusion in a viscous matrix under simple shear. From the computed stress distribution we took the local pressure (mean stress) in each grid point of the FEM calculation. This was used as input thermodynamic pressure in the Gibbs minimization and the result showed it is possible to have an equilibrium situation in which chlorite-amphibole is stable in the low pressure domain and kyanite in the high pressure domain of the stress field around the inclusion. Interestingly, the calculation predicts the redistribution of fluid from an average content of fluid in the system. The fluid in equilibrium tends to accumulate in the low pressure areas whereas it leaves the high pressure areas dry. Transport of fluid components occurs not necessarily by fluid flow, but may happen for example by diffusion. We conclude that an apparent disequilibrium texture may be explained by equilibrium under pressure variations, and apparent fluid addition by redistribution of fluid controlled by the local stress distribution.

[1] Mukai et al. (2014), Journal of Petrology, 55 (8), p. 1457-1477.
[2] Holland and Powell (1998), Journal of Metamorphic Geology, 16, p. 309-343
[3] Johnson et al. (1992), Computers & Geosciences, 18 (7), p. 899-947
[4] Connolly (2005), Earth and Planetary Science Letters, 236, p. 524-541