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Numerical simulation of garnet growth with THERIA_G: theory and applications

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We present the software program THERIA_G (Gaidies et al., 2007a), which allows for numerical simulation of garnet growth in a given volume of rock along any pressure–temperature–time (P–T–t) path. THERIA_G assumes thermodynamic equilibrium between the garnet rim and the rock matrix during growth and accounts for component fractionation associated with garnet formation as well as for intracrystalline diffusion within garnet. In addition, THERIA_G keeps track of changes in the equilibrium phase relations, which occur during garnet growth along the specified P–T–t trajectory. This is accomplished by the combination of two major modules: a Gibbs free energy minimization routine is used to calculate equilibrium phase relations including the volume and composition of successive garnet growth increments as P and T and the effective bulk rock composition change. With the second module intragranular multicomponent diffusion is modelled for spherical garnet geometry. THERIA_G allows simulating the formation of an entire garnet population, the nucleation and growth history of which is specified via the garnet crystal size frequency distribution. Garnet growth simulations with THERIA_G produce compositional profiles for the garnet porphyroblasts of each size class of a population and full information on equilibrium phase assemblages for any point along the specified P–T–t trajectory. The results of garnet growth simulation can be used to infer the P–T–t path of metamorphism from the chemical zoning of garnet porphyroblasts.

We present applications of THERIA_G modelling to garnet in metapelites from the

Austroalpine crystalline basement east of the Tauern Window. From these simulations, detailed information on the P–T–t evolution during prograde metamorphism is obtained (Gaidies et al., 2007b). We demonstrate that the coupling of THERIA_G modelling with monazite chemical Th–U–Pb microprobe ages offers the chance to link the trajectory of metamorphic P-T evolution with geochronological information. Based on compositional and textural relations between monazite and the major silicates this allows to relate metamorphic events in the earth history to their P–T evolution.

Gaidies, F., de Capitani, C. & Abart, R., 2007a. THERIA_G: a software program to numerically model prograde garnet growth. *Contributions to Mineralogy and Petrology*, doi:10.1007/s00410-007-0263-z.

Gaidies, F., de Capitani, C., Abart, R. & Schuster, R., 2007b. Prograde garnet growth along complex P-T-t paths: results from numerical experiments on polyphase garnet from the Wölz Complex (Austroalpine Basement). *Contributions to Mineralogy and Petrology*, doi:10.1007/s00410-007-0264-y.