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Modelling the size and spatial distribution of index minerals along P-T-t paths in amphibolite facies metapelites

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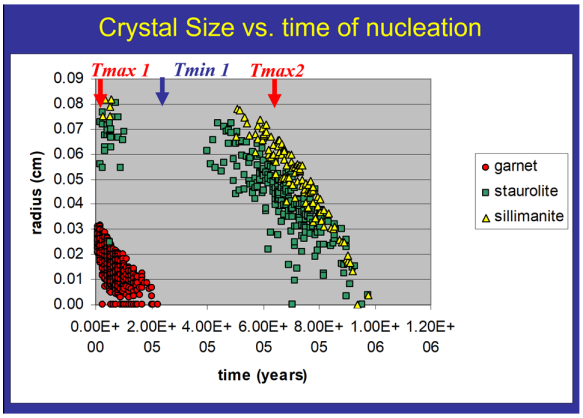

Over the last 20 years improvements in thermodynamic databases and accompanying software has led to the widespread use of programs like Thermocalc, PERPLEX and Theriak-Domino to calculate mineral assemblages, mineral modes and mineral compositions as a rock migrates along a P-T path during metamorphism. However, with the exception of garnet, very little progress has been made on quantitative models to interpret the meaning of observed spatial and size distributions of minerals in metamorphic rocks. The approach presented here permits the modelling of such features along a specified Pressure-Temperature-time path. Input parameters are: mineral modes and reactions at the whole rock scale along a specified P-T path (calculated from the program of your choice); detailed P-T-t conditions along the specified metamorphic path; and kinetic parameters that permit the calculation of mineral nucleation and diffusion controlled growth rates as a function of P-T-t. The present implementation of the approach focuses on predicting the size and location for individual crystals of index minerals that are commonly found in amphibolite facies metapelites (i.e. Grt, St, And, Ky, Sil & Crd). The method outputs the location (x, y z) and size (V) of each crystal in a cube of model rock for each time step along the P-T-t path. It also tracks the specific volume of rock within the model rock cube that contains reactant minerals which dissolved, specifying the source of components transported by diffusion to each growing crystal. At the present time the parameters that control nucleation rate, transport of components to/from a growing/dissolving crystal, and increasing size of domains of equilibrium around a growing crystal are not well known. Efforts are presently underway to obtain the necessary parameters by fitting crystal size distributions of well constrained natural examples. However, the method is currently useful to gain an understanding of how possible constraints such as rapid vs slow reaction overstepping, wet vs dry grain boundaries, and metastable vs equilibrium reactions might be expressed in rocks. An example of the type of output provided by the method, calculated for a pelite with two heating events, is shown in the figure.