Determination of single-mineral pressure and temperature using learning algorithms: an example from peridotitic garnet

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The adoption of FAIR data principles has created a quantity and quality of data that can be used for careful exploration with learning algorithms. These algorithms have diverse applications, such as sedimentary or volcaniclastic provenance, vectoring of ore deposits, tracing of magma storage processes, and quantification of sediment generation.

Learning algorithms applied to large geothermobarometric datasets can provide quantitative determinations of pressure and/or temperature, with several examples existing for magmatic and mantle rocks. Here we demonstrate our recent work developing a single-crystal thermometer and barometer for high-Cr pyrope garnet from peridotites in the sub-continental lithospheric mantle, which require only major element data. These models permit the acquisition of PT data from abundant single garnet xenocrysts, rather than much rarer xenoliths, permit study of the compositional stratification of the lithospheric mantle and thus understand its formation processes, and permit the determination of well-constrained geotherms through the lithospheric mantle with abundant crystals. Lastly, as garnet is the most physically and chemically robust rock forming phase from deep mantle peridotites at the Earth's surface, this information can be preserved and revealed in the sedimentary archive.

Our thermometer and barometer are trained on a global database of garnet peridotite xenoliths and have errors of 71 °C and 0.5 GPa respectively vs iteratively calculated Fe-Mg Grt-Opx exchange temperatures and Al-exchange Grt-Opx pressures, with no systematic skew at high or low T or P. Furthermore, our calculated temperatures for individual garnet agree very closely with the latest calibrations of the Ni-in-Grt single-crystal thermometer. In sum, these new tools enable the extraction of both P and T from all high-Cr peridotitic garnet xenocrysts, a feature previously only commonly possible in peridotite for single clinopyroxene crystals. However, as garnet also crystallise in cpx-free compositions, these new tools can uniquely enable us to construct "stratigraphies" of harzburgite, lherzolite and metasomatized peridotites through the lithospheric mantle which we demonstrate on example datasets from Finland, Australia and the USA.

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