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A new machine-learning single-crystal peridotitic garnet geobarometer & geothermometer

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For thirty-five years (Griffin et al., 1989) it has been possible to extract useful temperature estimates for peridotitic pyrope-rich garnet from the lithospheric mantle using the Nickel-in-garnet method. There have been amendments (Ryan et al., 1996; Canil et al., 1999; Nimis et al., 2024) to determine the best calibration but, overall, this method has proven to be a practical tool. Contrasting with thermometry, barometry in single peridotite pyrope crystals is underdeveloped. Cr-in-Grt barometry is the most disseminated method for estimating P from garnet separate, but Cr-in-Grt provides only minimum constraints on P from all but (rare) extremely depleted garnet compositions. Because of this, without additional constraints, it is not possible to determine whether a particular garnet xenocryst comes from the diamond stability field, or to construct reliable geotherms from garnet separate.

To extract P, scientists use several workarounds; such as by making educated guesses of P by projecting garnet Ni-in-Grt T onto known regional geotherms. And by relying only on Cr-in-Grt pressure estimates from ultra-depleted garnet. However, assumed geotherms may not always be valid, especially for very old pipes, and fully Cr-saturated garnet are rare at best, and absent in many kimberlite pipes. The current state-of-the-art in peridotitic garnet barometry is, therefore, unsatisfying; particularly as garnet is an ideal mineral for single-crystal methods – occurring in both depleted and fertile compositions, in both the graphite and diamond stability fields, abundantly in kimberlite separate and derived alluvium, and included in diamond.

In light of these issues, our solution for single-crystal pyrope-rich peridotitic garnet barometry is to use machine learning to calibrate garnet major element oxide compositions in natural peridotite xenoliths to pressures modelled from Grt-Opx cation-exchange barometry, based on the method of Higgins et al. (2022) for igneous thermobarometry. As we can extract temperatures using Grt-Opx cation exchange thermometry, we also determine a new single-crystal Grt thermometer that uses only major element oxide data (i.e., it does not employ Ni;). We created our barometer and thermometer by employing a random forest algorithm based on multiple regression trees on a database of approximately 1500 xenoliths containing G9, G10, G11, and G12 garnet. We successfully relate Grt-Opx pressure (Nickel and Green, 1985; NG85) and temperature (Sudholz et al., 2022; SH22) to major element composition, outputting the new single-crystal pressure and temperature estimates. Our barometer has a mean absolute error of ~ 4.6 kbar vs NG85 Grt-Opx cation exchange P (Figure 1a), and our thermometer has a mean absolute error of ~ 62 °C vs SH22 Grt-Opx cation exchange T. These errors are comparable to the errors on the exchange thermometers and barometers themselves. There is no skew at high or low T or P within the applicable range of the thermometer and barometer vs the cation-exchange models.

The xenolith database we use to train our models is global and covers a wide range of compositions, pressures, temperatures, geotherms and lithospheric thicknesses. Sheared Ti-metasomatised garnet (G11) are included. Firstly, as these may occur in separate and detritus, and estimates from these may inform diamond exploration. And secondly because their inclusion improves estimates from all other peridotitic garnet types. Off-craton (e.g. Patagonia, Namibia, Solomon Islands) and thinned-craton (e.g. North China)

garnet are also included, as we intend for our models to be fully applicable to *any* alluvial peridotitic garnet. If not included, spuriously deep estimates would be provided if such garnet were found in detrital assay.

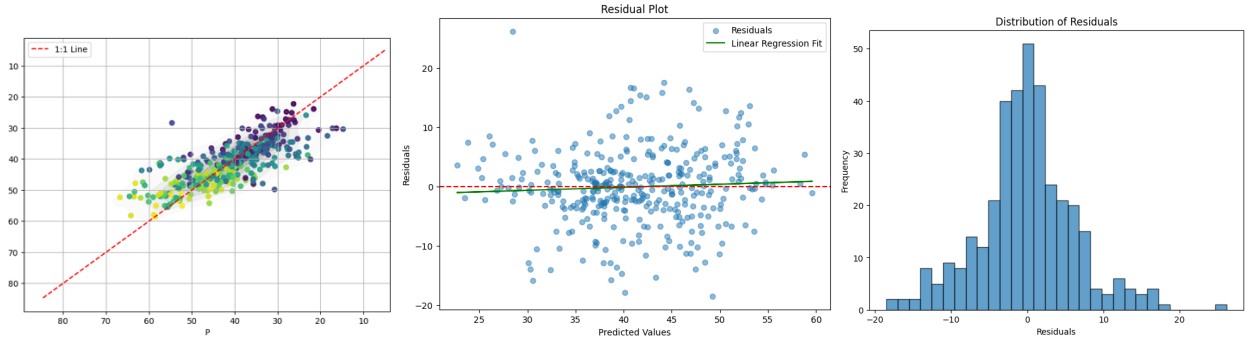

Figure 1. Comparison a) of Nickel and Green (1985) Grt-Opx cation exchange modelled pressures (x-axis) versus our machine learning single-crystal Grt pressures for out test dataset (y-axis) in kbar. Points are coloured by Cr2O3-content, with yellow = high and purple = low. b) residual fit from panel a to the 1:1 line with a linear regression fit. All values in kbar. Lack of slope indicates low skew; panel c) demonstrates that misfit (again, in kbar) is noramlly distributed around a zero value, with a mean absolute error of 4.6 kbar.

There are some caveats to the employment of our thermobarometer, which relate to the machine learning technique. The key point is that the barometer and thermometer can only be applied within the bounds of the data used to train the models, as the algorithm cannot make predictions outside the range of the training data. This applies both in compositional space (oxide composition) and PT space. Thus, our models are applicable within a range of pressure from about 2.25 – 6 GPa, and range of temperature of about 775 – 1350 °C. At 'real' higher or lower T or P, our model will output under- and over-estimates respectively. Despite this limitation, these ranges are very wide and cover the PT ranges of extant cratons. The PT range could be extended if further suitable xenolith data become available. Additionally, as flagged, our models filter for garnet with compositions matching the training dataset (G9, G10, G11, G12). Other garnet will yield spurious estimates and are thus rejected in our workflow.

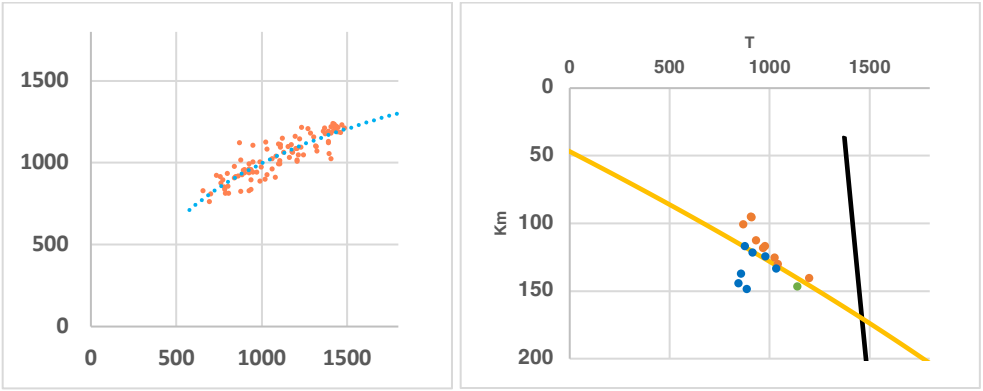

Figure 2. In plot a) Ni-in-Grt T in °C (Ryan et al., 1996) is shown (x-axis) vs our new machine learning Grt T in °C (y-axis). Our estimates match at low and moderate temperatures, but are substantially colder at temperatures >1100°C, in line with other calibrations of Ni-in-Grt T. In plot b) we demonstrate our machine learning barometer and thermometer for detrital garnet on a PT diagram for detrital peridotitic garnet from NE British Columbia (Simandl et al., 2004). With lherzolitic (G9, blue), harzburgitic (G10, orange) and sheared (G11, green) garnet. Yellow line = graphite/diamond stability; adiabat = black line.

As our technique uses only major element compositions (Al_2O_3, SiO_2, TiO_2, Cr_2O_3, FeO_t, MnO, MgO, and CaO) and not Ni, it can be applied to legacy datasets containing only microprobe data (Figure 2a). This means that large existing datasets may now be leveraged to extract information about diamond potential,

and lithospheric thickness and structure. It also means that our temperature estimates can be independently plotted versus Ni-in-Grt T (Figure 2b) for independent verification.

As pyrope are incredibly abundant in kimberlites and more resistant to weathering in detritus than other indicator minerals (e.g. Cr-diopside), there are obvious benefits from our method to diamond explorers on the basis of accurate pressure estimates for fertile and depleted peridotitic garnet compositions. There are opportunities to study mantle stratigraphy with greater accuracy than previously possible using only Ni-in-Grt modelled T. As an example of our model applied to data from the literature, Figure 3 shows the stratigraphy of the Fennoscandian lithosphere as recorded by c. 3000 garnets from the Lentiira kimberlite (Lehtonen et al., 2009). Properly leveraged and carefully applied, this new technique thus provides an opportunity to expand mantle geothermobarometry into the realm of 'big data'.

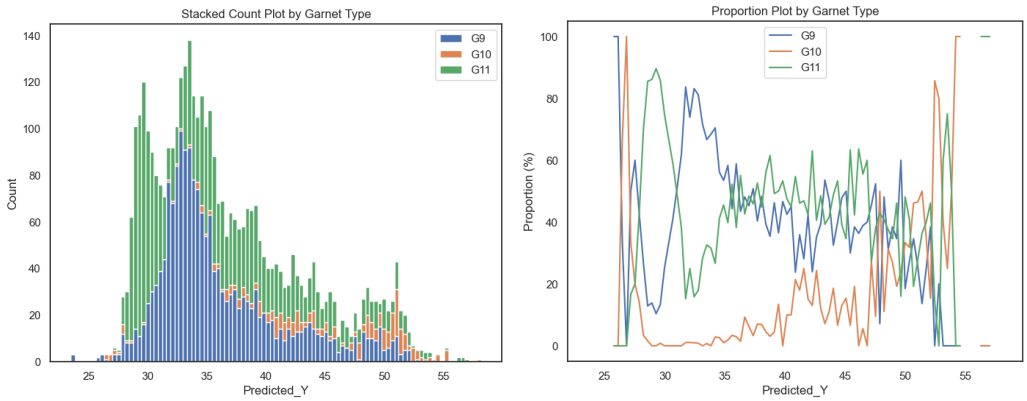

Figure 3. a) a stacked count bar chart of c. 3,000 garnet of different types from the Lentiira kimerlite (Finland, Lehtonen et al., 2009). X-axis is predicted pressure in kbar. This graph shows that our method can be used to determine the stratigragpy of the lithospheric mantle. On chart b) the relative abundance of each garnet type is shown vs predicted P in kbar (Predicted_Y). Below ~27 kbar and above ~54 kbar small n's make ratios unrealiable.

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