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Solid inclusion thermobarometry under fire: Heating experiments on encapsulated quartz inclusions in garnet

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Internal pressures of mineral inclusions (P_{incl}) result from differences in elastic properties of the inclusion mineral and its host mineral. Recent studies utilize pressure-sensitive Raman spectroscopic waveshifts to determine the retained P_{incl} and apply elastic theory to estimate pressure (or temperature) conditions of entrapment. Quartz inclusions are commonly utilized because quartz is a "soft," compressible mineral that is ubiquitous as an inclusion phase in continental metamorphic rocks. Garnet is a commonly used host because it is rigid and isotropic. Quartz inclusions trapped in garnet at *high-P*, *low-T* conditions will retain high P_{incl}; whereas those trapped at *low-P*, *high-T* conditions yield negative waveshifts equating to "negative" pressure, or net tensile stress on the inclusion.

While P_{incl} can be accurately calculated from Raman data, barometry relies also upon the quality of the elastic model, which fundamentally depends on the quality of the $P-V-T$ equations of state (EOS) applied. For quartz, EOS modeling is challenging due to the spontaneous strain that develops close to the lambda transition. In this study we conduct heating experiments on quartz inclusions in garnet from natural samples to assess the response of inclusion pressure to varying temperature (at ambient external pressure), and to evaluate predictions based on commonly applied EOS. Experiments were conducted on two quartz standards (a Herkimer "diamond" and Brazillian quartz) and four completely encapsulated inclusions of quartz in garnet from three tectonically diverse terranes, including: (i) a dilated quartz inclusion (P_{incl} = -4.3 kbar) from Port Leyden, Adirondack Mountains, New York, (ii) a Barrovian-sequence quartz inclusion from northern Scotland (P_{incl} = 3.1 kbar), and (iii) two high-pressure (blueschist) quartz inclusions from Sifnos, Greece (P_{incl} = 7.7 and 8.9 kbar). Standards were heated in 25 ˚C increments with smaller increments near the lambda transition. Quartz inclusions were heated in 50 ˚C increments. The standards were used to correct for thermal perturbations to the $\Delta\nu_{464}$ Raman band for quartz upon heating, allowing for determination of P_{incl} ($\Delta\nu_{464,measured} = \Delta\nu_{464,heating} + \Delta\nu_{464,pressure}$). Measurements were taken upon cooling to test for irreversible plastic deformation (which was not observed).

All samples exhibited a decrease in $\Delta\nu_{464}$ upon heating. The dilated inclusions from Port Leyden experienced the largest increase in P_{incl} (>2 kbar from 25 ˚C to 500 ˚C). The inclusion from Scotland developed moderate P_{incl} increase when heated to 500 ˚C ($\sim$1.4 kbar), whereas the Sifnos inclusion experienced little to no change in P_{incl} upon heating. These results reflect the anomalous increase in thermal expansivity of quartz near the lambda transition. For the low-P samples, the increased thermal expansivity during heating results in an increase in pressure as the inclusion expands more than the void space. For the Sifnos sample, the void space and inclusion expand by nearly the same amount, resulting in no additional pressurization. While the $P_{incl}-T$ trends match predictions, the magnitude of P_{incl} increase is notably less than that predicted by numerical modeling. These results suggest that improvements in $P-V-T$ EOS or more sophisticated elastic models are required to optimize quartz inclusion barometry for formation pressure constraints.