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P-V-T-K^S Equations of State for zircon and rutile

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Zircon ($ZrSiO_4$) and rutile (TiO_2) frequently occur as mineral inclusions entrapped in garnets host from high-pressure metamorphic rocks. In this case they may preserve remnant strains when measured at room conditions by micro-Raman spectroscopy or X-ray diffraction (XRD) that allow application of elastic geobarometry to retrieve the entrapment conditions (P_{trap}) and a constraint for the $P-T$ paths of ultrahigh-pressure metamorphic rocks (Angel et al., 2015). However, elastic geobarometry method requires accurate knowledge of the elastic properties for both host and inclusion phase. While for garnets a variety of consistent datasets and equations of state (EoS) have been already published and assessed, for zircon and rutile the large number of elastic properties that can be retrieved from literature are extremely variable and not consistent to one another.

In the present study the available literature data have been reassessed to derive self-consistent datasets for both zircon and rutile from which we obtained EoS parameters. Zircon data have been fit to a Birch-Murnaghan 3^{rd}-order (BM3) EoS combined with a Holland-Powell thermal pressure model yielding the following coefficients: isothermal bulk modulus K_0^T=225(2) GPa, $\partial K_0^T/\partial P$=$K'$=6.1(1.2), volume thermal expansion αV_0=1.048(7)*10^{-5} K^{-1}, $\partial K_0^T/\partial T$=-0.014(3) GPa/K. These parameters have been obtained after constraining the datasets only to 5 GPa and 730 ^{o}C according to the results of our ab initio models (hybrid Hartree-Fock/Density Functional Theory, HF/DFT) for the zircon-reidite phase transition. Rutile data were fit to a BM3-EoS combined with a Mie-Grüneisen-Debye model yielding the following coefficients: K_0^T=205 GPa (fixed), K'=8.8(3), αV_0=2.487*10^{-5} K^{-1}, $\partial K_0^T/\partial T$= -0.040(1) GPa/K. All datasets have been fit using EoSFit7 suite of programs (Angel et al., 2014).

Using our best estimate of EoS for zircon we calculated the remnant pressure (P_{inc}) for a Zircon trapped at an early stage of the prograde path (P_{trap}=0.5 GPa at T_{rap}=400˚C) and at the metamorphic peak (P_{trap}=4.3 GPa at T_{rap}= 800˚C) as 0.38 and 0.30 GPa, respectively. Our calculations suggest that the remnant strains associated to these P_{inc} would be experimentally distinguishable when measured through XRD, making zircon a good mineral phase to constrain different stages along the prograde path of metamorphic rocks. Underpressure conditions (negative P_{inc}) were calculated for rutile inclusions trapped in garnets, which in natural samples can only be sustained assuming no large-scale plastic or brittle deformation has occurred. Future XRD measurements will thus provide a safe means to control the quality of our results and the mechanism of deformation for natural inclusions.

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Keywords: Zircon, Rutile, Equation of State, HF/DFT, Elastic geobarometry

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