Elastic geobarometry of multiphase inclusions

Kira A. Musiyachenko[1], Mara Murri[2], Ross J. Angel[3], Mauro Prencipe[4], Matteo Alvaro[1], Hugo van Schrojenstein Lantman[1]

[1] Department of Earth and Environmental Sciences, University of Pavia, Via A. Ferrata, 1 27100 Pavia, Italy
[2] Department of Earth and Environmental Sciences, University of Milano-Bicocca, Piazza della Scienza 4, I-20126 Milano, Italy
[3] IGG CNR, Via Giovanni Gradenigo, 6, 35131 Padova, Italy
[4] Department of Earth Sciences, University of Torino, Via Valperga Caluso 35, 10125 Torino, Italy

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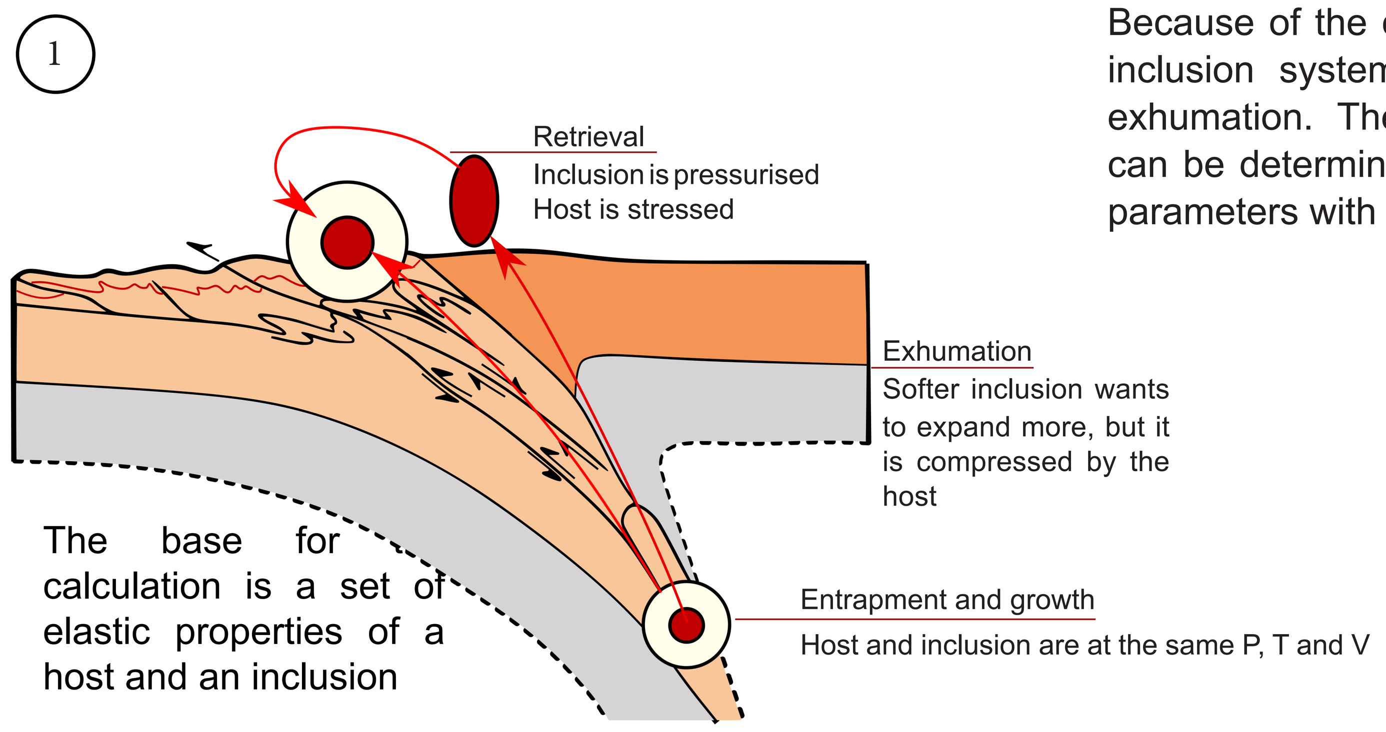
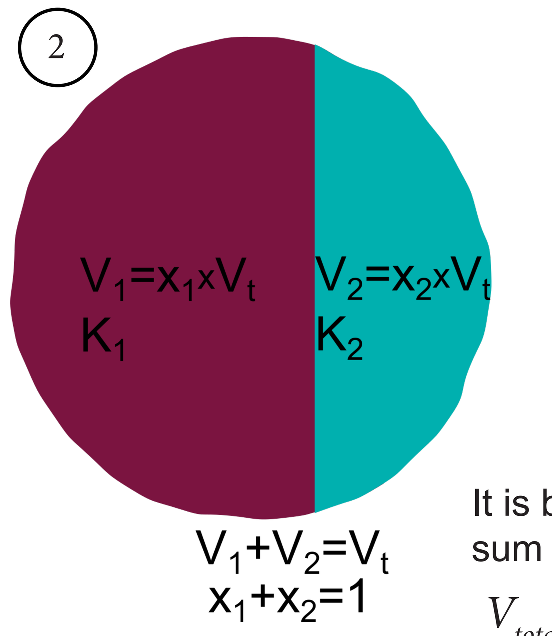
General concept: elastic geobarometry

The principles of elastic geobarometry provide an approach to recover the crystallization conditions of the system which does not require a chemical equilibrium, but it is based on the elastic interactions between the host–inclusion pair. Because of the contrast in the elastic properties, the host-inclusion system develops non-lithostatic stresses upon exhumation. The residual elastic strain in the inclusion can be determined directly (e.g. from the measured lattice parameters with single-crystal X-ray diffraction) or indirectly from the changes in the wavenumbers of Raman-active phonon modes relative to an unstrained crystal with the phonon-mode Grüneisen approach. The remnant inclusion stress is then calculated from the measured strains.



The references and more on elastic geobarometry: www.mineralogylab.com

Multiphase inclusions: elastic properties



The elastic properties of mixed-phase inclusions have Reuss and Voigt bounds. They represent the cases of equal stress or strain on all phases respectively

$K_{tot}=(x_1/K_1+x_2/K_2)^{-1}$ Reuss bound (all of the phases are at the same pressure)

$K_{tot}=x_1K_1+x_2K_2$ Voigt bound (all of the phases undergo the same volume strain)

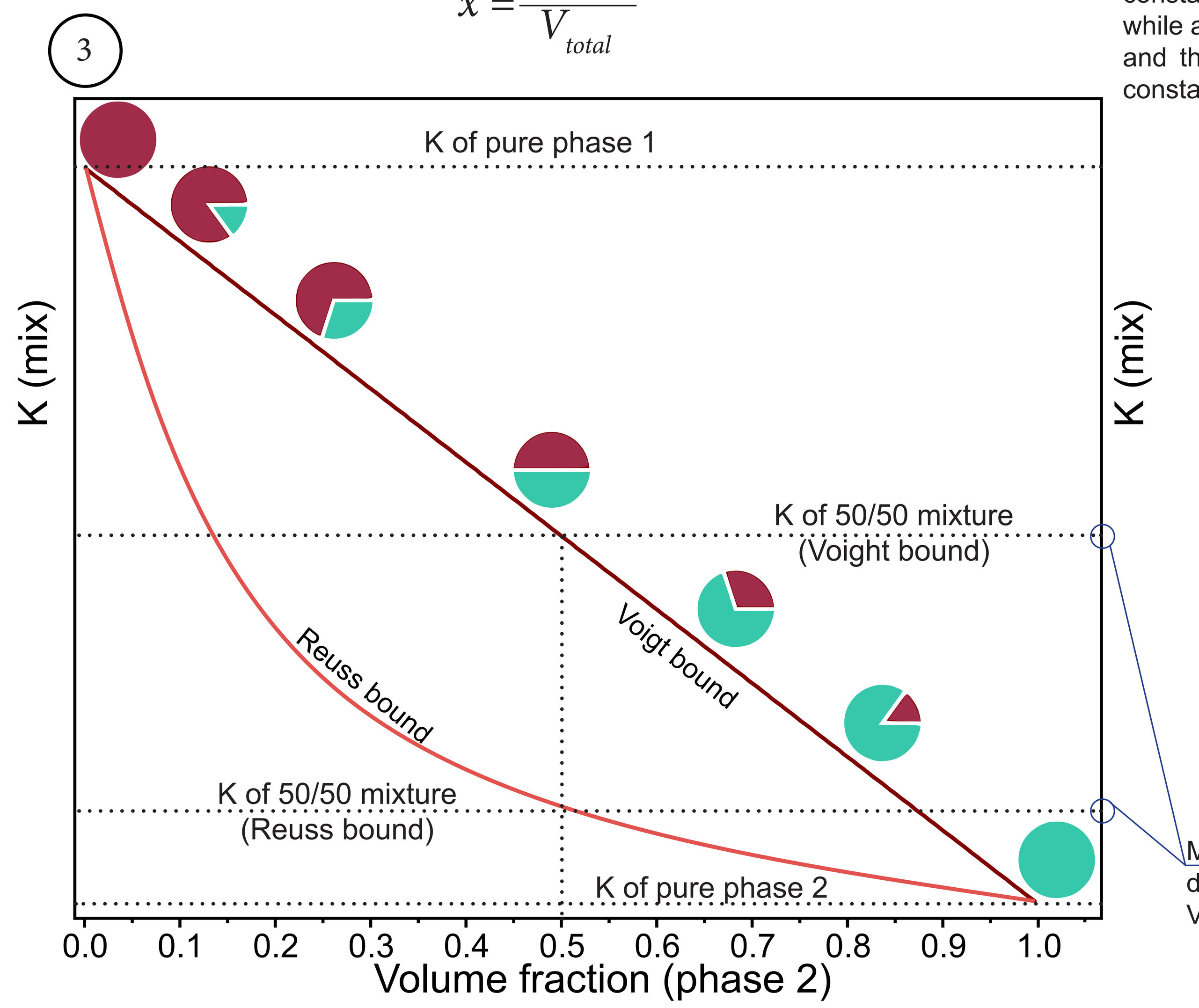
It is better to represent the volume of the mixture through the sum of the molar volumes per amount of moles of each phase:

$$V_{total}=\Sigma\, m_i V_{mi}$$

In that case the volume fraction x is given by:

$$x=\frac{m_i V_{mi}}{V_{total}}$$

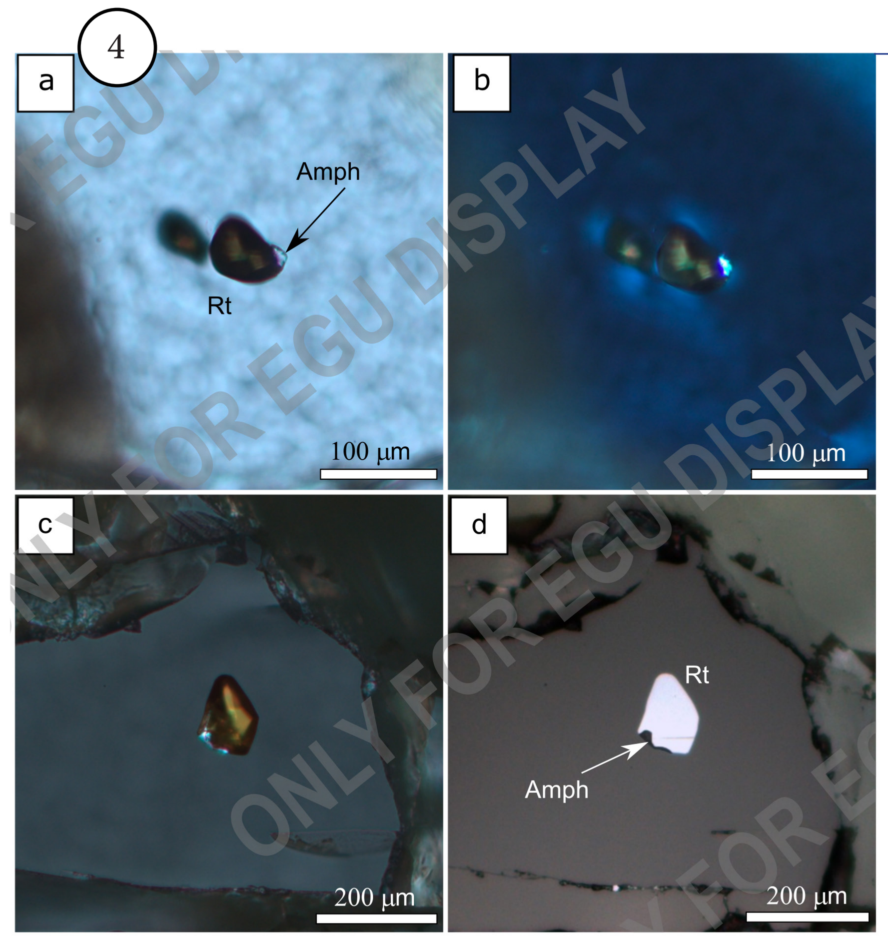
Volume fraction of the phase is not constant at different PT conditions while amounts of moles of each phase and therefore the molar fraction is a constant value



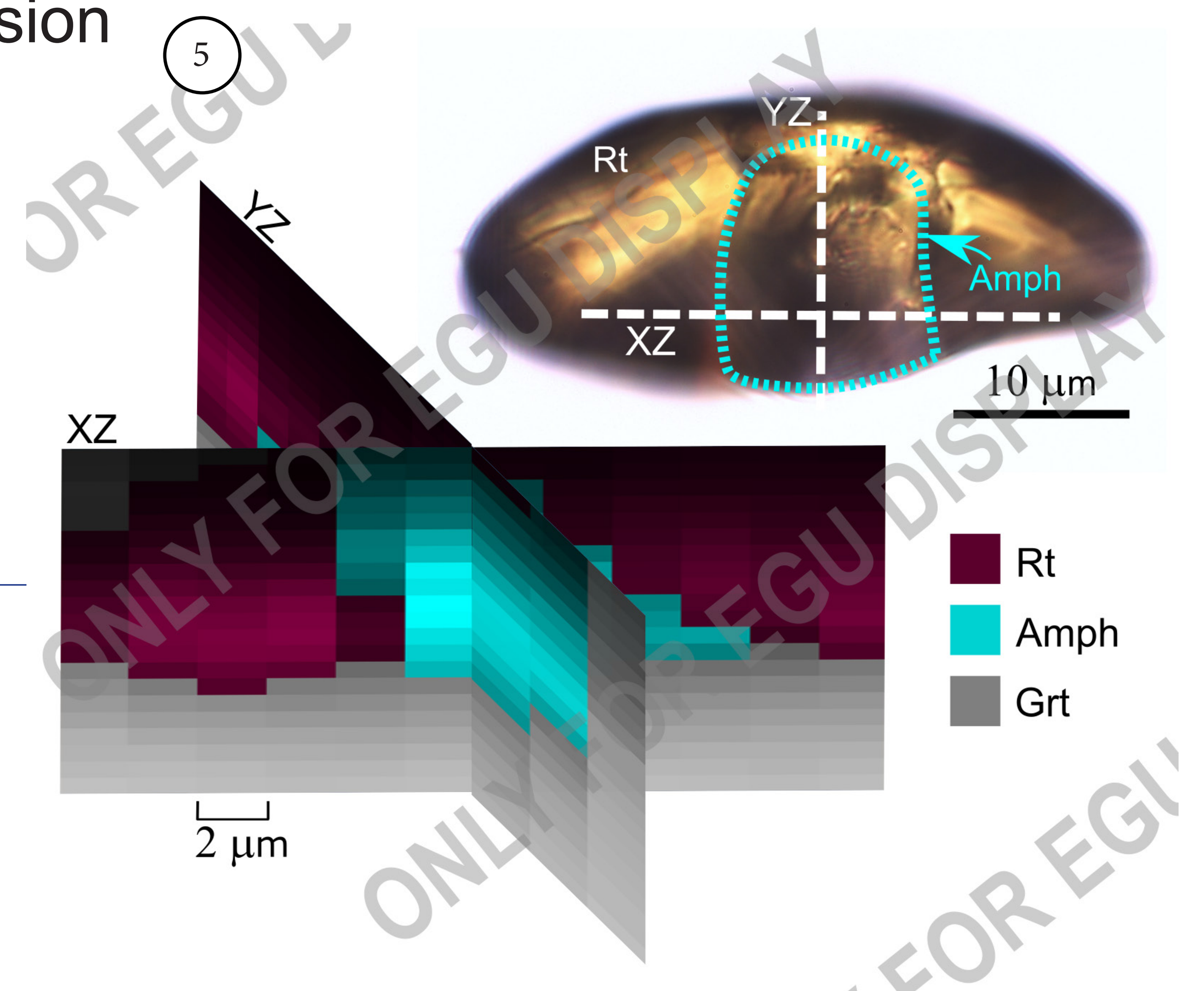
Mixture bulk modulus value differs if we use Reuss or Voigt bound for an estimation

Expression for the Voigt bound on the bulk modulus of a mixture is based on the sum of the bulk moduli of the component phases. By contrast, the Reuss bound on the bulk modulus of a mixture is based on the sum of the compressibilities of the phases. The Voigt bound on the bulk modulus is larger (i.e. stiffer) than the Reuss bound.

Natural samples: rutile+amphibole multiphase inclusion



Composite rutile + amphibole inclusions in garnet (eclogite from Pohorje massif). a, b – PPL and XPL microphotographs of the inclusions with the surrounding birefringent halo. c, d – Surface inclusion in garnet (XPL and RL microphotographs). Birefringent halo is absent on image c because the stress is released as the inclusion is exposed



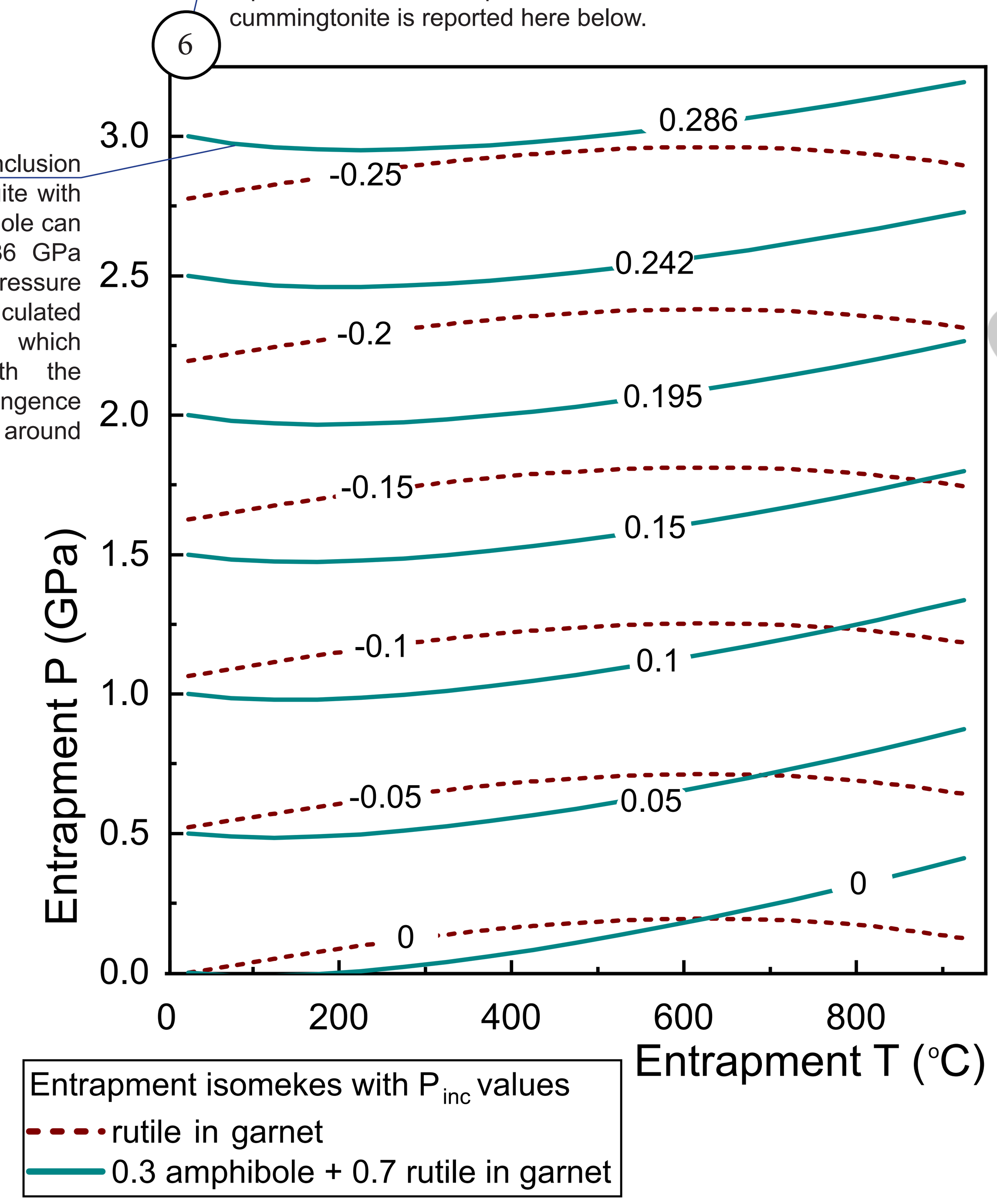
Raman imaging of a mixed rutile+amphibole inclusion along XZ and YZ planes. The blue area in the image indicate the presence of the 671 cm^{-1} characteristic peak of amphibole, while dark red and grey are related to the characteristic peaks at 141.6 and 917 cm^{-1} from rutile and garnet, respectively.

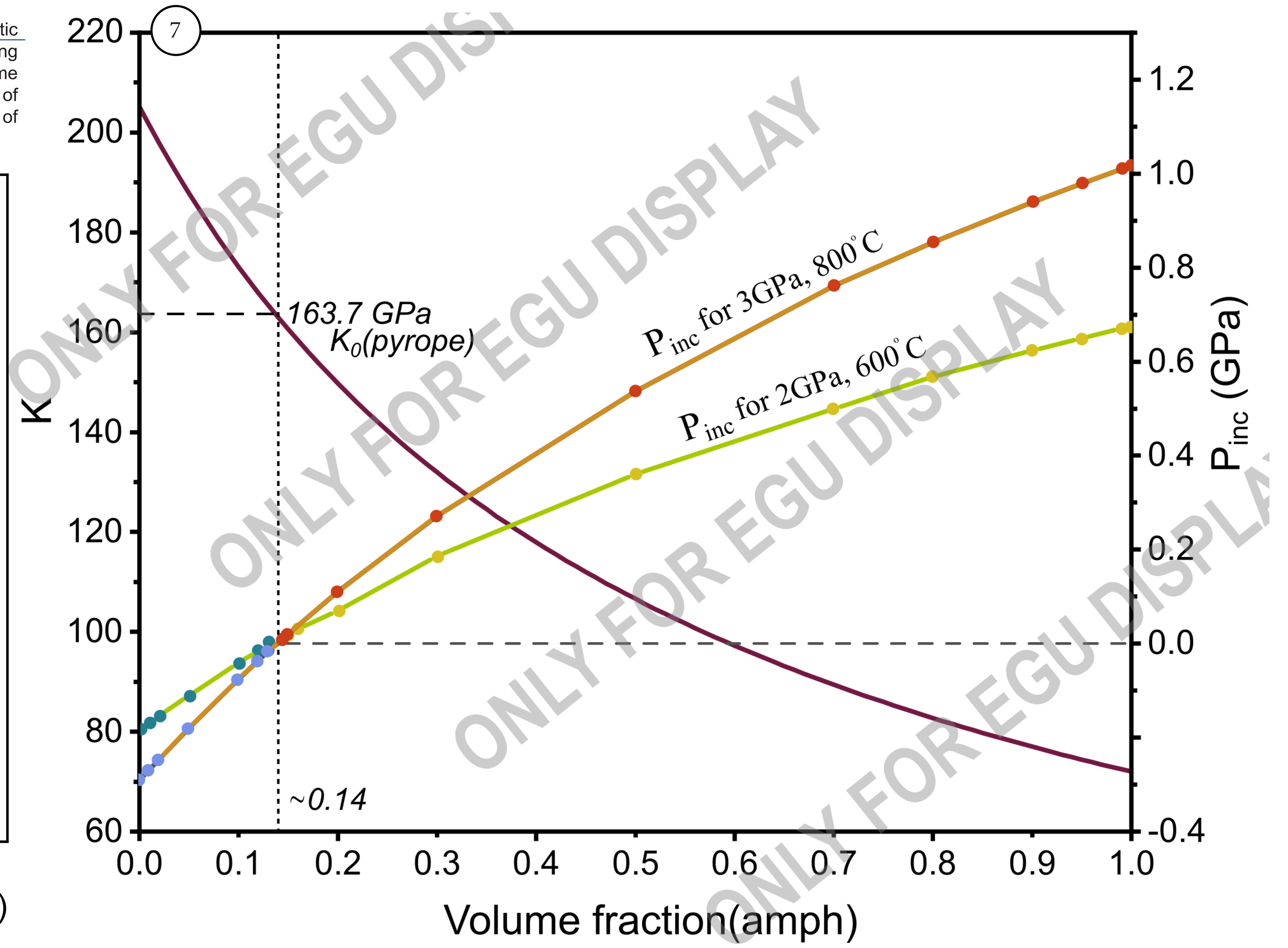
Rutile-in-garnet would be a good candidate for elastic geobarometry because of its common occurrence in high-pressure high-temperature (HP-HT) metamorphic rocks, its simple structure and chemistry and its broad PT stability field. However, recent work by Zaffiro et al. (2019) showed that rutile trapped in garnet should always exhibit negative pressure upon exhumation because rutile is stiffer than garnet, making this pair unsuitable for elastic geobarometry. Nevertheless, rutile inclusions in garnets from the Pohorje HP locality (Slovenia) seem to challenge this thermodynamic prediction - they appear to exhibit signs of residual pressure. These rutile inclusions are surrounded by a clearly distinguishable birefringence halo which reflects the elastic deformation of the host garnet in the immediate vicinity of the inclusion due to its elastic relaxation. High resolution 3D Raman mapping on one of these rutile inclusions revealed the presence of tiny (2-3 µm thick) amphibole crystals located between the garnet and rutile, with the amphibole occupying about 25-30% of the volume of the inclusion.

To treat this case we developed a methodology that is implemented in the MPHASE utility of EosFit7c, in which the volume of the mixture at all P and T is treated as the sum of the volumes of the individual phases calculated from their EoS weighted by their molar fractions. We used the Reuss approximation as we expect the two phases to be under the same pressure rather than the same strain (Voigt approximation). The presence of at least 14% in volume of amphibole is enough to reduce the bulk modulus (at ambient conditions) of the mixture to less than that of the garnet (Fig 9). This makes the inclusion softer than the host and should lead to the development of a positive inclusion pressure upon exhumation.

Presence in an inclusion of a second phase with a contrasting elastic properties changes significally the behaviour of the isomekes brigning to a positive residual pressure within the same host and the same entrapment conditions (PT). An example of entrapment isomekes of a pure rutile and a composite inclusion with 70 % of rutile and 30 % of cummingtonite is reported here below.

The multiphase inclusion from Pohorje eclogite with 30 vol.% of amphibole can exhibit up to 0.286 GPa of a residual pressure according to the calculated Pinc curves, which is consistent with the presence of birefringence haloes in the host around these inclusions.





Bulk modulus (red) and Pinc (orange and green) curves at room conditions of rutile plus cummingtonite mixtures as a function of volume fraction of the amphibole. Negative Pinc values are indicated with blue dots, while positive values with red and yellow dots. The bulk modulus curve corresponds to the Reuss expression for the bulk modulus of the two-phase mixture. Values of the Pinc are calculated for the entrapment condition at 3 GPa 800°C and at 2 GPa 600°C as an example. The volume fraction of the amphibole (0.14) leading to a zero Pinc is also the composition for which the bulk modulus of the inclusion is equal to that of the pyrope host.