EntraPT: an online application for elastic geothermobarometry

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Abstract

EntraPT is a web-based application for elastic geobarometry freely accessible at the "Fiorenzo Mazzi" experimental mineralogy lab website (www.mineralogylab.com/software). It provides an easy-to-use tool to calculate inclusion pressures with error propagation from the residual strain measured in mineral inclusions. EntraPT establishes a method and a workflow to import and analyze the measured residual strains, correctly calculate the mean stress in the inclusions, compute the entrapment isomekes with uncertainty estimation, and visualize all the results in relevant graphs. It enables the many possible errors arising from manual handling of the data and from the numerous steps required in geobarometry calculations to be avoided. All of the data, parameters and settings are stored in a consistent format and can be exported as project files and spreadsheets, and imported back to EntraPT for further analysis. This allows researchers to store and/or share their data easily, making the checking and the comparison of data and results reliable. EntraPT is an online tool that does not require any download and/or installation, and it will be updated in the future with new functionalities made available from advances in the development of elastic geobarometry.

EntraPT: an online application for elastic geothermobarometry

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Key Points

- We present EntraPT, a new online application for elastic geobarometry
- EntraPT establishes a workflow to calculate residual pressures and entrapment isomekes from the measured residual strain on inclusions
- Data can be imported and exported enabling the checking and the comparison of results

Abstract

EntraPT is a web-based application for elastic geobarometry freely accessible at the "Fiorenzo Mazzi" experimental mineralogy lab website (www.mineralogylab.com/software). It provides an easy-to-use tool to calculate inclusion pressures with error propagation from the residual strain measured in mineral inclusions. EntraPT establishes a method and a workflow to import and analyze the measured residual strains, correctly calculate the mean stress in the inclusions, compute the entrapment isomekes with uncertainty estimation, and visualize all the results in relevant graphs. It enables the many possible errors arising from manual handling of the data and from the numerous steps required in geobarometry calculations to be avoided. All of the data, parameters and settings are stored in a consistent format and can be exported as project files and spreadsheets, and imported back to EntraPT for further analysis. This allows researchers to store and/or share their data easily, making the checking and the comparison of data and results reliable. EntraPT is an online tool that does not require any download and/or installation, and it will be updated in the future with new functionalities made available from advances in the development of elastic geobarometry.

Plain Language Summary

During geodynamic processes minerals in rocks can recrystallize at depth in the Earth at high pressures and temperatures, and new minerals form. During crystallization growing minerals can trap other minerals within them as inclusions. After millions of years, some of these rocks are exposed on the Earth's surface and become available to researchers for direct observation. The inclusions deform during exhumation because of the removal of external pressure and temperature. By measuring the residual deformation in the inclusion and with specific calculations it is possible to estimate the conditions (pressure and temperatures) of the recrystallization; the time when the inclusion was entrapped in its host. This in turn gives us a wealth of information to understand large scale geological processes such as the subduction and the collision of tectonic plates. Here we present EntraPT, a new freely accessible online application that eases the interpretation of the residual deformation of inclusions and performs the calculations to estimate the entrapment conditions. EntraPT gives a standardized procedure to make it easier for researchers to check, store and share their data.

1 Introduction

Mineral inclusions entrapped in their mineral host in several rock types provide fundamental information on geological processes such as subduction and exhumation. A residual strain is developed in the inclusion during exhumation of a host-inclusion pair to the Earth's surface, because of the contrast in elastic properties between the two minerals **(**Angel, Nimis, et al., 2015). The inclusion does not expand in response to changes in *P* and *T* as would a free crystal. Instead it is restricted by the host mineral, and this confinement can result in a residual strain, whose magnitude depends on the entrapment conditions and on the elastic properties of the mineral pair. If the residual strain is interpreted correctly, the conditions at entrapment ($\boldsymbol{P_{trap}}$, $\boldsymbol{T_{trap}}$) can be estimated through the elastic geobarometric approach by using the elastic properties of the host and the inclusion.

The basic concept has been known for long time (e.g. Angel, Mazzucchelli, et al., 2014; Angel, Nimis, et al., 2015; Rosenfeld and Chase, 1961). It is based on the assumption of isotropic elasticity for both the host and the inclusion. Angel, Mazzucchelli, et al. (2017) have formulated this problem in a way that can include non-linear elasticity. The entrapment conditions are calculated as the conditions under which there are no stress gradients across the host and inclusion. All the possible entrapment conditions for a specific host-inclusion system lie on the entrapment isomeke, a line in P-T space along which, in isotropic systems, the strain and the stress are uniform in the system. However, the determination of the entrapment isomeke requires the knowledge of the residual pressure in the inclusion.

The methods to measure residual pressure of minerals have been discussed recently by Murri et al. (2018) and Bonazzi et al. (2019). They showed that the elastic anisotropy of minerals affects the definition of residual pressure. Since anisotropic mineral inclusions are usually under non-hydrostatic stress (detailed explanation in Angel et al., 2019; Mazzucchelli et al., 2019; Murri et al., 2018), common approaches that determine the residual pressure by interpreting Raman shifts (wave-numbers) with hydrostatic calibrations (Ashley et al., 2016; Enami et al., 2007) can lead to significantly inaccurate estimates of the residual "pressure" and, in turn, of the entrapment conditions, leading to fundamental misinterpretations of geological processes. Changes in the Raman shifts of a crystal arise from the strains imposed upon it (e.g. Angel et al., 2019; Barron et al., 1980; Grüneisen, 1926). The phonon-mode Grüneisen tensor describes the relationship

between the change in the position of each Raman peak and the strain in a crystal. The full state of strain of an inclusion relative to a free crystal in air can therefore be determined from the measurement of the changes in the Raman shifts relative to the free crystal. Once the strains are known, the residual stress and the residual pressure in the inclusion can be determined. Bonazzi et al. (2019) showed that for quartz inclusions entrapped in garnet hosts, the entrapment conditions determined with this definition of residual pressure are reliable even in presence of deviatoric stress.

We here present EntraPT, a web application which implements the method developed by Angel et al. (2019) and Murri et al. (2018) and applied by Bonazzi et al. (2019), to correctly calculate the mean stress in inclusions from the measured strains, and then to calculate entrapment isomekes with the isotropic model including the propagation of uncertainties. EntraPT is freely accessible after registration. It can be used effectively to process strain data from a single inclusion or large datasets of residual strains of multiple inclusions to obtain entrapment conditions and to easily generate plots, without introducing external errors. In this paper we will guide the reader through the step-by-step analysis using EntraPT of a typical dataset (Bonazzi et al. 2019) of quartz inclusions entrapped in almandine .

2 Program description

The successful determination of the *P-T* of metamorphism using elastic geothermobarometry ideally requires the analysis of a large number of inclusions (Bonazzi et al., 2019). Because of the contrast in elastic properties between the two minerals, some host-inclusion systems are good geothermometers (e.g. zircon in garnet) while other are good barometers (e.g. quartz in garnet), and their coexistence in the same rock might provide a constraint on the metamorphic *P-T* path of the rock, because of the different slopes of their isomekes (e.g. Zhong et al., 2019). Furthermore, to interpret correctly the conditions of metamorphism it is necessary to account for all the uncertainties from the measurement of the residual strain to the calculation of the entrapment conditions. EntraPT is a MATLAB® based online application with a Graphical User Interface (GUI) that can be used to: (1) import and visualize the residual strain and the associated

uncertainties from measurements in inclusions; (2) correctly calculate the mean stress in inclusions from the measured strains; (3) calculate entrapment isomekes with the isotropic model of Angel, Mazzucchelli, et al. (2017) with uncertainty propagation; (4) plot the entrapment isomekes for multiple inclusions simultaneously; (5) export all the data and results as project files or spreadsheets to store and share them.

EntraPT is freely accessible upon registration as an online application at the website of the "Fiorenzo Mazzi" Experimental Mineralogy Lab (www.mineralogylab.com/software). EntraPT is supported on most of the common browsers and operating systems (Windows®, macOS®, Linux®) and no download and/or installation is required. The app was developed with MATLAB® AppDesigner and deployed with MATLAB® Compiler on Web App Server. For all of the calculations based on the equations of state (EoS) of the minerals (e.g. the calculation of the residual pressure and of the entrapment isomeke), EntraPT relies on Eosfit7 (Angel, Alvaro, et al., 2014) a stable and efficient Fortran code that has been validated over many years. Eosfit7n, a fast version of the program without a console or GUI for direct user interaction, is embedded in EntraPT. The instructions and EoS parameters for calculations are sent from EntraPT to Eosfit7n as files. Once the calculations are terminated, the output generated by Eosfit7n is read back into the app. The use of EosFit7n as a separate executable ensures that EntraPT will be able to access new EoS forms and other developments introduced into the EosFit library and program suite in the future.

EntraPT consists of three main tabs: *Add New Analyses*, *Calculate Entrapment* and *View Data* (Fig. 1a, b, c). The workflow, from the definition of the host-inclusion system to the calculation of entrapment conditions and the data visualization, is illustrated in detail in Section 3. EntraPT works on *analyses*. Each *analysis* is a container of all of the information relative to one measurement of residual strain and the calculations performed on it. An *analysis* is defined at least by:

- A label
- A pair of mineral phases: the host and the inclusion phase
- The elastic properties of the host and the inclusion (EoS, stiffness tensors)
- The geometry of the host-inclusion system
- The relative orientation between the host and the inclusion

- The residual strain state defined by the components of residual strain vector, and its covariance matrix

Other data that can be optionally associated with an *analysis* are:

- The labels of the sample, thin section, host, inclusion and of the point analysis
- A text description
- The results of the calculation of its entrapment conditions (i.e. *P* and *T* of the entrapment isomeke, and all the intermediate results, such as residual stress, unrelaxed strain, their covariance matrices, etc..)

With this definition, two measurements of residual strain taken in the same inclusion crystal are stored and treated as separate *analyses* in EntraPT. In fact, even if they belong to the same host-inclusion system (same mineral phases, geometry and orientation) they can differ in the residual strain. For the same reason, measurements from several inclusions in the same host crystal are also considered as separate *analyses*. This allows for great flexibility in storing and processing the measurements, since each of them can have different data and metadata and can be handled separately.

EntraPT makes use of the Voigt notation (Voigt, 1910) to represent tensors, and this notation will be assumed thoughout this paper. Therefore 2^{nd}-rank tensors are represented as vectors and 4^{th}-rank tensors as matrices. The mapping of the indices between the tensor notation and the vector (Voigt) notation is the following:

Tensor notation	11	22	33	23	13	12
Voigt notation	1	2	3	4	5	6

2.1 Properties of the host-inclusion system and residual strain

In EntraPT the user first needs to add one or more new *analyses* to the project from the *Add New Analyses* tab (Fig. 1a), where the host and the inclusion minerals, the geometry of the system and their relative orientation must be chosen. The calculation of the entrapment conditions requires the elastic properties of the minerals. EntraPT is based on an internally-consistent database of elastic properties (Table 1). The database contains for each mineral phase the volume EoS and, for

inclusions, the 4th-rank elastic tensor at room conditions. The elastic tensors are taken from experimental determinations reported in the literature, and, if necessary, their components are rescaled to ensure that the Reuss bulk modulus equals that of the volume EoS (Table 1) at room conditions. This ensures consistency throughout the entire calculation. During the rescaling, care is taken that the degree of anisotropy (evaluated through the Universal anisotropic index, Ranganathan and Ostoja-Starzewski, 2008) is not altered (see Mazzucchelli et al., 2019 for further details). Only phases with published and validated elastic properties and EoS are included in the program database. In the current version aluminosilicate garnet endmembers (e.g. pyrope, almandine and grossular) and diamond are available as hosts. The inclusion can be chosen among quartz, zircon, diamond and garnet. Addtional hosts and inclusion minerals will be added as more internally consistent elastic data and EoS become available.

Table 1. Equations of State (EoS) and independent components of the at room-conditions elastic (stiffness) tensor of the minerals currently available in the database of EntraPT. For internal consistency, the components of the stiffness tensor from literature were rescaled to ensure that the Reuss bulk modulus equals that of the corresponding volume EoS. The rescaling does not alter the anisotropy evaluated through the universal anisotropic index (Ranganathan and Ostoja-Starzewski, 2008). The elastic properties (EoS parameters and the components of the elastic tensors) are shown to the user in the application once a host-inclusion system is selected (see Fig. 1).

Mineral	Type	EoS from:	C_{ij} (GPa)	C_{ij} modified after:
Almandine	Host/inclusion	Milani et al. (2015)	$C_{11} = 300.2$; $C_{12} = 108.8$; $C_{44} = 93.3$;	Jiang et al. (2004)
Diamond	Host/inclusion	Angel, Alvaro, et al. (2015)	$C_{11} = 1078.4$; $C_{12} = 126.8$; $C_{44} = 575.7$;	Zouboulis et al. (1998)
Grossular	Host/inclusion	Milani et al. (2017)	$C_{11} = 316.7$; $C_{12} = 91.5$; $C_{44} = 102.2$;	Isaak et al. (1992)
Pyrope	Host/inclusion	Milani et al. (2015)	$C_{11} = 291.1$; $C_{12} = 100$; $C_{44} = 93$;	Sinogeikin and Bass (2002)
Zircon	Host/inclusion	Unpublished	$C_{11} = 422.0$; $C_{12} = 70.0$; $C_{13} = 148.9$; $C_{33} = 488.0$; $C_{44} = 113.1$; $C_{66} = 48.3$;	Özkan et al. (1974)
Quartz	inclusion	Angel, Alvaro, et al. (2017)	$C_{11} = 86.1$; $C_{12} = 7.2$; $C_{13} = 11.7$; $C_{14} = 17.7$; $C_{33} = 105.6$; $C_{44} = 59.2$;	Lakshtanov et al. (2007)

Once the properties of the system are set, the user must input the residual strain measured in the inclusion for each *analysis*. As shown by Murri et al. (2019) and Angel et al. (2019) the strain state can be obtained from the measured Raman shifts by applying the concept of the phonon-mode

Gruneisen tensor. This can be done easily for inclusions such as quartz and zircon using stRAinMAN (Angel et al., 2019), a free program that can be downloaded at http://www.rossangel.com/. stRAinMAN allows the user to load the measured Raman shifts and to export the resulting strain components and the associated standard deviations and correlations in a logfile. For a uniaxial inclusion without symmetry breaking, stRAinMAN provides an output with the sum of the strain components (in Voigt notation) $\varepsilon_1 + \varepsilon_2$, the component ε_3, their estimated standard deviations (esd) and the covariance between $\varepsilon_1 + \varepsilon_2$ and ε_3. If the strain is measured with X-ray diffraction, measurements need to be carefully interpreted because irregular and faceted inclusions may exhibit stress and strain gradients. In this case, diffraction measurements only provide some average value of strain over the whole inclusion volume that cannot be used directly in elastic geobarometry (e.g. Alvaro et al., 2020; Campomenosi et al., 2018; Mazzucchelli et al., 2018; Murri et al., 2018). However, with XRD the value of each strain component (together with their esd and covariances) can be potentially determined independently. The user can input in EntraPT the components of the residual strain and the associated uncertainties, for each *analysis*. The esd and the covariances associated with the residual strain are needed to propagate the uncertainties into the residual pressure and the entrapment isomeke. Since the application of elastic geobarometry usually requires the processing of several measurements performed on several inclusions, the user has the option of importing a file with a list of *analyses* with their strains and the associated uncertainties (esd's and covariances). The input file can be selected with a file-browser window and it is uploaded to the server via a secure SSL connection. The input file must have a **.dat* extension, and be a tab-delimited text file. Template files are provided with the program on the website mineralogylab.com and can be edited with a spreadsheet editor, to preserve the tab delimited structure. Each row of this file stores the data of one *analysis*, i.e. of one measurement. All of the *analyses* in one input file must belong to the same host-inclusion system (i.e. same host and inclusion phases). The content of each column is specified by the headers. Five columns are reserved for the labels to identify the *analysis* (sample, thin section, host, inclusion and point analysis) and one column for the notes associated to the *analysis*. The content of the remaining columns depends on the symmetry of the residual strain, which corresponds to the symmetry of the inclusion in absence of symmetry breaking. A general-purpose file, suitable for any symmetry of the strain, contains one column for each strain component (6 columns), and one column for each independent entry of the covariance matrix (21 columns). If

the inclusion is uniaxial without symmetry breaking both the strain and the covariance matrix have fewer independent components. In this case a specific template is provided (see Table 2 for an example). The measured strain components and the statistical parameters (esd, covariances) can be easily copied and pasted from the stRAinMAN logfile to this input file using any spreadsheet editor. When the inclusion is cubic (without symmetry breaking), the volume strain is enough to describe the strain state of the inclusion (e.g. Angel et al., 2019). Therefore, the volume strain and its esd can be specified in the appropriate input file for cubic inclusions. During the import process, EntraPT checks that the file is readable and consistent. Depending on the symmetry of the inclusion selected by the user in the app, a minimum number of independent strain components is required. Moreover, the symmetry of the inclusion prescribes the equality between some of the components of the strain. A check is also performed on the consistency of the provided esd and covariances, since the resulting covariance matrix must be positive definite. Analyses that do not satisfy these requirements are discarded during the import process, and a detailed message describing the errors is shown to the user.

Table 2. Example of input file to import into EntraPT the components of the residual strain and the associated esd and covariances of uniaxial inclusions without symmetry breaking. In this example, the Raman shifts were measured in quartz inclusions in almandine host synthetized by Bonazzi et al. (2019), and they were converted into residual strains using the program stRAinMAN. The first row reports the headers that must be included in the input file even when the associated columns are not used. The labels allow the user to identify each *analysis* by giving the codes of the sample, thin section, host and inclusion to which it belongs. The *PointAnalysis_label* can be used when more than one *analysis* are measured in the same inclusion. The complete template **.dat* file is reported in the Data Repository.

Sample_label	ThinSection_label	Host_label	Inclusion_label	PointAnalysis_label	e1_plus_e2	esd_e1_plus_e2	e3	esd_e3	cov_e1_plus_e2_e3
Alm1		Grt1	I1		-0.02210	0.00451	-0.00810	0.00291	-1.2995E-05
Alm1		Grt1	I2		-0.02430	0.00451	-0.00620	0.00291	-1.2995E-05
Alm1		Grt1	I4		-0.05960	0.00451	0.02310	0.00291	-1.2995E-05
Alm1		Grt1	I5		-0.02490	0.00451	-0.00720	0.00291	-1.2995E-05
Alm1		Grt1	I6		-0.02800	0.00451	-0.00540	0.00291	-1.2995E-05
Alm1		Grt2	I1		-0.04490	0.01041	0.00920	0.00673	-6.9345E-05
Alm1		Grt2	I2		-0.02120	0.00451	-0.00810	0.00291	-1.2995E-05
Alm1		Grt2	I3		-0.03990	0.00451	0.00750	0.00291	-1.2995E-05
Alm2		Grt1	I1		-0.02520	0.00451	-0.00218	0.00291	-1.2995E-05
Alm2		Grt1	I2		-0.02670	0.00451	0.00004	0.00291	-1.2995E-05
Alm2		Grt1	I3		-0.02630	0.00451	-0.00100	0.00291	-1.2995E-05
Alm2		Grt2	I5		-0.02720	0.00451	0.00063	0.00291	-1.2995E-05
Alm2		Grt3	I1		-0.02480	0.00451	-0.00262	0.00291	-1.2995E-05
Alm2		Grt3	I2		-0.02500	0.00451	-0.00244	0.00291	-1.2995E-05
Alm2		Grt4	I1		-0.01600	0.00451	-0.00574	0.00291	-1.2995E-05
Alm2		Grt4	I2		-0.02100	0.00451	-0.00449	0.00291	-1.2995E-05
Alm2		Grt5	I1		-0.01950	0.00451	-0.00517	0.00291	-1.2995E-05
Alm2		Grt6	I1		-0.02400	0.00451	-0.00185	0.00291	-1.2995E-05
Alm2		Grt7	I1		-0.02270	0.00451	-0.00247	0.00291	-1.2995E-05
Alm2		Grt8	I2		-0.03340	0.00601	0.00491	0.00388	-2.3131E-05
Alm2		Grt9	I2		-0.02240	0.00451	-0.00254	0.00291	-1.2995E-05

EntraPT requires the full 6 x 6 covariance matrix $\boldsymbol{V}^{\varepsilon}$ of the residual strain values in order to propagate the uncertainties through the calculations of the residual pressure and the entrapment isomeke. For a general state of residual strain with six independent components in Voigt notation $(\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4, \varepsilon_5, \varepsilon_6)$, the fully-symmetric covariance matrix $\boldsymbol{V}^{\varepsilon}$ is defined as:

$$\boldsymbol{V}^{\varepsilon} = \begin{bmatrix} esd(\varepsilon_1)^2 & cov(\varepsilon_1,\varepsilon_2) & cov(\varepsilon_1,\varepsilon_3) & cov(\varepsilon_1,\varepsilon_4) & cov(\varepsilon_1,\varepsilon_5) & cov(\varepsilon_1,\varepsilon_6) \\ & esd(\varepsilon_2)^2 & cov(\varepsilon_2,\varepsilon_3) & cov(\varepsilon_2,\varepsilon_4) & cov(\varepsilon_2,\varepsilon_5) & cov(\varepsilon_2,\varepsilon_6) \\ & & esd(\varepsilon_3)^2 & cov(\varepsilon_3,\varepsilon_4) & cov(\varepsilon_3,\varepsilon_5) & cov(\varepsilon_3,\varepsilon_6) \\ & & & esd(\varepsilon_4)^2 & cov(\varepsilon_4,\varepsilon_5) & cov(\varepsilon_4,\varepsilon_6) \\ & Symmetric & & & esd(\varepsilon_5)^2 & cov(\varepsilon_5,\varepsilon_6) \\ & & & & & esd(\varepsilon_6)^2 \end{bmatrix} \quad (1)$$

Where $esd(\varepsilon_i)$ is the estimated standard deviation on the *i-th* component of the strain vector (in Voigt notation), and $cov(\varepsilon_i, \varepsilon_j)$ is the covariance between the strain components *i* and *j*.

The esds and the covariances of the residual strain of uniaxial and cubic inclusions are automatically translated by EntraPT into the full 6 x 6 covariance matrix $\boldsymbol{V}^{\varepsilon}$ of the residual strain. For uniaxial inclusions (i.e. trigonal, tetragonal and hexagonal crystal systems) without symmetry breaking, two normal strain components are equal ($\varepsilon_1 = \varepsilon_2$), while the third ($\varepsilon_3$) is different. The shear components are absent ($\varepsilon_4 = \varepsilon_5 = \varepsilon_6 = 0$). When the residual strain of uniaxial inclusions is determined from Raman spectroscopy through the stRAinMAN program, the strain sum $\varepsilon_1 + \varepsilon_2$ and ε_3 are given as output together with the corresponding uncertainties $esd(\varepsilon_1 + \varepsilon_2)$, $esd(\varepsilon_3)$. The covariance between $\varepsilon_1 + \varepsilon_2$ and ε_3 is also computed and reported as $cov(\varepsilon_1 + \varepsilon_2, \varepsilon_3)$. Given these parameters, and assuming that $\varepsilon_1 = \varepsilon_2$ are completely correlated, the full covariance matrix of the residual strain $\boldsymbol{V}^{\varepsilon}$ is assembled by EntraPT as:

$$\boldsymbol{V}^{\varepsilon} = \begin{bmatrix} \left(\frac{esd(\varepsilon_1+\varepsilon_2)}{2}\right)^2 & \left(\frac{esd(\varepsilon_1+\varepsilon_2)}{2}\right)^2 & \frac{1}{2}cov(\varepsilon_1+\varepsilon_2,\varepsilon_3) & 0 & 0 & 0 \\ & \left(\frac{esd(\varepsilon_1+\varepsilon_2)}{2}\right)^2 & \frac{1}{2}cov(\varepsilon_1+\varepsilon_2,\varepsilon_3) & 0 & 0 & 0 \\ & & esd(\varepsilon_3)^2 & 0 & 0 & 0 \\ & & & 0 & 0 & 0 \\ & symmetric & & & 0 & 0 \\ & & & & & 0 \end{bmatrix} \quad (2)$$

For cubic crystals without symmetry breaking, the normal strain components are equal $\varepsilon_1 = \varepsilon_2 = \varepsilon_3$, the shear components are absent ($\varepsilon_4 = \varepsilon_5 = \varepsilon_6 = 0$) and the residual volume strain is $\varepsilon_V = \varepsilon_1 + \varepsilon_2 + \varepsilon_3$. Given the uncertainty on the volume strain $esd(\varepsilon_V)$, the full covariance matrix of the residual strain $\boldsymbol{V}^{\varepsilon}$ is:

$$\boldsymbol{V}^{\varepsilon} = \begin{bmatrix} \left(\frac{1}{3}esd(\varepsilon_V)\right)^2 & \left(\frac{1}{3}esd(\varepsilon_V)\right)^2 & \left(\frac{1}{3}esd(\varepsilon_V)\right)^2 & 0 & 0 & 0 \\ & \left(\frac{1}{3}esd(\varepsilon_V)\right)^2 & \left(\frac{1}{3}esd(\varepsilon_V)\right)^2 & 0 & 0 & 0 \\ & & \left(\frac{1}{3}esd(\varepsilon_V)\right)^2 & 0 & 0 & 0 \\ & & & 0 & 0 & 0 \\ & symmetric & & & 0 & 0 \\ & & & & & 0 \end{bmatrix} \quad (3)$$

Once the strains are imported or set in the program, the user can add the *analyses* to the current project.

2.2 Calculation of the entrapment isomeke with uncertainties

The possible entrapment conditions, i.e. points on the entrapment isomeke (Rosenfeld and Chase, 1961; Angel, Mazzucchelli, et al., 2014; Angel, Nimis, et al., 2015), of each *analysis* can be calculated from the *Calculate Entrapment* tab (Fig. 4). This calculation using isotropic elasticity and the full non-linear EoS of the host and inclusion requires the knowledge of the residual pressure of the inclusion (Angel, Mazzucchelli, et al., 2017). As shown by Bonazzi et al. (2019), when the residual strain of the inclusion is used there are two possible definitions of residual pressure (P_{inc}) for anisotropic inclusions:

1) The residual stress can be calculated from the residual strain as:

$$\sigma_i = C_{ij}\varepsilon_j \quad (4)$$

where C_{ij} is the matrix representation in Voigt notation of the 4th rank elastic modulus tensor of the inclusion determined at room conditions. The pressure is then the negative of the mean normal stress:

$$P_{inc}^{strain} = -\frac{(\sigma_1 + \sigma_2 + \sigma_3)}{3} \quad (5)$$

2) Alternatively, the residual volume strain can be found as the sum of the normal components of the strain:

$$\varepsilon_V = \varepsilon_1 + \varepsilon_2 + \varepsilon_3 \quad (6)$$

from which the residual pressure is obtained using the EoS of the inclusion as:

$$P_{inc}^{V} = f_{EoS}(\varepsilon_V) \quad (7)$$

By default, EntraPT uses model (1) for the calculation of residual pressure. However, the user can enable the *Expert mode* panel from the *Settings* menu and choose model (2) or both the models to explore a comparison of the results.

The covariance matrix of the residual strain is used to propagate the uncertainties on the calculated residual pressures and the isomekes. If model (1) is selected (eq. 4), the covariance matrix on the residual stress ($\boldsymbol{V^{\sigma}}$) in the inclusion is obtained from that on the residual strain ($\boldsymbol{V^{\varepsilon}}$) as:

$$\boldsymbol{V^{\sigma}} = \boldsymbol{C}\,\boldsymbol{V^{\varepsilon}}\,\boldsymbol{C}^{T} \quad (8)$$

Where $\boldsymbol{C}$ is the matrix representation in Voigt notation of the 4th rank elastic modulus tensor of the inclusion, and $\boldsymbol{C^{T}}$ its transpose. Eq. (8) assumes that the uncertainties on the elastic components are negligible compared to the uncertainties of the measured strains. The typical uncertainty on the elastic components is usually less than 2% (e.g. Lakshtanov et al., 2007) compared to a typical uncertainty on the strain larger than 5% (Bonazzi et al., 2019). Moreover, the covariances of the

elastic components determined experimentally are often not reported in literature and cannot therefore be used for error propagation.

Once the residual stress and its covariance matrix are known, the standard deviation on the residual pressure P_{inc}^{strain} (eq. 5) can be found as:

$$esd(P_{inc}^{strain}) = \frac{1}{3}\sqrt{V_{1,1}^{\sigma} + V_{\mathbf{2},2}^{\sigma} + V_{3,3}^{\sigma} + 2V_{1,2}^{\sigma} + 2V_{1,3}^{\sigma} + 2V_{\mathbf{2},3}^{\sigma}} \quad (9)$$

On the other hand, if model (2) is selected, the uncertainty on the strain components is propagated into the estimated standard deviation of the volume strain $esd(\varepsilon_V)$ as:

$$esd(\varepsilon_V) = \sqrt{V_{1,1}^{\varepsilon} + V_{\mathbf{2},2}^{\varepsilon} + V_{3,3}^{\varepsilon} + 2V_{1,2}^{\varepsilon} + 2V_{1,3}^{\varepsilon} + 2V_{\mathbf{2},3}^{\varepsilon}} \quad (10)$$

Given this uncertainty on the volume strain the standard deviation on the residual pressure P_{inc}^{V} (eq. 7) is found as:

$$esd(P_{inc}^{V}) = (1/2)\left[\left|f_{EoS}\left(\varepsilon_V + esd(\varepsilon_V)\right) - f_{EoS}(\varepsilon_V)\right| + \left|f_{EoS}\left(\varepsilon_V - esd(\varepsilon_V)\right) - f_{EoS}(\varepsilon_V)\right|\right] \quad (11)$$

The calculation of the possible entrapment conditions for the host-inclusion pair is performed assuming isotropic elasticity with the model proposed by Angel, Mazzucchelli, et al. (2017), using the non-linear elasticity of the host and the inclusion. The calculation of the entrapment isomeke is performed calling the specific routines in the Eosfit7n program. The *Pend* and *Tend* are the pressure and temperature at which residual strain is measured and are assumed to be room conditions (25 °C or 298 K and 0 GPa). Since the calculation of the residual pressure (eq. 4 - 5) requires the elastic tensors ($\boldsymbol{C}$) of each inclusion, which are mostly only known for room *P*,*T*, EntraPT is necessarily restricted to calculations from strain measured when the host is at room conditions. The user can set the range of temperatures for the calculation of the entrapment isomeke using the *Tmin*, *Tmax* and *Tstep* fields in the application (see Fig. 4). Initially, the units for temperature (Tscale) and for the pressure (Pscale) are set to °C and GPa respectively, but they can be set to K and kbar, respectively, from the *Settings* menu. The uncertainties on the entrapment

isomeke are estimated from the standard deviation on the residual pressure $esd(P_{inc})$. The extreme values of the residual pressure are evaluated assuming an uncertainty on the residual pressure equivalent to one standard deviation as:

$$P_{inc}^{max} = P_{inc} + esd(P_{inc}) \qquad P_{inc}^{min} = P_{inc} - esd(P_{inc}) \tag{12}$$

The entrapment isomeke is computed for each value of residual pressure. Therefore, for each temperature step along the isomeke (T_{iso}), P_{iso} is the mean value of the pressure on the isomeke, while P_{iso}^{max} and P_{iso}^{min} are the boundaries on the uncertainty, associated with one standard deviation on the residual pressure. For each T_{iso} on the isomeke the corresponding uncertainty on the P_{iso} is obtained as:

$$esd(P_{iso}) = \frac{1}{2}\left(|P_{iso}^{max} - P_{iso}| + \left|P_{iso}^{min} - P_{iso}\right|\right) \tag{13}$$

Once the calculation is completed, the results of the calculation (residual stress, pressure, P-T points on the entrapment isomekes) of each *analysis* are stored in the current project.

2.3 Viewing and plotting data

In the *View Data* tab (Fig. 1c) the user can view all of the data relative to each *analysis* and generate relevant plots. The details of the selected analysis are reported in the *Details* page. The residual strain of one or more *analyses* can be analyzed visually in a scatter plot (Fig 3) from the *Plot Strain* page. For each *analysis*, the associated confidence ellipse is shown, as obtained from the variance-covariance matrix $\boldsymbol{V}^{\varepsilon}$ determined from the measurement of the residual strain. For a visual reference, the isochors and the lines of isotropic strain and hydrostatic stress state of a crystal of the same phase as the inclusion can be added to the plot. The results of the calculation of the entrapment isomeke are shown in the *Results* page (Fig. 5c). The user can also generate a *P-T* plot with the isomeke(s) of one *analysis* together with the estimated uncertainty shown as a shaded area from the *Plot Isomekes* page (Fig. 5d,e). The isomekes of multiple *analyses* can also be plotted at the same time, even if they belong to different host-inclusion systems. This is particularly useful

for constraining the metamorphic conditions if several host-inclusion systems within the same rock were measured. Since some host-inclusion systems are good barometers (e.g. quartz in garnet) while others are good thermometers (e.g. zircon in garnet), the intersection of their isomekes can provide constraints on the *P-T* path of the rock (e.g. Zhong et al., 2019).

2.4 Export and import of data

Project files, that contain all of the data from all of the *analyses* (elastic properties, strain given as input, covariance matrices, calculation parameters, results, notes etc.) are stored in a database-like format and can be downloaded to the user's computer from the *File>Export Project* menu. By default, the project is saved to a binary file with **.ept* extension. Project files can be imported back into EntraPT, using the *File>Import Project* menu, to view the data, generate the plots. Importing a project file puts EntraPT in the same configuration as when the project file was created. Once a project is loaded, new *analyses* can be added or existing *analyses* can be deleted. Moreover, multiple project files can be merged in EntraPT to create larger databases. Such project files can be easily shared, making the checking and the comparison of data and results reliable. The project file can be easily imported into MATLAB® and custom scripts can be developed to further process the data. An example of these scripts is reported in the Data Repository and the generated plot is shown in Fig. 6. During the export procedure from EntraPT, the user can also choose to save the data to spreadsheets (with **.xlsx* extension) that can be read by any commonly used spreadsheet application, such as Microsoft Excel® or LibreOffice®. In this case an individual spreadsheet is created for each *analysis.* A compressed folder, with **.zip* extension, is created that contains the **.ept* project file and one or more folders containing the spreadsheet files. To preserve the privacy of the users and the complete control of their data, all of the data are deleted from the server when the EntraPT session is terminated and cannot be recovered even by the server administrators. Therefore, downloading the project to the users computer is the only way to have access to the data after the EntraPT session is terminated. The upload and the download of the data to and from the server is always performed over a secure SSL connection.

3 Example

In this section we show how EntraPT can be used in practice to: (i) interpret the residual strain measured in several inclusions; (ii) calculate the residual pressure and the entrapment conditions evaluating the uncertainties for each step of the calculation; (iii) store all of the data in a consistent way and use them for further analysis. In this example we will focus on the data published by Bonazzi et al. (2019), obtained from hydrothermal synthesis experiments with a piston-cylinder press to produce quartz inclusions in pure almandine garnet (>99%) at eclogite facies metamorphic conditions. In the study two experiments were performed and labelled Alm-1 (synthesis performed at P = 3.0 GPa and T= 775 °C) and Alm-2 (at P= 2.5 GPa and T= 800 °C). From each experiment they recovered several host crystals, each containing one or more crystals of quartz as inclusions. Isolated, fully-enclosed quartz inclusions in the recovered garnets were then investigated using micro-Raman spectroscopy. The changes in the Raman peak positions were measured at the central point of the inclusion and interpreted by applying the phonon-mode Grüneisen tensors of quartz (Murri et al., 2018) to obtain the full strain state of each inclusion, using the program stRAinMAN (Angel et al., 2019). From the residual strain they calculated the full residual anisotropic stress state and the mean stress by using the elastic properties of quartz. The authors showed that the entrapment pressures calculated from this mean stress with the isotropic model for host-inclusion systems differ from the known synthesis pressure by <0.2 GPa, which is on the order of the combined experimental uncertainties. Their results show that the most significant effect of the elastic anisotropy of quartz is on the Raman shifts of the inclusion, and not on the subsequent calculation of entrapment conditions.

3.1 Add new analyses: set the host-inclusion system and import the measured residual strains

The user can add new *analyses* from the *Add New Analyses* tab. This tab has a panel on the right to navigate through the *Host&Inclusion*, *Geometry*, *Orientation* and *Strain* pages where all of the parameters that define an *analysis* can be set. Since all of the measurements refer to quartz inclusions in almandine, the user has first to set these phases as host and inclusion in the *Host&Inclusion* page (Fig. 1d). The analysis in the current version of EntraPT is based on the assumptions that the inclusion is spherical and far away from fractures and the external surface of the host. Therefore, we will show the application to those inclusions measured by Bonazzi et al.

(2019) that have an "ideal" geometry (almost spherical and far from the surface of the host). As a consequence, the geometry can be left as a sphere in the *Geometry* page (Fig. 1e). Since the orientation between the host and inclusion is not relevant for isotropic elastic geobarometry, the *Orientation* page (Fig. 1f) is set by default to an inclusion unrotated with respect to the host.

Once all of the parameters are set, the user needs to confirm them from the *Orientation* page and moves to the next page, *Strain* (Fig. 2a). Since we want to analyse multiple measurements all belonging to the same host-inclusion systems with the same features (mineral phases, geometry and orientation) we can choose to import the strains for multiple *analyses* (Fig 2b). By clicking on *Import File* (Fig 2c), a file-dialog is opened to choose an input file (with **.dat* extension) from the computer of the user. In Bonazzi et al.(2019) the residual strain of each inclusion was obtained from the stRAinMAN program using the measured Raman shifts. Since the inclusion (quartz) is uniaxial, the values $\varepsilon_1 = \varepsilon_2$ and ε_3 (together with their esd and covariance) are given in the output file of stRAinMAN. It was formatted into the input file for EntraPT (Table 2) using a spreadsheet editor and is available in the Data Repository. The input file is then loaded to the server and the consistency check is performed (see Section 2.1). If the check is passed, the imported data will be listed in the application. The user can now click on *Add Analyses to Workspace* (Fig 2d) and all the imported *analyses* will appear in the *Workspace* on the left side of the app (Fig 2e).

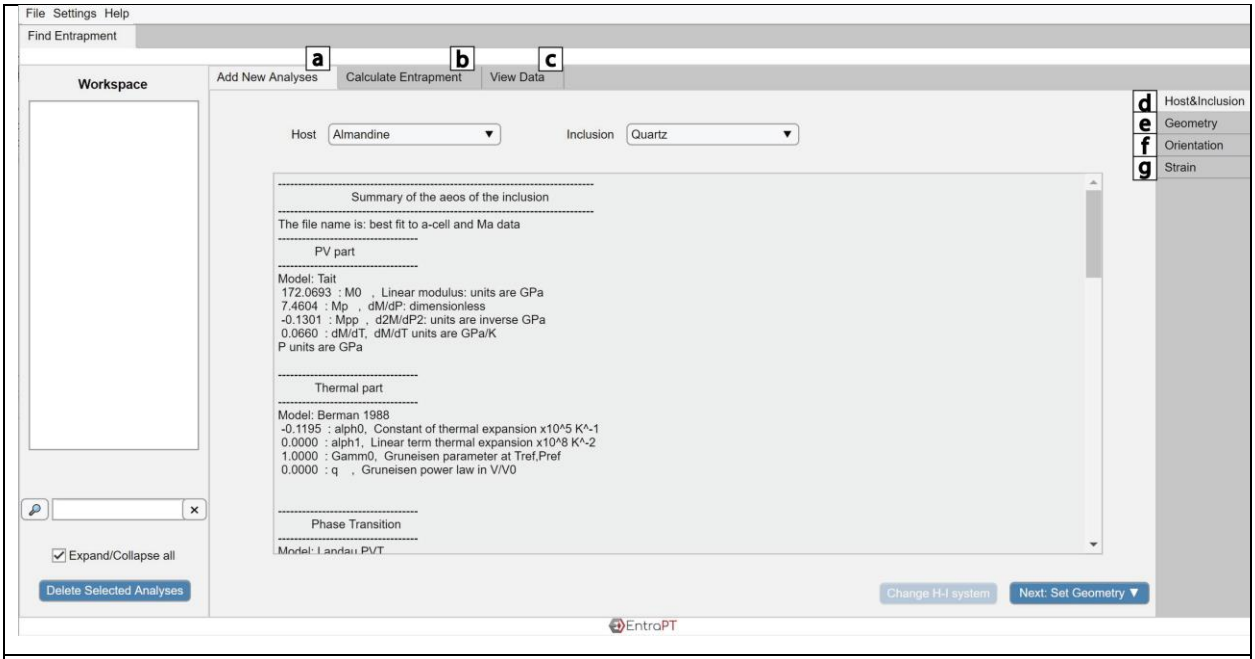

Figure 1. EntraPT is structured with three main tabs: *Add New Analyses* (a), *Calculate Entrapment* (b) and V*iew Data* (c). The user has first to define one or more new analyses from

the *Add New Analyses* tab. Using the panel on the right side the user can set the host and inclusion minerals (d), the geometry (e), the orientation (f) and the measured residual strains (g). This figure shows the Host&Inclusion page (d) where the host and the inclusion minerals are set, and a summary of their EoS is shown to the user.

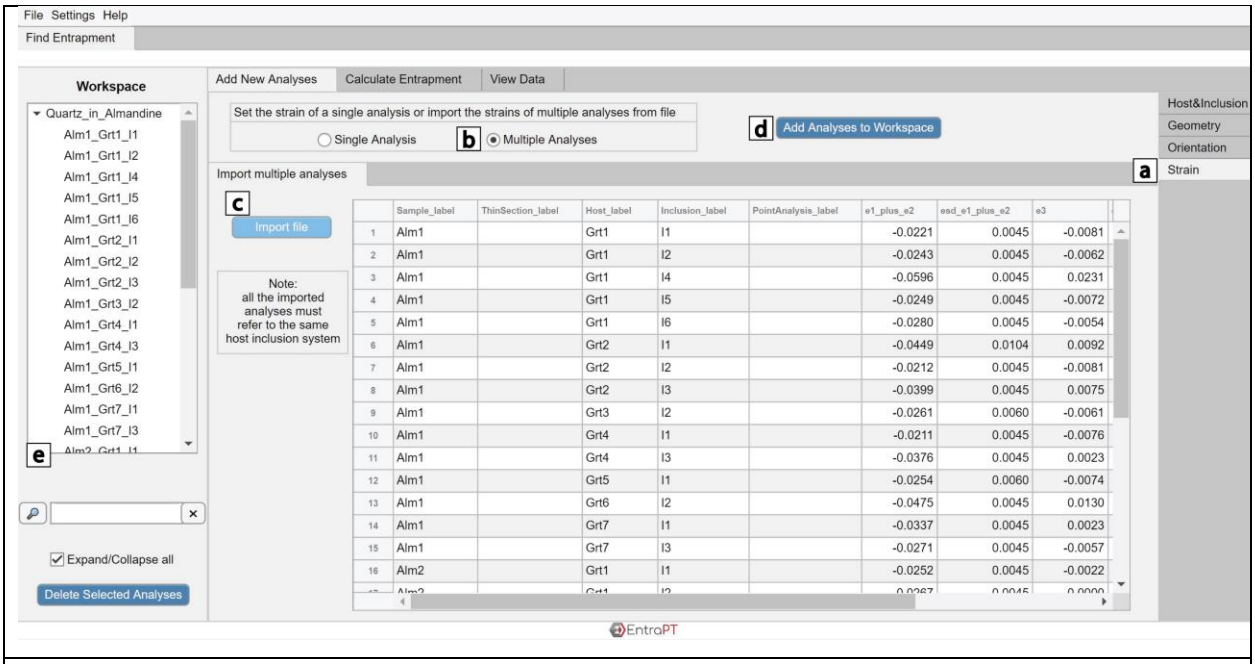

Figure 2. The user can import several measurements of the residual strain measured in the same host inclusion system (i.e. same minerals, geometry and orientation) from the *Strain* page (a) under *Add New Analyses.* The user has first to choose the option *Multiple analyses* (b) and then click on *Import file* (c). A file dialog is opened to choose the input file (with *.dat extension) from the user's computer. If the file is imported successfully, the imported data are listed in the app and the analyses can be added to the current project by clicking on *Add Analyses to Workspace* (d). The analyses will appear in the *Workspace* (e).

3.2 Visual analysis of the residual strain

Once the measured strains are stored in the project, the user can at any time perform a visual analysis of the residual strain from *Plot Strain* (Fig. 3a) in the *View Data* tab. By selecting all of the *analyses* from the *Workspace* (Fig. 3b), their strains are shown by default in a plot of ε_1 vs ε_3 with error bars and confidence ellipses obtained from the esd and covariances on the residual strain (Fig 3c). Other choices for the axes can be done, e.g. $\varepsilon_1 + \varepsilon_2$ vs ε_3. The isochors and the lines of isotropic strain and hydrostatic stress can be added to the plot (Fig 3e) and the range of the axes can be modified as needed by using the Plot Settings (Fig 3f). The user can show the plot of specific

groups of analyses by using the search field (Fig. 3g) below the *Workspace*. For example, searching for the keyword "Alm1" will display in the *Workspace* only those analyses belonging to the sample Alm1, which can be selected and displayed in the current plot. As already noted by Bonazzi et al., (2019), the measured strain values lie sub-parallel to the isochors and are clustered above the line of hydrostatic conditions (Fig 3c). The presence of a non-hydrostatic stress in these inclusions is expected from the symmetry of the inclusion and purely elastic behavior: when the quartz is trapped in a cubic host such as garnet, the inclusion will be subject to isotropic strains imposed by the host and therefore, because it is elastically anisotropic, the inclusion will develop deviatoric stresses unless the deviatoric stress is decreased by a plastic deformation (e.g. Zhong et al., 2018; Zhong et al., 2020).

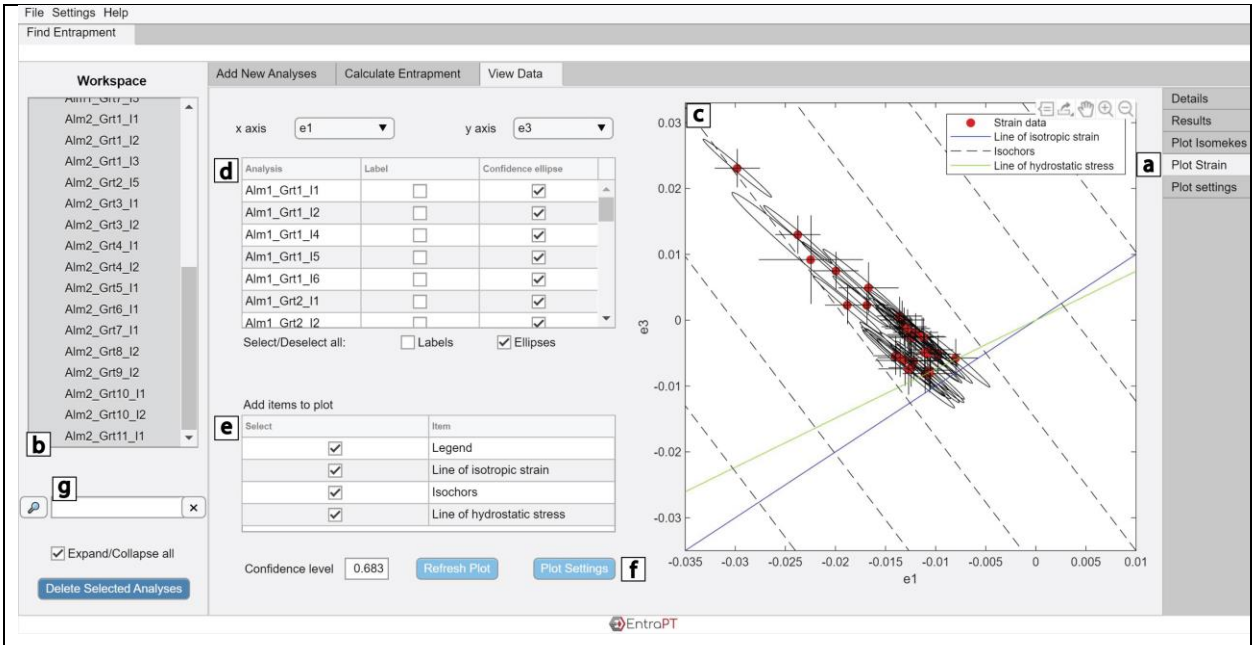

Figure 3. Once the analyses are added to the current project, a visual inspection of the measured residual strains can be performed from the *Plot Strain* page (a) under *View Data*. Here the user needs to select one or more analyses from the *Workspace* (b). By default, the strain data are shown in a ε_3 vs ε_1 plot (c), but other choices of axes can also be made in the app. The values of the strains are plotted together with their error bars and confidence ellipses obtained from their covariance matrices. The labels of the analyses and the confidence ellipses can be shown or hidden (d). The lines of isotropic strain and hydrostatic stress and the isochors can be also added to the plot (e). The range of the axes can be adjusted as needed (f). The search field (g) allows the user to search for specific analyses by typing a full label or part of it. The searched analyses are listed in the *Workspace*. The strain components determined at room temperature for quartz inclusions from experiments Alm-1 and Alm-2 by Bonazzi et al. (2019) are shown in

the plot with the confidence ellipses corresponding to one standard deviation. They lie sub-parallel to the isochors and are clustered above the strains for hydrostatic conditions.

3.3 Calculate the entrapment isomekes

The entrapment conditions are calculated in the *Calculate Entrapment* tab. The user has to select one or more *analyses* from the *Workspace* to calculate their entrapment isomekes (Fig. 4a). The parameters for the calculation of the isomeke (*Tmin, Tmax, Tstep*) have to be set (Fig. 4b). Since the inclusions were synthetized by Bonazzi et al. (2019) in two experiments conducted at 3 GPa, 775 °C (Alm1) and 2.5 GPa, 800 °C (Alm2), in our example we choose *Tmin* = 750 °C, *Tmax*=850 °C, *Tstep* =5 °C as the temperature range for the calculation of the entrapment isomeke. The final conditions at which the residual strain was measured are always assumed to be room conditions (*T* = 25 °C or 298 K, *P* = 0 GPa or 0 kbar, Fig. 4c). One or both of the models discussed in section 2.2 can be chosen to get the residual pressure from the measured strain (Fig. 4d), by enabling the *Expert Mode* panel from the *Settings* menu. The chosen residual pressure(s) will be used for the calculation of the entrapment isomeke. For the current example, the residual pressure was calculated using both methods. By selecting all the *analyses* from the *Workspace*, the calculation of the entrapment isomeke is run at once (Fig. 4e) and the results are saved to the project. However, the user can calculate the entrapment isomekes for each *analysis* independently by selecting one at time from the *Workspace* and setting the appropriate calculation parameters.

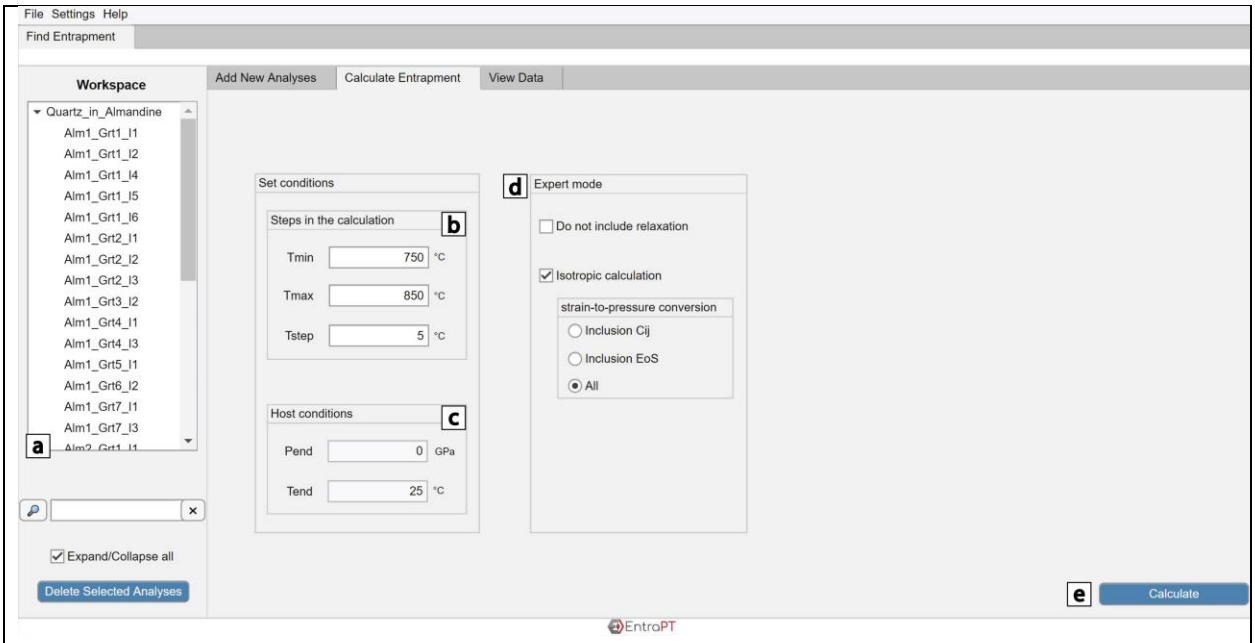

Figure 4. In the *Calculate Entrapment* tab the user can calculate the entrapment isomekes of one or more analyses by selecting them from the *Workspace* (a). The T limits and steps in the calculation of the isomekes can be adjusted as needed (b). Other P and T scales (K and kbar) can be selected from the *Settings* menu. The final conditions of the host are always assumed to be room conditions (c). The *Expert mode* panel (d) allows the user to not include the elastic relaxation (see Angel, Mazzucchelli, et al., 2014) in the calculation and to choose the model to obtain the residual pressure from the measured strain (see Section 2.2). Once the parameters are set, the calculation is started by clicking on the *Calculate* button (e).

3.4 View and plot the results

The results from each *analysis* can be viewed in the *View Data* tab (Fig. 5). By selecting one *analysis* from the *Workspace* (Fig. 5a), the *Details* page (Fig. 5b) shows all of the details of the selected analysis such as the label, the notes, the host-inclusion system, and the residual strain. The *Results* page (Fig. 5c) shows all of the numerical results (residual pressure found with each model, *P-T* points on the isomekes, and all of the uncertainties). The *Plot Isomekes* page (Fig. 5d) shows a *P-T* graph reporting the isomekes obtained using models (1) and (2) described in Section 2.2 with their estimated uncertainties shown as a shaded area (Fig. 5e). As discussed in section 2.2, the uncertainties on the isomekes are estimated assuming an uncertainty equal to one standard deviation on the residual pressure. The user can selectively choose to hide one or more objects from the plot (isomekes, shaded area of the uncertainty, legend, labels, see Fig. 5f and g), and set

the *P* and *T* range for the plot (Fig. 5h). The plot can be exported to the user's computer using the toolbar at the top-right of the plot (Fig. 5i). The buttons in the toolbar allow the user to select any point on the plot to get its coordinates, zoom in and out, and export the plot as a picture. Plots can be customized and exported to various formats (png, jpeg). They can also be exported as pdf which can be easily edited in common vector graphics programs to produce publication-quality plots. The user can also generate a plot with the isomekes of multiple *analyses* by selecting two or more from the *Workspace*. Specific *analyses* or groups of *analyses* can be searched by using the tool (Fig. 5j) below the *Workspace*.

The entrapment conditions determined using EntraPT agree with those reported by Bonazzi et al., 2019 (e.g. compare the P_{trap} calculated at 775 °C in Fig. 6 with Fig. 6a in Bonazzi et al., 2019). For each *analysis* the isomekes calculated from the two different definitions of residual pressure, can be plotted simultaneously. As noted by Bonazzi et al. (2019), the isomekes calculated using the P_{inc}^{V} obtained from the inclusion EoS (model 2 in section 2.2) tend to overestimate the expected entrapment pressure, especially for those inclusions with a high differential residual strain (inclusions in the top left sector of the plot in Fig. 3). This is because the effective bulk modulus of quartz is lower in presence of differential stresses and strains above the hydrostatic line in ε_3 vs ε_1 plots (e.g. as shown in Fig 3). Therefore, for such inclusions the P_{inc}^{V} becomes larger as a consequence of the Reuss bulk modulus of the EoS being larger than that of the strained inclusion. For the same reason, the uncertainty on the P_{inc}^{V} obtained from eq. (11) is in general larger than the uncertainty on the P_{inc}^{strain} (found with the stiffness tensor and eq. 9), especially for soft inclusions under differential stress. This is illustrated in Fig. 5e taking as an example the quartz Alm1_Grt6_I2 which has a high measured differential strain (≈ 0.037). Its P_{inc}^{V} is 1.453 ± 0.079 GPa while the pressure P_{inc}^{strain} obtained from the strain through the stiffness tensor (eq. 4 and 5) is 1.104 ± 0.038 GPa. As a consequence, the isomeke calculated from P_{inc}^{V} overestimates the synthesis pressure of P_{trap} = 3 GPa at T_{trap} = 775°C (Fig. 5e), and has a larger associated uncertainty compared to the isomeke obtained from P_{inc}^{strain}. The same observation is shown synthetically in Fig. 6 for all of the *analyses* belonging to the synthesis Alm1 of Bonazzi et al. (2019). Because the residual pressure P_{inc}^{V} obtained from the volume strain is overestimated in presence of large differential stresses in the inclusion, the entrapment pressures P_{trap}^{V} calculated from P_{inc}^{V} clearly diverge from the synthesis conditions with the increasing differential stress in

503 the inclusion (Fig. 6). On the other hand, the P_{trap}^{strain} obtained from the measurements of strain
504 are in good agreement with the experimental pressure of the synthesis, independently of the degree
505 of differential stress in the inclusion.

506

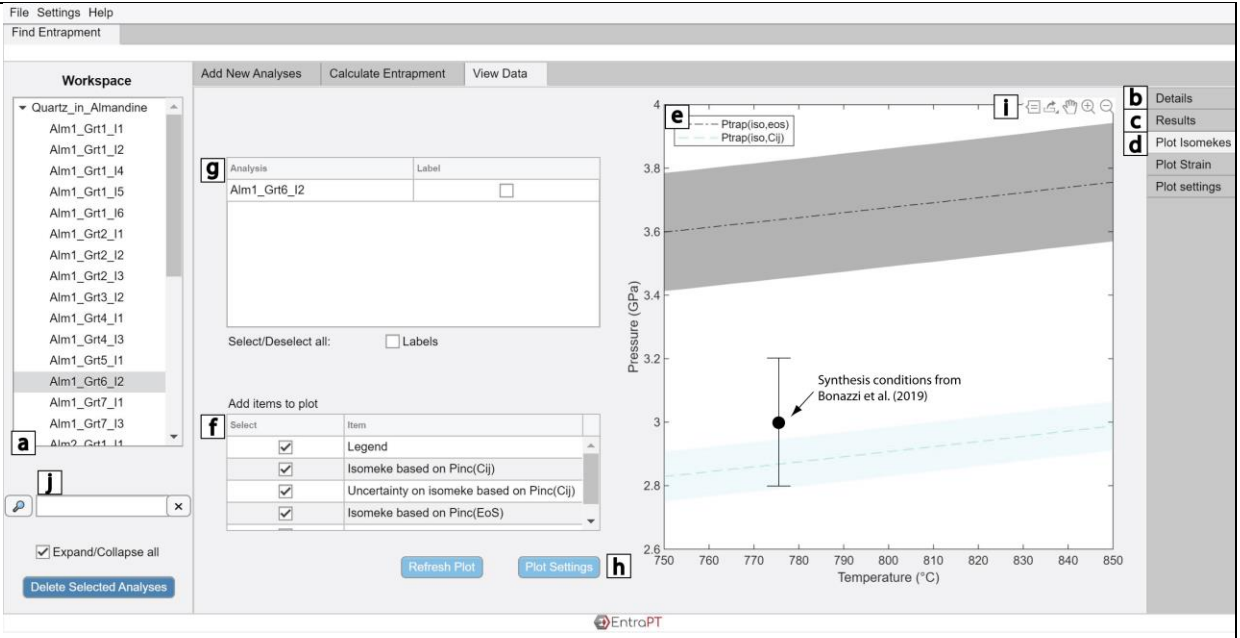

Figure 5. The data relative to each analysis and the results of the calculation of the entrapment conditions can be viewed at any time from the *View Data* tab.When the user selects one analysis from the *Workspace* (a) its details are shown in the *Details* page (b). The numerical results of the calculation are shown under *Results* (c). The isomeke(s) can be plot from *Plot Isomekes* (d). In the *Plot Isomekes* page, the graph (e) reports one or two isomekes depending on the models chosen for the calculation (see panel in Fig 4d) together with the estimated uncertainties on them represented by a shaded area. The isomekes, the shaded areas and the labels of the analysis can be optionally hidden from the specific panels (f and g). The range of the axes can be adjusted as needed (h). A toolbar on the right-top side of the plot (i) allows the user to get the coordinates on the plot of the selected points, to export the figure in various formats and to enable the zoom. The search field (j) allows the user to search for specific analyses by typing a full label or part of it. The searched analyses are listed in the *Workspace*. The plot in (e) shows the isomekes and the associated uncertainties for the *analysis* Alm1_Grt6_I2 of Bonazzi et al. (2019) calculated starting from P_{inc}^{V} (black line) and P_{inc}^{strain} (light blue line). The point at 3 GPa, 775 °C is added as visual reference to represent the synthesis conditions of the experiment Alm1, with the error bar associated with the experimental uncertainties.

507

508

509 ### 3.5 Export project: save data to the user's computer and further processing

510

511 As explained in section 2.4, the data can be exported to the computer of the user from the
512 *File>Export Project* menu as **.ept* and spreadsheet files that contain all of the *analyses* with their
513 data. The **.ept* project file can be opened and processed using MATLAB®. Short scripts can be
514 implemented to rapidly produce custom plots that are not directly displayed in EntraPT, taking
515 advantage that all of the data are structured consistently in the project file. An example is the plot
516 of the entrapment pressures as a function of the residual differential stress (Fig. 6) that was
517 generated externally with the MATLAB® script provided in the Data Repository using the data
518 contained in the project file.

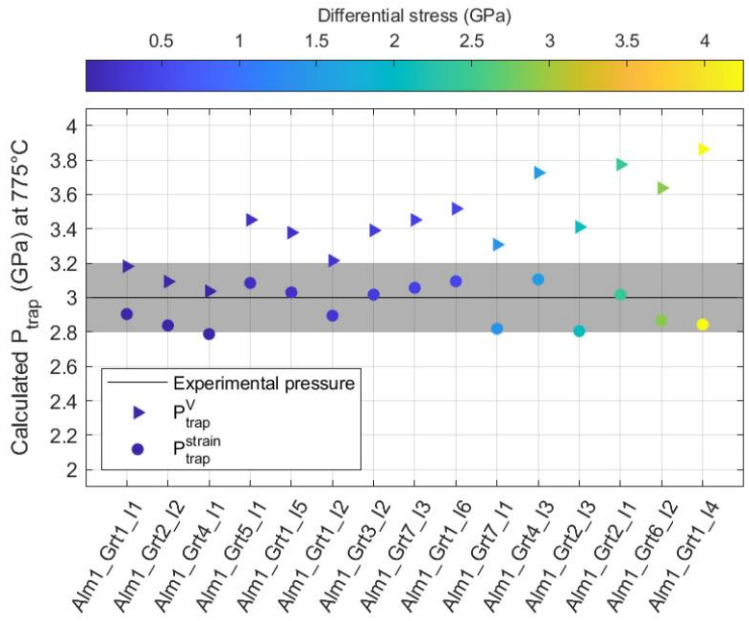

Figure 6. Entrapment pressure P_{trap} calculated at 775 °C for all the analyses belonging to the experiment Alm1 of Bonazzi et al. (2019), reported as a function of the residual differential stress measured in the inclusion. The quartz inclusions in garnet were synthetized at 3± 0.2 GPa at 775 °C (black line in the plot). The shaded area represents the maximum estimated uncertainty propagated through the calculation of P_{trap}. The pressures P_{trap}^{V} calculated from P_{inc}^{V} (triangles) always overestimate the synthesis conditions, especially in presence of large differential stress in the inclusion. The P_{trap}^{strain} obtained from the measurements of strain show a good agreement with the experimental pressure of the synthesis, independently of the differential stress in the inclusion. The plot was generated with an external MATLAB® script provided in the Data Repository together with the project file with all the data.

519

4 Conclusions

EntraPT is a web-based application freely accessible at www.mineralogylab.com/software that provides an easy-to-use tool to calculate entrapment pressures with error propagation from the residual strain measured in mineral inclusions, avoiding the many possible errors arising from manually handling large amounts of data in the multi-step calculations required for elastic geobarometry. EntraPT establishes a consistent workflow to import and visually analyze the measured residual strains, correctly calculate the mean stress in the inclusions, compute the entrapment isomekes with uncertainty estimation and plot the results. With EntraPT all of the data are stored in a consistent format and can be exported as project files and spreadsheets. This allows the data to be shared easily, making the checking and the comparison of data and results reliable. EntraPT will be constantly updated, without requiring the user to download any program. EntraPT is designed on a modular basis, which will allow its functionalities to be expanded in the future, such as the correction for the geometry of the system and to perform calculations of elastic geobarometry including the full elastic anisotropy of the host and the inclusion. The possibility to add more functions that generate additional plots or that perform specific data processing can be explored upon request.

Acknowledgments and Data

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Data Repository: The files (input and project files and the Matlab script) used for the Example section of this paper are temporarily available at https://www.mineralogylab.com/data_repository_mazzucchellietal2020/. After acceptance, they will be made available at the 4TU.Centre Data Repository.

References

Alvaro, M., Mazzucchelli, M. L., Angel, R. J., Murri, M., Campomenosi, N., Scambelluri, M., et al. (2020). Fossil subduction recorded by quartz from the coesite stability field. Geology, 48(1), 24–28. https://doi.org/10.1130/G46617.1

Angel, R. J., Alvaro, M., & Gonzalez-Platas, J. (2014). EosFit7c and a Fortran module (library) for equation of state calculations. Zeitschrift Für Kristallographie-Crystalline Materials, 229(5), 405–419.

Angel, R. J., Mazzucchelli, M. L., Alvaro, M., Nimis, P., & Nestola, F. (2014). Geobarometry from host-inclusion systems: The role of elastic relaxation. American Mineralogist, 99(10), 2146–2149. https://doi.org/10.2138/am-2014-5047

Angel, R. J., Alvaro, M., Nestola, F., & Mazzucchelli, M. L. (2015). Diamond thermoelastic properties and implications for determining the pressure of formation of diamond-inclusion systems. Russian Geology and Geophysics, 56(1–2). https://doi.org/10.1016/j.rgg.2015.01.014

Angel, R. J., Nimis, P., Mazzucchelli, M. L., Alvaro, M., & Nestola, F. (2015). How large are departures from lithostatic pressure? Constraints from host–inclusion elasticity. Journal of Metamorphic Geology, 33(8), 801–813. https://doi.org/10.1111/jmg.12138

Angel, R. J., Alvaro, M., Miletich, R., & Nestola, F. (2017). A simple and generalised P–T–V EoS for continuous phase transitions, implemented in EosFit and applied to quartz. Contributions to Mineralogy and Petrology, 172(5), 29. https://doi.org/10.1007/s00410-017-1349-x

Angel, R. J., Mazzucchelli, M. L., Alvaro, M., & Nestola, F. (2017). EosFit-Pinc: A simple GUI for host-inclusion elastic thermobarometry. American Mineralogist, 102(9), 1957–1960. https://doi.org/10.2138/am-2017-6190

Angel, R. J., Murri, M., Mihailova, B., & Alvaro, M. (2019). Stress , strain and Raman shifts. Zeitschrift Für Kristallographie-Crystalline Materials., 234(2), 129–140. https://doi.org/10.1515/zkri-2018-2112

Ashley, K. T., Steele-MacInnis, M., Bodnar, R. J., & Darling, R. S. (2016). Quartz-in-garnet inclusion barometry under fire: Reducing uncertainty from model estimates. Geology, 44(9), 699–702. https://doi.org/10.1130/G38211.1

Barron, T. H. K., Collins, J. G., & White, G. K. (1980). Thermal expansion of solids at low temperatures. Advances in Physics, 29(4), 609–730. https://doi.org/10.1080/00018738000101426

Bonazzi, M., Tumiati, S., Thomas, J. B., Angel, R. J., & Alvaro, M. (2019). Assessment of the reliability of elastic geobarometry with quartz inclusions. Lithos, 350–351. https://doi.org/10.1016/j.lithos.2019.105201

Campomenosi, N., Mazzucchelli, M. L., Mihailova, B. D., Scambelluri, M., Angel, R. J., Reali, A., & Alvaro, M. (2018). How geometry and anisotropy affect residual strain in host inclusion system: coupling experimental and numerical approaches. American Mineralogist, 103(12), 2032–2035. https://doi.org/10.2138/am-2018-6700CCBY

Enami, M., Nishiyama, T., & Mouri, T. (2007). Laser Raman microspectrometry of metamorphic quartz: A simple method for comparison of metamorphic pressures. American Mineralogist, 92(8–9), 1303–1315. https://doi.org/10.2138/am.2007.2438

Grüneisen, E. (1926). Zustand des festen Körpers. In Drucker C. (Ed.), Thermische Eigenschaften der Stoffe (pp. 1–59). Springer Berlin Heidelberg. https://doi.org/10.1007/978-3-642-99531-6_1

Isaak, D. G., Anderson, O. L., & Oda, H. (1992). High-temperature thermal expansion and elasticity of calcium-rich garnets. Physics and Chemistry of Minerals, 19(2), 106–120. https://doi.org/10.1007/bf00198608

Jiang, F., Speziale, S., & Duffy, T. S. (2004). Single-crystal elasticity of grossular- and almandine-rich garnets to 11 GPa by Brillouin scattering. Journal of Geophysical Research: Solid Earth, 109(B10). https://doi.org/10.1029/2004JB003081

Lakshtanov, D. L., Sinogeikin, S. V., & Bass, J. D. (2007). High-temperature phase transitions and elasticity of silica polymorphs. Physics and Chemistry of Minerals, 34(1), 11–22. https://doi.org/10.1007/s00269-006-0113-y

606 Mazzucchelli, M. L., Reali, A., Morganti, S., Angel, R. J., & Alvaro, M. (2019). Elastic
607 geobarometry for anisotropic inclusions in cubic hosts. Lithos, 350–351.
608 https://doi.org/10.1016/j.lithos.2019.105218

609 Mazzucchelli, Mattia Luca, Burnley, P., Angel, R. J., Morganti, S., Domeneghetti, M. C.
610 C., Nestola, F., & Alvaro, M. (2018). Elastic geothermobarometry: Corrections for the geometry
611 of the host-inclusion system. Geology, 46(3), 231–234. https://doi.org/10.1130/G39807.1

612 Milani, S., Nestola, F., Alvaro, M., Pasqual, D., Mazzucchelli, M. L., Domeneghetti, M.
613 C., & Geiger, C. A. (2015). Diamond–garnet geobarometry: The role of garnet compressibility
614 and expansivity. Lithos, 227(0), 140–147. https://doi.org/10.1016/j.lithos.2015.03.017

615 Milani, S., Angel, R. J., Scandolo, L., Mazzucchelli, M. L., Ballaran, T. B., Klemme, S.,
616 et al. (2017). Thermo-elastic behavior of grossular garnet at high pressures and temperatures.
617 American Mineralogist, 102(4), 851–859. https://doi.org/10.2138/am-2017-5855

618 Murri, M., Mazzucchelli, M. L., Campomenosi, N., Korsakov, A. V., Prencipe, M.,
619 Mihailova, B. D., et al. (2018). Raman elastic geobarometry for anisotropic mineral inclusions.
620 American Mineralogist, 103(11), 1869–1872. https://doi.org/10.2138/am-2018-6625CCBY

621 Özkan, H., Cartz, L., & Jamieson, J. C. (1974). Elastic constants of nonmetamict
622 zirconium silicate. Journal of Applied Physics, 45(2), 556–562.
623 https://doi.org/10.1063/1.1663283

624 Ranganathan, S. I., & Ostoja-Starzewski, M. (2008). Universal elastic anisotropy index.
625 Physical Review Letters, 101(5), 3–6. https://doi.org/10.1103/PhysRevLett.101.055504

626 Rosenfeld, J. L., & Chase, A. B. (1961). Pressure and temperature of crystallization from
627 elastic effects around solid inclusions in minerals? American Journal of Science, 259(7), 519–
628 541.

629 Sinogeikin, S. V, & Bass, J. D. (2002). Elasticity of pyrope and majorite-pyrope solid
630 solutions to high temperatures. Earth and Planetary Science Letters, 203(1), 549–555.

631 Voigt, W. (1910). Lehrbuch der Kristallphysik. Kristalloptik. Leipzig: Teubner.

632 Zhong, X., Moulas, E., & Tajčmanová, L. (2018). Tiny timekeepers witnessing high-rate
633 exhumation processes. Scientific Reports, 8(1), 1–9. https://doi.org/10.1038/s41598-018-20291-7

Zhong, X., Andersen, N. H., Dabrowski, M., & Jamtveit, B. (2019). Zircon and quartz inclusions in garnet used for complementary Raman thermobarometry: application to the Holsnøy eclogite, Bergen Arcs, Western Norway. Contributions to Mineralogy and Petrology, 174(6), 50. https://doi.org/10.1007/s00410-019-1584-4

Zhong, X., Moulas, E., & Tajčmanová, L. (2020). Post-entrapment modification of residual inclusion pressure and its implications for Raman elastic thermobarometry. Solid Earth, 11(1), 223–240. https://doi.org/10.5194/se-11-223-2020

Zouboulis, E., Grimsditch, M., Ramdas, a., & Rodriguez, S. (1998). Temperature dependence of the elastic moduli of diamond: A Brillouin-scattering study. Physical Review B, 57(5), 2889–2896. https://doi.org/10.1103/PhysRevB.57.2889