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SEISMIC, a Python-based code of the QUANTAS package to calculate the phase and group acoustic velocities in crystals

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ABSTRACT

The present work reports the theoretical background and the capabilities of *SEISMIC*, a Python code specifically developed to calculate the propagation of the sound waves inside crystalline materials. *SEISMIC* is a tool integrated in the QUANTAS package and provides a series of useful information for engineers and geophysicists, such as the phase and group velocities, the power flow angle, the enhancement factors, and the polarization vectors, using as input the elastic moduli and the density of the material. Numerical treatments of the derivatives were avoided, using analytical methods to obtain numerically stable results. The code relies only on Python numerical and graphical libraries to ensure a full cross-platform usability.

1. Introduction

The analysis of the elastic moduli of crystalline solids, physically represented by a $3 \times 3 \times 3 \times 3$ (4th-rank) tensor, can yield several information about the behaviour of crystalline materials. From the experimental point of view, the elastic moduli can be obtained from the analysis of the propagation of sound velocities inside the medium, e.g., by Brillouin scattering techniques (Kojima, 2022). Vice versa, if the stiffness tensor is known, it is possible to calculate how the acoustic waves travel inside a material by solving the Christoffel's equation (Musgrave, 1970), which is a very useful knowledge that is widely employed by engineers and geophysicists.

Thanks to the continuous advancement of both computing power and technology, the elastic moduli can be readily calculated from *ab initio* simulations for a wide range of crystalline materials. Some code, for example CRYSTAL (Dovesi et al., 2018), VASP (Kresse and Hafner, 1993) and SIESTA (Soler et al., 2002), implemented automated routines to calculate the components of the stiffness tensor from stress-strain relationships. However, typically these quantum chemistry codes do not implement advanced post-processing routines to extract all the useful information from the elastic tensor. To this aim some specific softwares were developed, such as MTEX (Mainprice et al., 2011), which is a toolbox for Matlab®, and the Fortran code AWESOME (Acoustic Wave Evaluator in Solid Media) (Munoz-Santiburcio et al., 2015), which was recently added to CRYSTAL. Only recently, a Python code called `christoffel` (Jaeken and Cottenier, 2016) was developed, intended as a cross-platform utility that, like AWESOME, still requires an external code, i.e., GNUPlot, to produce the graphical representations of the results.

For all these reasons, and starting from the code of Jaeken and Cottenier (2016), it was decided to develop a code that relies only on Python and its libraries to analyse the acoustic (i.e., seismic) wave velocities within crystalline media. The program was called *SEISMIC*, and it is an open-source code implemented as a module of the QUANTAS package (Ulian and Valdrè, 2022), both freely available on Github under the New Berkeley Software Distribution (BSD) software license.

The structure of the present article is the following: after the introduction in Section 1, Section 2 provides the necessary background to understand the principles behind the calculation of the acoustic wave velocities in solids; Section 3 shows how the involved quantities are obtained, i.e., the adopted computational strategy, how the code works and the results that are produced. Section 4 reports two test cases used to demonstrate the capability of the software to obtain valuable data, and, finally, Section 5 provides a summary and the future perspectives of the code.

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2. Theoretical background

The basic property used to calculate the acoustic wave propagation in a homogeneous crystalline material (e.g., a perfect crystal) is the elastic tensor, which describes the relationship between stress σ and strain ε according to the following formula:

$$\sigma_{ij} = \sum_{kl} C_{ijkl}\varepsilon_{kl}, \tag{1}$$

where the C_{ijkl} terms are the component of the $3 \times 3 \times 3 \times 3$ stiffness tensor (see Nye, 1957). For the sake of clearness, all the sums here reported run over the three Cartesian coordinates x, y and z. Generally, Eq. (1) is written using the 6×6 Voigt's matrix notation of elastic tensor:

$$\begin{pmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\\ \sigma_4\\ \sigma_5\\ \sigma_6\end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16}\\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26}\\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36}\\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46}\\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56}\\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66}\end{pmatrix}\begin{pmatrix}\varepsilon_1\\ \varepsilon_2\\ \varepsilon_3\\ 2\varepsilon_4\\ 2\varepsilon_5\\ 2\varepsilon_6\end{pmatrix} \tag{2}$$

with the subscripts being mapped as $1 \rightarrow xx$, $2 \rightarrow yy$, $3 \rightarrow zz$, $4 \rightarrow yz$, $5 \rightarrow xz$, $6 \rightarrow xy$, and the double counting is accounted by the factor 2 in the strain tensor.

To access information on the elastic (acoustic) waves that travel through the material, it is necessary to solve the Christoffel's equation (see Musgrave, 1970). Let's define $\mathbf{q}$ a monochromatic wave vector with angular frequency ω and polarization $\hat{\mathbf{s}}$ that travels inside a crystalline material with density ρ. The Christoffel equation is an eigenvalue problem defined as:

$$\sum_{ij}\left[M_{ij} - \rho\omega^2\delta_{ij}\right] s_j = 0 \tag{3}$$

where M_{ij} are the terms of the Christoffel matrix $\mathbf{M}$ that are written as

$$M_{ij} = \sum_{kl} q_k C_{iklj} q_l \tag{4}$$

Eq. (3) can be solved for any given $\mathbf{q}$. From now on, we will use the notation suggested by Jaeken and Cottenier (2016), which introduces the reduced stiffness tensor $\mathbf{C}' = \mathbf{C}/\rho$ and the reduced Christoffel matrix $\mathbf{M}' = \mathbf{M}/\rho$. For convenience, the prime on these two tensor quantities will be omitted in the following expressions. In addition, Eq. (3) and Eq. (4) show $\omega(\mathbf{q})$ is a linear function of q in a single direction, which means the sound velocities are independent of the wavelength $\mathbf{q}$ but its direction. Hence, $\mathbf{q}$ will be considered in the following as a dimensionless unit vector that describes only the travel direction of the monochromatic plane wave. Thus, Eq. (3) can be rewritten as:

$$\sum_{ij}\left[M_{ij} - v_p^2\delta_{ij}\right] s_j = 0 \tag{5}$$

with v_p the velocity of the monochromatic plane wave that travels in the direction given by $\hat{\mathbf{q}}$. The subscript p denotes this quantity as the *phase* velocity. The non-trivial solutions of Eq. (5) are three eigenvalues, i.e. three velocities subdivided into one primary (P-mode) and two secondary (S-mode), which are related to the (pseudo-) longitudinal and (pseudo-) transversal polarizations, respectively. As a convention, the two secondary velocities are one fast S-mode and a slow S-mode, so that in general $v_{p,P} > v_{p,S_{fast}} > v_{p,S_{slow}}$, and the difference $v_{p,S_{fast}} - v_{p,S_{slow}}$ is called shear-wave splitting. The three eigenvector solutions of the Christoffel equation are associated with the polarization directions.

The above formulas consider the sound as a monochromatic plane wave, an ideal situation. However, a more realistic approach is representing sound as a wave packet whose wavelength and travelling direction show a certain amount of spreading. Thus, the sound (acoustic) energy) travels through a homogeneous medium as a wave packet given by the superposition of several phase waves, whose velocity is described by the following formula:

$$\mathbf{v}_g = \vec{\nabla} v_p \tag{6}$$

where $\mathbf{v}_g$ is the so-called *group velocity*, whose direction is the travel direction of (acoustic) energy if the medium does not dissipate energy (see Auld, 1973). The gradient (in reciprocal space) is given by the derivative of the components of the dimensionless vector $\hat{\mathbf{q}}$. It is worth noting that $\mathbf{v}_g$ is a vector that typically does not line in the direction of $\hat{\mathbf{q}}$, and the power flow angle ψ describes the angular difference between the directions of the group and phase velocity according to:

$$v_p = v_g \cos(\psi) \tag{7}$$

If we introduce the normalized directions of the phase velocity, $\hat{\mathbf{n}}_p$, and of the group velocity, $\hat{\mathbf{n}}_g$, we can re-write Eq. (7) as:

$$\cos(\psi) = \hat{\mathbf{n}}_p \cdot \hat{\mathbf{n}}_g. \tag{8}$$

Since the energy travelling direction typically is not the same of the phase velocity, the power flow concentration changes depending on the direction. To quantify this effect on a directional basis, it is introduced the enhancement factor, A, which is calculated using the following formula:

$$A = \frac{\Delta\Omega_p}{\Delta\Omega_g} \tag{9}$$

In Eq. (9), $\Delta\Omega_p$ and $\Delta\Omega_g$ are the solid angles subtended by beams of phase $\hat{\mathbf{n}}_p$ and group $\hat{\mathbf{n}}_g$ wave vectors, respectively. Fig. 1 shows the quadrangle that is formed on a unit sphere when the vectors $\hat{\mathbf{n}}_p$ and $\hat{\mathbf{n}}_g$ are normalized.

The most simple way to determine the enhancement factor is to consider its infinitesimal value, which is easily described in spherical coordinates, as suggested by Jaeken and Cottenier (2016). With this approach, the solid angle is equal to the area of a quadrangle described on the unit sphere by the partial derivatives of the phase vector $\hat{\mathbf{n}}_p$ or group vector $\hat{\mathbf{n}}_g$ to θ and φ. This translates into

$$d\Omega_p = \sin(\theta) d\theta d\varphi \tag{10}$$

and

$$d\Omega_g = \left\| \frac{\partial \hat{\mathbf{n}}_g}{\partial\theta} \times \frac{\partial \hat{\mathbf{n}}_g}{\partial\varphi} \right\| \sin(\theta) d\theta d\varphi \tag{11}$$

Thus, the enhancement factor is given by

$$A = \left\| \frac{\partial \hat{\mathbf{n}}_g}{\partial\theta} \times \frac{\partial \hat{\mathbf{n}}_g}{\partial\varphi} \right\|^{-1}, \tag{12}$$

which can be also expressed as

$$\begin{aligned}\left(\hat{\theta}\cdot\vec{\nabla}\hat{\mathbf{n}}_g\right) \times \left(\hat{\varphi}\cdot\vec{\nabla}\hat{\mathbf{n}}_g\right) &= \det\left(\vec{\nabla}\hat{\mathbf{n}}_g\right)\left(\vec{\nabla}\hat{\mathbf{n}}_g\right)^{-T}\cdot\left(\hat{\theta}\times\hat{\varphi}\right)\\ &= \det\left(\vec{\nabla}\hat{\mathbf{n}}_g\right)\left(\vec{\nabla}\hat{\mathbf{n}}_g\right)^{-T}\cdot\hat{\mathbf{q}}\\ &= \mathrm{Cof}\left(\vec{\nabla}\hat{\mathbf{n}}_g\right)\cdot\hat{\mathbf{q}}\end{aligned} \tag{13}$$

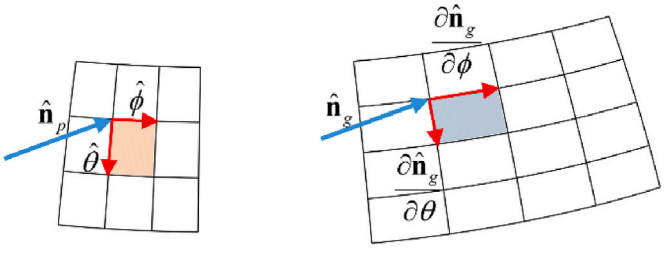

Fig. 1. Graphical representation of the $d\Omega_p$ and $d\Omega_g$ values.

where Cof indicates the matrix of cofactors, and

$$\widehat{\theta}=\frac{\partial\widehat{\mathbf{q}}}{\partial\theta}\cdot,\ \widehat{\varphi}=\frac{\partial\widehat{\mathbf{q}}}{\partial\varphi}\cdot. \tag{14}$$

By substituting Eq. (13) into Eq. (14), the enhancement factor is given by the following expression

$$A=\left\|\mathrm{Cof}\left(\vec{\nabla}\widehat{\mathbf{n}}_g\right)\cdot\widehat{\mathbf{q}}\right\|^{-1}, \tag{15}$$

which is not dependent on the spherical coordinates and can be evaluated from the derivatives of the Christoffel's matrix eigenvalues.

3. Algorithm and implementation

3.1. Computational strategy

A schematic workflow of the analysis of the second-order elastic moduli to obtain the seismic wave velocities is shown in Fig. 2. As previously suggested by Jaeken and Cottenier (2016), the implemented computational approach uses the eigenvalues of the Christoffel's matrix, λ, as the key quantity to obtain all the measurable properties (phase velocity v_p, group velocity $\mathbf{v}_\mathrm{g}$ and enhancement factor A). Hence, the phase velocity is defined as

$$v_p=\sqrt{\lambda} \tag{16}$$

that can be substituted in Eq. (6) to give

$$\mathbf{v}_g=\vec{\nabla}v_p=\vec{\nabla}\sqrt{\lambda}=\frac{\vec{\nabla}\lambda}{2\sqrt{\lambda}} \tag{17}$$

Except for the phase velocities, all the other quantities are obtained from the first and second derivatives of the matrix λ. The gradient of the generic eigenvalue λ_i can be expressed as

$$\frac{\partial\lambda_i}{\partial q_k}=\widehat{\mathbf{s}}_i\cdot\frac{\partial\mathbf{M}}{\partial q_k}\cdot\widehat{\mathbf{s}}_i \tag{18}$$

with $\hat{\mathbf{s}}_i$ the normalized eigenvector related to λ_i. The Hessian matrix $\mathbf{H}(\lambda)$ is given by the second-order derivatives of the Christoffel's eigenvalues, according to the following expression

$$\mathbf{H}(\lambda)_i=\frac{\partial^2\lambda_i}{\partial q_k\partial q_m}=\widehat{\mathbf{s}}_i\cdot\frac{\partial^2\mathbf{M}}{\partial q_k\partial q_m}\cdot\widehat{\mathbf{s}}_i+2\widehat{\mathbf{s}}_i\cdot\frac{\partial\mathbf{M}}{\partial q_k}\cdot\left(\lambda_i\mathbf{I}-\mathbf{M}\right)^{+}\cdot\frac{\partial\mathbf{M}}{\partial q_m}\widehat{\mathbf{s}}_i, \tag{19}$$

which is obtained from the derivative of the gradient of the eigenvectors given by (Petersen and Pedersen, 2012)

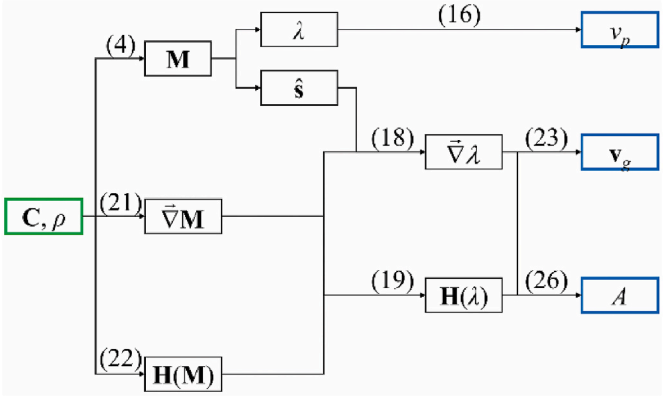

Fig. 2. Workflow of the implementation of the analysis of the seismic wave velocities in crystalline solids. The green box reports the input data (tensor of the elastic moduli in Voigt's notation and crystal density), whereas the blue ones are the output of the calculation. The numbers in parentheses are references to the equations shown along the text.

$$\frac{\partial\widehat{\mathbf{s}}_i}{\partial q_k}=\left(\lambda_i\mathbf{I}-\mathbf{M}\right)^{+}\cdot\frac{\partial\mathbf{M}}{\partial q_k}\widehat{\mathbf{s}}_i. \tag{20}$$

In this framework, the derivative of the Christoffel's matrix, $\vec{\nabla}\mathbf{M}$ (third-order tensor), is simply

$$\vec{\nabla}\mathbf{M}=\frac{\partial M_{ij}}{\partial q_k}=\sum_m\left(C_{ikmj}+C_{imkj}\right)q_m, \tag{21}$$

and its Hessian is

$$\mathbf{H}(\mathbf{M})=\frac{\partial^2 M_{ij}}{\partial q_k\partial q_m}=C_{ikmj}+C_{imkj} \tag{22}$$

It is worth noting that (i) Eq. (21) depends on $\mathbf{q}$, whereas Eq. (22) does not, and (ii) the group velocities can be straightforwardly obtained from the solution of Eqs. (17), (18) and (21), which require just the eigenvalues and eigenvectors of $\mathbf{M}$:

$$\mathbf{v}_g^i=\frac{\widehat{\mathbf{s}}_i\cdot\vec{\nabla}\mathbf{M}\cdot\widehat{\mathbf{s}}_i}{2\sqrt{\lambda_i}}. \tag{23}$$

The calculation of the enhancement factor considers the gradient of the vector field of the normalized group velocity with respect to λ,

$$\vec{\nabla}\widehat{\mathbf{n}}_g=\vec{\nabla}\frac{\mathbf{v}_g}{\|\mathbf{v}_g\|}=\vec{\nabla}\frac{\vec{\nabla}v_p}{\|\vec{\nabla}v_p\|}=\vec{\nabla}\frac{\vec{\nabla}\lambda}{\|\vec{\nabla}\lambda\|} \tag{24}$$

Considering that the gradient of a differentiable and positive vector field $\mathbf{v}$ is given by

$$\vec{\nabla}\frac{\mathbf{v}}{\|\mathbf{v}\|}=\frac{\vec{\nabla}\mathbf{v}}{\|\mathbf{v}\|}-\frac{\mathbf{v}\otimes\left(\vec{\nabla}\mathbf{v}\right)\cdot\mathbf{v}}{\|\mathbf{v}\|^3}, \tag{25}$$

where $\otimes$ is the Kronecker's product, it follows that

$$\vec{\nabla}\widehat{\mathbf{n}}_g=\frac{\mathbf{H}(\lambda)}{\|\vec{\nabla}\lambda\|}-\frac{\vec{\nabla}\lambda\otimes\mathbf{H}(\lambda)\cdot\vec{\nabla}\lambda}{\|\vec{\nabla}\lambda\|^3}. \tag{26}$$

It is important to highlight that the outer product in Eq. (26) does not commute, hence $\vec{\nabla}\widehat{\mathbf{n}}_g$ is not equal to its transposed matrix, i.e., the matrix is not symmetric, as explained by Jaeken and Cottenier (2016).

3.2. SEISMIC Python module

The code that performs the analysis of the seismic wave velocities in crystalline materials was entirely written in Python, as a module of the QUANTAS (QUANTitative Analysis of Solids) software (Ulian and Valdrè, 2022). The module is subdivided into three components, i.e., (i) a *Seismic* object, which implements all the previously discussed formulas to obtain v_p, v_g, ψ and A from the elastic moduli, (ii) plotting utilities to automatically generate 2D and 3D representations of the wave velocities, and (iii) the interface to the QUANTAS code.

The calculation of the acoustic wave velocities can be initialized using the *ad hoc* command line interface of QUANTAS, i.e.

QUANTAS seismic input_file [options]

where input_file is a text file containing the stiffness tensor in Voigt's notation (complete, upper triangular or lower triangular) and the density of the crystalline material. The code performs a matrix-to-tensorial form conversion that preserves the Cartesian reference frame that was employed to obtain the elastic tensor in the Voigt's notation. The analysis of the seismic waves is automatic, i.e., the acoustic wave velocities are calculated by scanning the surface of a unit sphere between the $0\leq\theta\leq\pi/2$ and $0\leq\varphi\leq2\pi$. At the end of the analysis, the code can produce plots of the results.

3.3. Output and visualization

The results of the analysis performed by *Seismic* are saved in a single

binary file in HDF5 format with three datasets, one for each solution of the Christoffel's equation (one primary and two secondary waves), which store.

- Column 1 – the spherical coordinate θ (radians),
- Column 2 – the spherical coordinate φ (radians),
- Column 3 – the phase velocity v_p (km s^{-1})
- Column 4 – the relative phase velocity with respect to the isotropic acoustic wave velocity (%)
- Columns 5–7 – the phase polarization along x, y, and z
- Column 8 – the group velocity v_g (km s^{-1})
- Column 9 – the relative group velocity with respect to the isotropic acoustic wave velocity (%)
- Columns 10–12 – the x, y, and z coordinates of the ray surface (km s^{-1})
- Column 13 – the power flow angle ψ (degrees)
- Column 14 – the enhancement factor A ($\log_{10}A$).

The isotropic wave velocities cited above are given by:

$$v_{\mathrm{iso,P}} = \sqrt{\frac{K + 4\mu/3}{\rho}} \tag{27}$$

$$v_{\mathrm{iso,S}} = \sqrt{\frac{\mu}{\rho}} \tag{28}$$

with K and μ the bulk and shear modulus, respectively, calculated according to the Voigt-Reuss-Hill averaging scheme (see Nye, 1957).

The calculated data can be plotted with the routines implemented in *Seismic*, which uses the Plotly graphical library (Plotly Technologies Inc, 2015) for the 3D (spherical) representations, whereas the Matplotlib package (Hunter, 2007) is employed for the 2D (polar) plots of the results. The latter are projections of the spherical results on two dimensions that were implemented considering both the Lambert equal-area and stereographic projections, which preserve, respectively, the local area and the local shape of the data.

4. Test cases: fluorite and quartz

4.1. Fluorite CaF_2

Fluorite, the cubic polymorph of calcium fluoride (space group $Fm\bar{3}m$), was used a simple test case, using the *SEISMIC* code of the QUANTAS package to calculate the acoustic wave velocities and to produce their graphical representations. The input data were taken from the experimental work of Speziale and Duffy (2002), who reported the following elastic moduli in Voigt's notation:

$$C = \begin{pmatrix} 170.9 & 47.5 & 47.5 & \cdot & \cdot & \cdot \\ 47.5 & 170.9 & 47.5 & \cdot & \cdot & \cdot \\ 47.5 & 47.5 & 170.9 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 34.0 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 34.0 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 34.0 \end{pmatrix}, \tag{29}$$

with a crystal density of 3222 kg m^{-3}. The dots in Eq. (29) are the null values of C_{ij} due to the symmetry of the material.

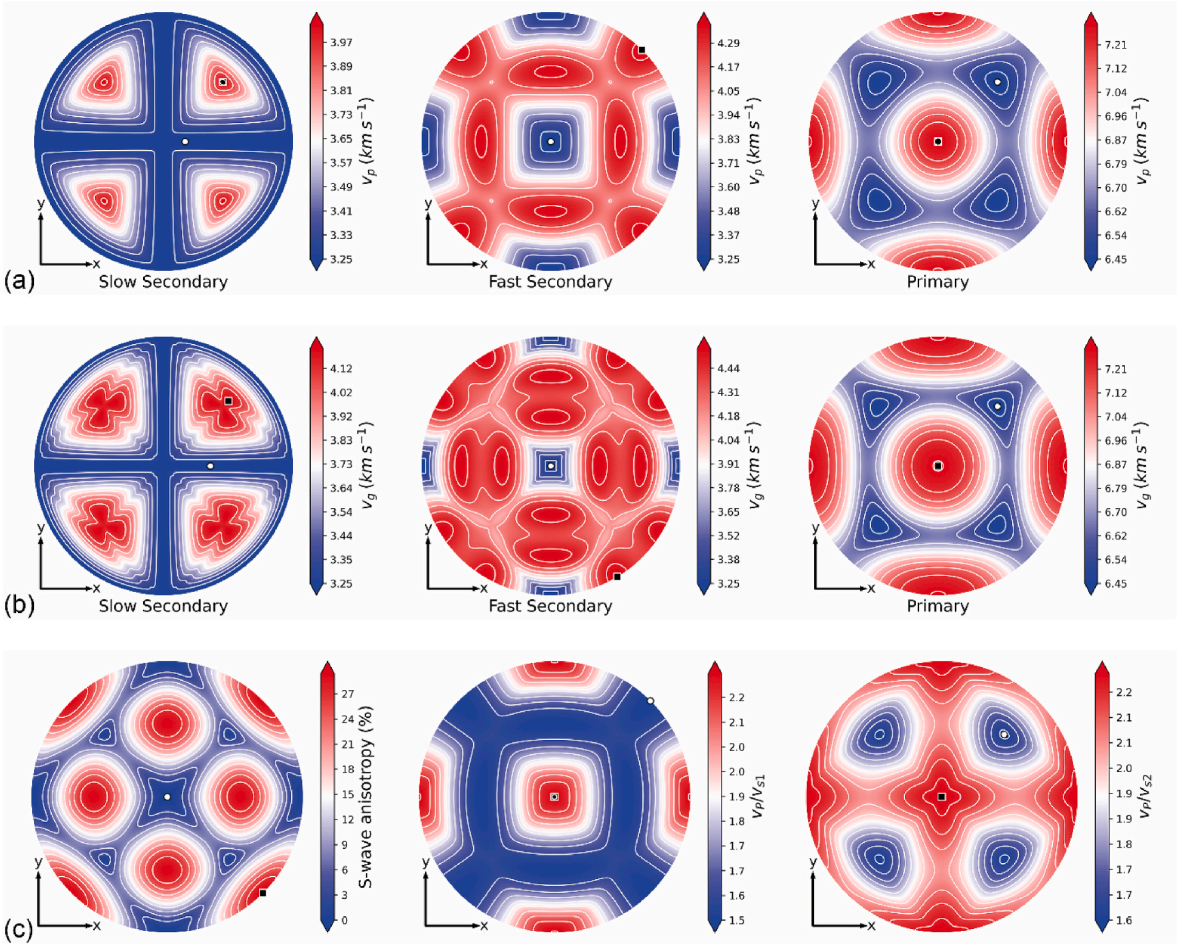

Fig. 3. (a) Phase velocities v_p, (b) group velocities $\mathbf{v}_g$, and (c) S-wave anisotropy and ratios between the phase velocities (P/S1 and P/S2) of fluorite CaF_2, reported as Lambert equal area 2D projection. The black square and the white dot show the maximum and minimum value calculated in each plot, respectively.

Fig. 3 reports the Lambert equal area 2D projection of the phase velocities v_p, group velocities $\mathbf{v}_g$, the S-wave anisotropy (or shear wave splitting), defined as

$$200 \cdot \frac{v_{p,S1} - v_{p,S2}}{v_{p,S1} + v_{p,S2}}, \tag{30}$$

and the ratio between the primary and the secondary phase velocities. To interpret the relationship between the phase and the group velocities, it is useful to also analyse the enhancement factor A and the power flow angle ψ (Fig. 4). The $\mathbf{v}_g$ is shown as a function of the wavefront $\mathbf{q}$, however the actual direction of the group velocities forms the ψ angle with $\mathbf{q}$. The focussing of the acoustic waves in fluorite depends on the considered wave, as evinced from the enhancement factor (Fig. 4a). The primary mode shows the highest A values along the [001] crystallographic direction, whereas the lowest value lies on the [111] propagation direction. The minimum A value for the secondary modes is also on the [111] crystallographic direction, but the general pattern is more complex with respect to the one calculated for the primary mode.

Finally, Fig. 5 shows the three-dimensional plots of the quantities described above, which could be further useful to analyse and interpret the results, in particular when less symmetrical materials (in the crystallographic perspective) are considered.

4.2. .Quartz SiO_2

Quartz (SiO_2, space group $P3_221$, trigonal crystal system) is a framework silicate and one of the most abundant minerals in the Earth's crust, with several important technological applications, among which various exploiting mechanical properties, e.g., it is employed as a piezoelectric material (Wang et al., 2015). The experimental data of Wang et al. (2015) were used to calculate the acoustic wave velocities with *SEISMIC*, with the following second-order elastic moduli:

$$C = \begin{pmatrix} 86.6 & 6.74 & 12.4 & 17.8 & \cdot & \cdot \\ 6.74 & 86.6 & 12.4 & -17.8 & \cdot & \cdot \\ 12.4 & 12.4 & 106.4 & \cdot & \cdot & \cdot \\ 17.8 & -17.8 & \cdot & 58.0 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 58.0 & 17.8 \\ \cdot & \cdot & \cdot & \cdot & 17.8 & 39.9 \end{pmatrix}, \tag{31}$$

and a crystal density of 2648 kg m^{-3}.

Fig. 6 shows the Lambert equal area 2D projection of the phase velocities v_p, group velocities $\mathbf{v}_g$, power flow angle ψ and enhancement factor A. The trigonal symmetry of quartz is easily recognizable in each panel of Fig. 6. In fact, differently from fluorite (belonging to the cubic system), the patterns of the group velocity $\mathbf{v}_g$, power flow angle ψ and enhancement factor A are more complex. The results are in good agreement with the single crystal velocities experimentally determined by Braun et al. (1991). For example, in the cited work, the maximum (minimum) longitudinal wave velocity was 7.1 (5.5) km s^{-1} along the [011] ([201]) crystallographic direction, which is in line with those calculated with SEISMIC, i.e., 7.0 (5.3) km s^{-1}. Also, the calculated anisotropy of the primary (28%), fast secondary (31%) and slow secondary (34%) are in good agreement with those calculated by Braun and collaborators (1991), i.e., 25%, 27% and 32%, respectively. This good agreement is also reflected in the 2D projection of the primary, fast secondary and slow secondary seismic wave velocities shown in Fig. 6a in the present work, which perfectly match the graphical results reported in the study of Braun et al. (1991).

5. Conclusions

The present paper showed the capabilities of *SEISMIC*, a Python code implemented within the Quantas framework that was developed to provide a simple tool to calculate the acoustic wave velocities in crystalline media knowing the elastic moduli and the density of the material. The code was built as a module of the Quantas package, which already implement some routines to analyse the stiffness tensor, and does not require other software to provide the three-dimensional and two-dimensional plots of the calculated quantities. As in the `christoffel` code (Jaeken and Cottenier, 2016), derivatives are calculated in an accurate and efficient way, and the amount of details can be increased or decreased according to the size of the sampling grid of (spherical) directions. At present, the code is serial, i.e., it computes the seismic waves one direction at a time, which means that the computational cost increases linearly with the number of sampling points requested by the user. In the present paper, *SEISMIC* was tested against two different crystal structures, fluorite (cubic symmetry) and quartz (trigonal), finding a very good agreement with experimental data.

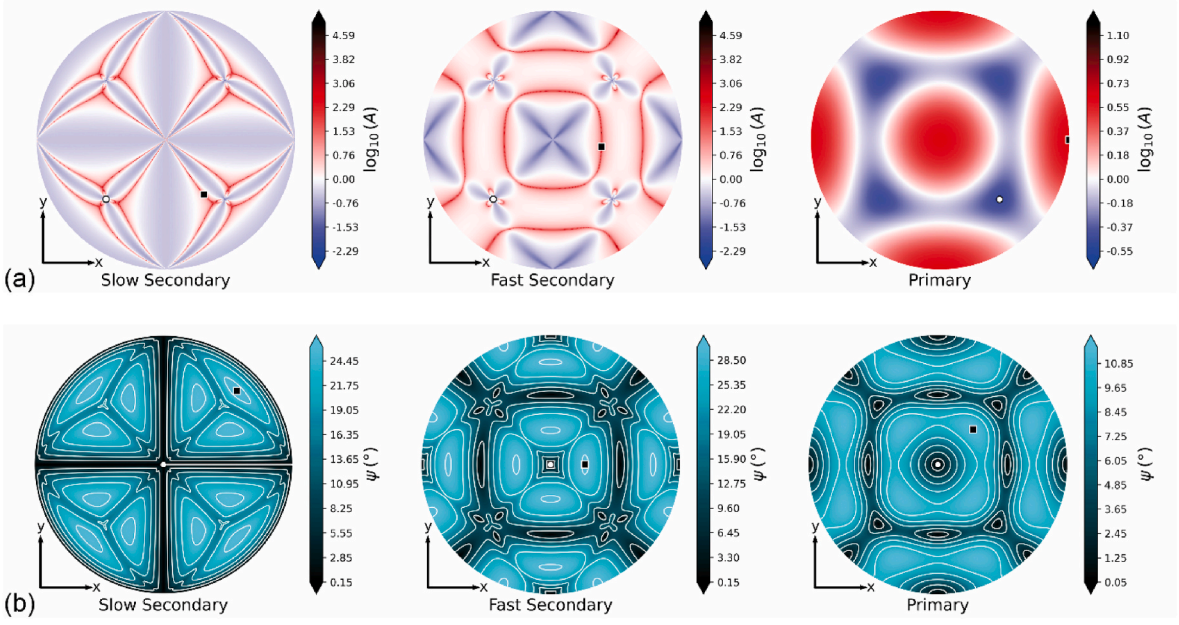

Fig. 4. Lambert equal area 2D projection of (a) enhancement factor A (as $\log_{10}A$) and (b) power flow angle ψ of fluorite. The black square and the white dot show the maximum and minimum value calculated in each plot, respectively.

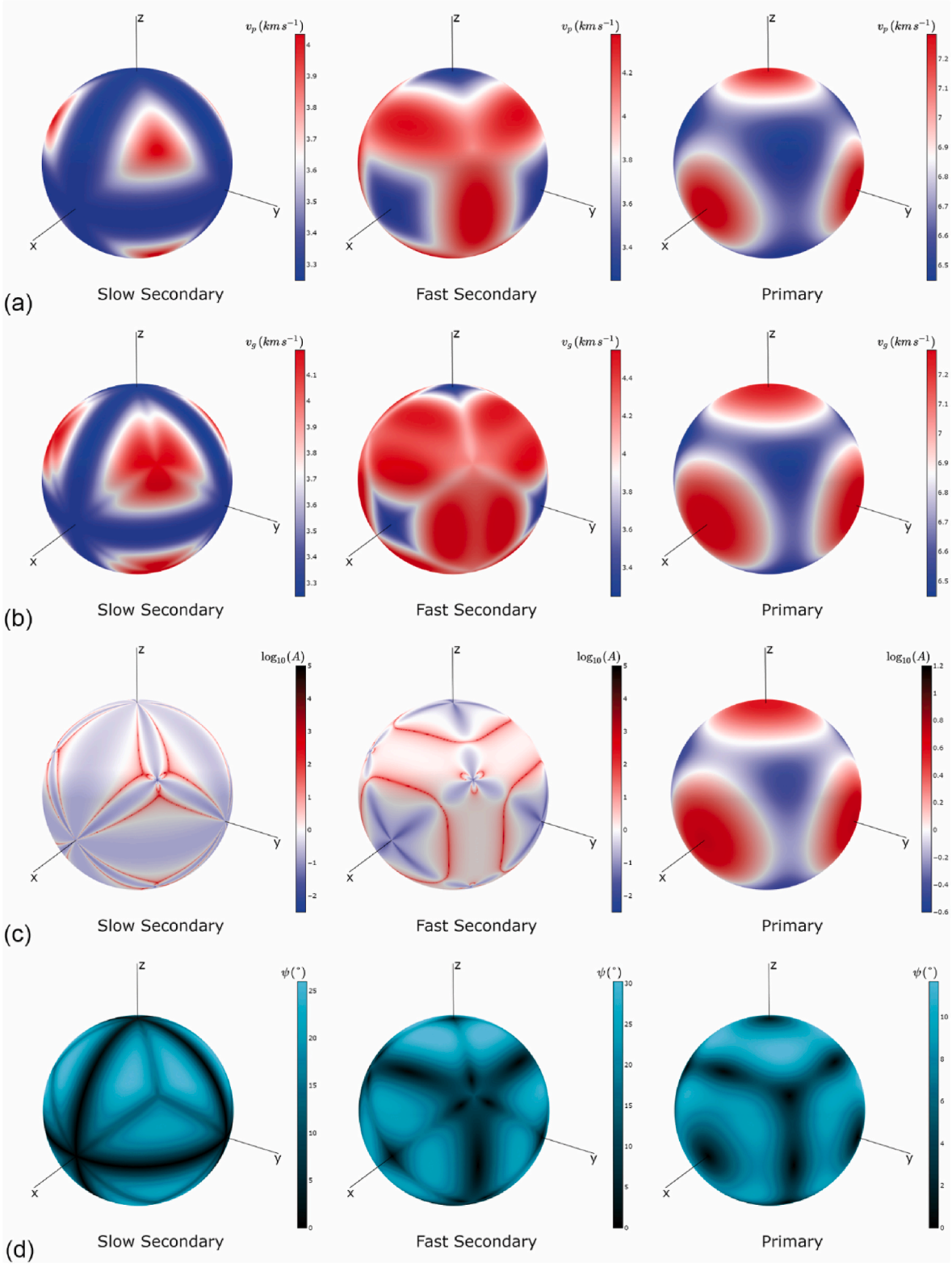

Fig. 5. Three-dimensional representations of (a) phase velocity, (b) group velocity, (c) enhancement factor, and (d) power flow angle of fluorite.

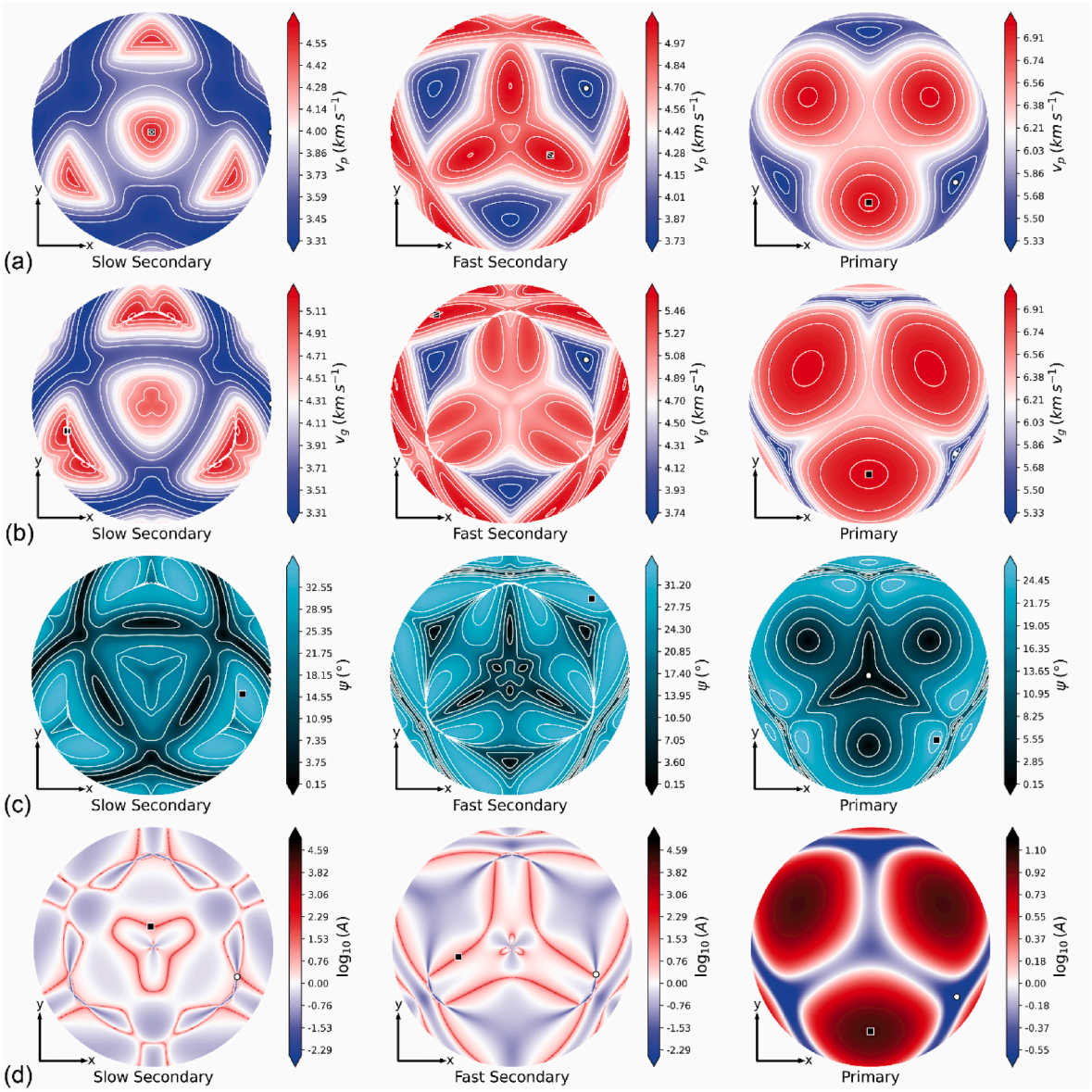

Fig. 6. (a) Phase velocities v_p, (b) group velocities $\mathbf{v}_g$, (c) power flow angle ψ, and (d) enhancement factor A (as $\log_{10}A$) of quartz SiO_2, reported as Lambert equal area 2D projection. The black square and the white dot show the maximum and minimum value calculated in each plot, respectively.

In future, other features will be added to *SEISMIC*, i.e., the number of analyses, text reports and 2D/3D plots of the results that can be produced. In addition, it will be included the estimation of the calculation errors from the uncertainties associated with the elastic tensor components, which will give the reliability range of the results.

The performance of the code could be increased using parallelization support, either using the multiprocessing library of Python or other more advanced ones.

Code availability section

SEISMIC (part of the *QUANTAS* library)

Contact: gianfranco.ulian2@unibo.it, 0039-0512094934 - giovanni.valdre@unibo.it 0039-0512094943.

Hardware requirements: PC with at least 2 GB of memory, supporting Unix, MacOS or Windows operative systems.

Program language: Python.

Software required: Python >3.7, NumPy, SciPy, Matplotlib, Plotly.

Program size: 15.2 MB (including the source files for the documentation)

The source codes are available for downloading at the link: https://github.com/gfulian/quantas/tree/development.

CRediT authorship contribution statement

Gianfranco Ulian: Writing – review & editing, Visualization, Validation, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Giovanni Valdrè:** Writing – review & editing, Validation, Supervision, Investigation, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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References

Auld, B.A., 1973. Acoustic Fields and Waves in Solids. John Wiley & Sons Publications, New York.

Braun, G., Siegesmund, S., Dahms, M., 1991. The influence of quartz textures on the seismic anisotropy in lower crustal granulites. J. Struct. Geol. 13, 955–966. https://doi.org/10.1016/0191-8141(91)90090-6.

Dovesi, R., Erba, A., Orlando, R., Zicovich-Wilson, C.M., Civalleri, B., Maschio, L., Rerat, M., Casassa, S., Baima, J., Salustro, S., Kirtman, B., 2018. Quantum-mechanical condensed matter simulations with CRYSTAL. Wiley Interdiscip. Rev.-Comput. Mol. Sci. 8, E1360. https://doi.org/10.1002/Wcms.1360.

Hunter, J.D., 2007. Matplotlib: a 2D graphics environment. Comput. Sci. Eng. 9, 90–95. https://doi.org/10.1109/Mcse.2007.55.

Jaeken, J.W., Cottenier, S., 2016. Solving the Christoffel equation: phase and group velocities. Comput. Phys. Commun. 207, 445–451. https://doi.org/10.1016/j.cpc.2016.06.014.

Kojima, S., 2022. 100th anniversary of Brillouin scattering: impact on materials science. Materials 15. https://doi.org/10.3390/ma15103518.

Kresse, G., Hafner, J., 1993. Ab-initio molecular-dynamics for open-shell transition-metals. Phys. Rev. B 48, 13115–13118. https://doi.org/10.1103/PhysRevB.48.13115.

Mainprice, D., Hielscher, R., Schaeben, H., 2011. Calculating Anisotropic Physical Properties from Texture Data Using the MTEX Open-Source Package, 360. Geological Society, London, Special Publications, pp. 175–192. https://doi.org/10.1144/SP360.10.

Munoz-Santiburcio, D., Hernandez-Laguna, A., Soto, J.I., 2015. AWESoMe: a code for the calculation of phase and group velocities of acoustic waves in homogeneous solids. Comput. Phys. Commun. 192, 272–277. https://doi.org/10.1016/j.cpc.2015.02.024.

Musgrave, M.J.P., 1970. Crystal Acoustics: Introduction to the Study of Elastic Waves and Vibrations in Crystals. Holden-Day, San Francisco, CA, USA.

Nye, J.F., 1957. Physical Properties of Crystals. Oxford University Press, Oxford.

Petersen, K.B., Pedersen, M.S., 2012. The Matrix Cookbook version 15 November 2012. http://matrixcookbook.com.

Plotly Technologies Inc, 2015. Collaborative Data Science.

Soler, J.M., Artacho, E., Gale, J.D., García, A., Junquera, J., Ordejón, P., Sánchez-Portal, D., 2002. The SIESTA method for ab initio order-N materials simulation. J. Phys. Condens. Matter 14, 2745–2779. https://doi.org/10.1088/0953-8984/14/11/302.

Speziale, S., Duffy, T.S., 2002. Single-crystal elastic constants of fluorite (CaF_2) to 9.3 GPa. Phys. Chem. Miner. 29, 465–472. https://doi.org/10.1007/s00269-002-0250-x.

Ulian, G., Valdrè, G., 2022. *Quantas* : a Python software for the analysis of thermodynamics and elastic behavior of solids from *ab initio* quantum mechanical simulations and experimental data. J. Appl. Crystallogr. 55, 386–396. https://doi.org/10.1107/S1600576722000085.

Wang, J., Mao, Z., Jiang, F., Duffy, T.S., 2015. Elasticity of single-crystal quartz to 10 GPa. Phys. Chem. Miner. 42, 203–212. https://doi.org/10.1007/s00269-014-0711-z.