

Elastic geobarometry for anisotropic inclusions in anisotropic host minerals: quartz-in-zircon

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Introduction

These supplementary materials provide further details about the elastic properties, axial conventions, and relative orientation of the host zircon and the quartz inclusion. The datasets provide all the results of the quartz-in-zircon calculations in table format. The datasets include the unrelaxed and relaxed strains, and the relaxation tensors.

Text S1.

Elastic properties, axial conventions and relative orientations for quartz and zircon

Elastic properties

The anisotropic elastic properties are described by the 4th-rank stiffness tensor (\mathbf{C}). Here we report the components C_{ij} of the corresponding matrix in Voigt notation (Voigt, 1910) for quartz and zircon. The elastic constants (C_{ij}) and the Equation of State (EoS) usually are not determined on the same crystal and with the same experimental settings. Moreover, the EoS is obtained from isothermal measurements while the elastic constants are obtained from adiabatic measurements (Angel et al. 2009). This has the consequence that the value of the isothermal Reuss bulk modulus determined at room conditions ($K_{TR,0}$) from the EoS does not coincide exactly with that of the adiabatic Reuss bulk modulus that is calculated from the elastic tensor. To keep consistency among the different steps of the calculation, which involve both the elastic tensor and the EoS (see Appendix A), for each mineral its C_{ij} components were rescaled to obtain a new elastic tensor that gives a $K_{TR,0}$ equal to that obtained from its EoS. To this aim, all the C_{ij} were multiplied by a scalar value (close to 1) that was adjusted until the agreement in the value of $K_{TR,0}$ was reached. This approach guarantees that the anisotropy of the mineral is not modified by the rescaling.

Zircon

Zircon crystallizes in the tetragonal systems, point group 4/mmm (centrosymmetrical class). The elastic properties of nonmetamict natural and synthetic crystals of zircon were

measured by Özkan et al. (1974) using the pulse superposition and the phase comparison method. Their adiabatic elastic constants were rescaled to obtain the same value of $K_{TR,0} = 224.4$ GPa as that given by the EoS of Ehlers et al. (2021). The anisotropy, as evaluated by the universal anisotropic index (Ranganathan and Ostoja-Starzewski 2008) $A^U = 1.12$, is left unchanged by the rescaling. The independent components of the stiffness tensor are reported in Table S1.

Quartz

Quartz crystallizes in the trigonal system, point group 32. The adiabatic elastic constants of a natural quartz were determined by Lakshtanov et al. (2007). The room P,T adiabatic elastic constants were rescaled to obtain the same value of $K_{TR,0} = 37.15$ GPa as in the EoS of Angel et al. (2017). The anisotropy, as evaluated by the universal anisotropic index (Ranganathan and Ostoja-Starzewski 2008) $A^U = 0.84$, is left unchanged by the rescaling. The independent C_{ij} components of the stiffness tensor are reported in Table S2.

Axial conventions

For each mineral we follow the axial convention that was assumed for the experimental determination of its stiffness tensor C_{ijkl} , and we maintain it for all of our calculations. For zircon (tetragonal) the Cartesian x, y, z are taken parallel to the crystallographic $\mathbf{a}, \mathbf{b}, \mathbf{c}$ axes respectively, according to the convention of the stiffness tensor followed by Özkan et al. (1974). For quartz (trigonal) the Cartesian z is taken parallel to the crystallographic \mathbf{c} , while x is parallel to \mathbf{a} . As a consequence y is in the crystallographic $\mathbf{a-b}$ plane, parallel to \mathbf{b}^* . This convention is the standard for quartz proposed by the ANSI/IEEE (1987) and it is the axial convention assumed by Lakshtanov et al. (2007) for their stiffness tensor. Both

these axial conventions can be represented by the same matrix \mathbf{A} that transforms the unit cell onto a Cartesian reference basis which in general puts z parallel to \mathbf{c} and the y axis parallel to the reciprocal lattice axis \mathbf{b}^* :

$\mathbf{A} = \begin{pmatrix} a \sin(\beta) & b(\cos(\gamma) - \cos(\alpha) \cos(\beta))/\sin(\beta) & 0 \\ 0 & V/(a c \sin(\beta)) & 0 \\ a \cos(\beta) & b \cos(\alpha) & c \end{pmatrix}$	(eq. S1)
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Where a, b, c are the lengths of the unit-cell axes, V is the unit-cell volume, and the α, β, γ are the angles between the unit-cell axes. For trigonal and tetragonal crystals without symmetry breaking, equation S1 is simplified by letting $\alpha = \beta = 90^\circ$.

Choice of the relative orientations

Both quartz and zircon are elastically anisotropic. As a consequence the residual strain developed in the inclusion is a function of the relative orientation of the two minerals. In our analysis we illustrate this orientation dependency by considering three specific relative orientations. The orientations are chosen by aligning the directions of highest and lowest Young's modulus of the inclusion to the direction with highest Young's modulus of the host. The Young's modulus of an anisotropic crystal is direction-dependent and its value along any direction is calculated as (Nye 1985):

$E = 1/(S'_{1111}) = 1/(U_{1m}U_{1n}U_{1p}U_{1q}S_{mnpq})$	(eq. S2)
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where the indicial notation with summation over repeated indices is assumed (the Einstein summation convention). The matrix \mathbf{U} is the transformation matrix (as defined above) while \mathbf{S} is the 4th-rank compliance tensor of the mineral. The directions of largest

and smallest Young's modulus do not necessarily coincide with the crystallographic axes of the crystal (Nye 1985). With the elastic properties of quartz defined in Table S2, the Young's modulus is largest ($E = 130.04$ GPa) along the $[0.00 \ -0.77 \ 0.64]$ direction and equivalents (in Cartesian coordinates) and smallest ($E = 69.47$ GPa) along the $[1.00 \ -0.58 \ 0.42]$ direction and equivalents. The equivalent directions are found considering that elasticity is a centrosymmetrical property, which for quartz is described in the Laue group $\bar{3}m$. With the properties of zircon reported in Table S1 its' Young's modulus is largest ($E = 397.87$ GPa) in the Cartesian $[0 \ 0 \ 1]$ direction, that coincides with the c unit-cell axis.

Under the constraint of aligning one specific direction of the inclusion to a specific direction of the host, infinite relative orientations are possible, which are generated by rotating the local reference system of the inclusion around that chosen direction. Therefore, in defining a unique orientation, one should add a second constraint that orients another direction of the inclusion with respect to the host. Table S3a shows the transformation matrix \mathbf{U} (see equation A1) that describes the orientation of the inclusion assuming that the direction of largest Young's modulus of the quartz inclusion is parallel to the direction of largest Young's modulus of zircon, while the Cartesian $[1 \ 0 \ 0]$ of the host and the inclusion are kept parallel. For the case where the direction with the smallest Young's modulus of quartz aligned with the direction of the largest Young's modulus of zircon, no other condition is imposed. Therefore, one of the possible orientation matrices that satisfies this condition was used (Table S3b). The identity transformation matrix is the orientation matrix that keeps the local Cartesian reference system parallel to the global reference system (Table S3c).

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Supplementary Data Tables

Table S1.					
C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}
422.0	70.0	148.9	488.0	113.1	48.3

Table S1. Components of the stiffness tensor in Voigt notation of zircon (C_{ij} , GPa), modified from Özkan et al., (1974).

Table S2.					
C_{11}	C_{12}	C_{13}	C_{14}	C_{33}	C_{44}
86.1	7.2	11.7	17.7	105.6	59.2

Table S2. Components of the stiffness tensor in Voigt notation of quartz (C_{ij} , GPa). Modified from Lakshtanov et al., (2007), as described in the text.

Table S3.		
stiff-stiff orientation	$\mathbf{U} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0.639200 & -0.769041 \\ 0 & 0.769041 & 0.639200 \end{pmatrix}$	(a)
soft-stiff orientation	$\mathbf{U} = \begin{pmatrix} 0.507240 & 0.285802 & 0.813034 \\ 0.285802 & 0.834234 & -0.471561 \\ -0.813034 & 0.471561 & 0.341475 \end{pmatrix}$	(b)
identity orientation	$\mathbf{U} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	(c)

Table S3. Transformation matrices for the three choices of relative orientations between the quartz inclusion and the zircon host.

Supplementary Data Sets

Data Set S1. The unrelaxed strain results for all of the quartz-in-zircon models. Model results are grouped according to the P-T of the simulation as described in the text. Strain tensors are represented using the notation of Voigt (1910).

Data Set S2. The relaxation tensors calculated using Finite Element Modeling following the methods outlined in Mazzucchelli et al., (2019) and Morganti et al., (2020).

Data Set S3. The relaxed strain results for all of the quartz-in-zircon models. Model results are grouped according to the P-T of the simulation as described in the text. Strain tensors are represented using the notation of Voigt (1910).