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Key Points:

- MATLAB toolbox and Excel workbook calculates rock physical properties for any composition
- Quartz has complex properties due to highly unusual properties at the alpha-beta transition
- Calculations of rock seismic velocities from mineralogy can be integrated with other effects

Supporting Information:

- Supporting Information S1
- Supporting Information S2

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A MATLAB toolbox and Excel workbook for calculating the densities, seismic wave speeds, and major element composition of minerals and rocks at pressure and temperature

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Abstract To interpret seismic images, rock seismic velocities need to be calculated at elevated pressure and temperature for arbitrary compositions. This technical report describes an algorithm, software, and data to make such calculations from the physical properties of minerals. It updates a previous compilation and Excel[®] spreadsheet and includes new MATLAB[®] tools for the calculations. The database of 60 mineral end-members includes all parameters needed to estimate density and elastic moduli for many crustal and mantle rocks at conditions relevant to the upper few hundreds of kilometers of Earth. The behavior of α and β quartz is treated as a special case, owing to its unusual Poisson's ratio and thermal expansion that vary rapidly near the α - β transition. The MATLAB tools allow integration of these calculations into a variety of modeling and data analysis projects.

1. Introduction

Seismic imaging provides a wealth of data on the subsurface at many scales primarily by in the form of P and S wave speeds or their contrasts across interfaces. These data potentially provide information on the composition and mineralogy of the crust and mantle, which can vary considerably. The connection between seismic wave speeds and composition can be made in at least two ways. First, velocities can be measured in the laboratory for natural rocks recovered from the field. However, retrogression and alteration of exposed natural samples tend to reduce their wave speeds relative to the same rocks at depth [Carlson, 2014] and accurate pressure and temperature derivatives are required to extrapolate to conditions at depth. Alternatively, seismic velocities can be predicted for any arbitrary rock composition if mineral abundances are known and mineral elastic properties can be adequately described [e.g., Bina and Helffrich, 1992]. The latter approach is taken here.

This technical report updates Hacker and Abers [2004], a Microsoft Excel[®] worksheet, and macro for calculating rock and mineral physical properties at pressure (P) and temperature (T) relevant to the Earth's crust and mantle. Several improvements have been made to this rock velocity calculator from the 2004 version. First, the calculations have been rewritten as a suite of MATLAB[®] functions, allowing the user to rapidly construct complex calculations and create figures. An optional MATLAB graphical user interface (GUI) allows simple calculations to be made in a manner suitable for classroom use. Second, the underlying mineral database has been updated to include new mineral-physics data published over the last decade; a more accurate model for quartz elasticity is the biggest change. Third, the rock major element composition is now calculated. Except for quartz, the underlying models of the temperature and pressure sensitivity of density and elastic moduli remain the same, as does the multicomponent mixing approach; the reader is referred to Hacker and Abers [2004] for specifics. An updated macro and spreadsheet is also included for users who prefer to use Excel. The Excel spreadsheet continues to be the primary organizational tool for the underlying mineral elasticity and composition database, and is exported for use by the MATLAB functions. This approach makes it easy for users to update the database and include other minerals as they see fit.

Although this approach has widespread application, it has shortcomings. One obvious limitation is the lack of any anelastic or physical dispersion effects for finite-frequency signals, which can be as important as

anharmonic effects at mantle adiabatic conditions [Karato, 1993]. Unfortunately, anelasticity is well calibrated for only a few minerals, principally olivine [e.g., Jackson and Faul, 2010], so we could not systematically include these effects here. It is possible that generalizations of scaling laws may allow extrapolation to other mineral systems [McCarthy et al., 2011], should such extrapolations be sufficiently validated. A second limitation is the assumption of isotropy; the reader is referred to a variety of other toolboxes [e.g., Mainprice, 1990; Walker and Wookey, 2012] for estimating elasticity in mineral aggregates with sufficient data. Third, these calculations deal with minerals, whereas in many situations, poroelastic effects can be important. A rich literature exists describing the effects of water and melt within pores in calculations of elastic moduli, including recipes and toolboxes for MATLAB [e.g., Mavko et al., 2009; Schmeling et al., 2012]. One advantage of the MATLAB toolbox provided here is that it may be easier to interface with calculations that take into account some of these effects. Fourth, this toolbox includes mineral physics and compositional data for only a small subset of natural minerals, most of which are end-member compositions. Data for many end-members are missing (e.g., Mn-garnet, K-amphibole, Na-mica, Cr-spinel, and Fe-pumpellyite), meaning that the effects of these minerals—in velocities, densities, and rock compositions—are ignored, and the relative influence of other end-members enhanced. The reader is referred to Hacker and Abers [2004] for a discussion of other limitations.

We caution the user that this toolbox will calculate elastic properties for any chosen minerals and mineral compositions, and it does not test whether the mineral assemblage is stable at the specified P and T (except for the α - β quartz transition as discussed below)—or, indeed, at any P and T. This can be of great use, but caution is warranted. Also, the end-member mineral names in the spreadsheets need not have a 1:1 correlation with minerals in rocks, so some understanding of mineral systematics is required. To give two common examples, (i) a plagioclase feldspar may contain K_2O , in which case that part must be represented in the spreadsheet by orthoclase or sanidine and (ii) an orthopyroxene may contain CaO, in which case that part must be represented in the spreadsheet by Ca-Tschermak or diopside.

2. Database

The database of thermoelastic properties for 60 minerals is similar to that in Hacker and Abers [2004], with updated values from the literature, and a half a dozen new minerals. Supporting information Table S1 summarizes all of these references. Many recent experiments and ab initio calculations have improved the mineral database. These new values and the related references are highlighted in red in the Excel spreadsheet, and the related references are noted in supporting information Table S1 by a “*.”

3. Quartz

The updated algorithm pays particular attention to quartz because it is a common crustal mineral with unusual elastic properties (e.g., a Poisson's ratio <0.1 at STP) requiring special treatment. In the lower crust of hot orogenic belts, α quartz should transform to the hexagonal, high-temperature polymorph β quartz [Shen et al., 1993]; the transition from α quartz to β quartz has a remarkable elastic signature [Ohno, 1995] that is expected to be visible in V_p or V_p/V_s measurements [Mainprice and Casey, 1990; Mechie et al., 2004; Kuo-Chen et al., 2012; Sheehan et al., 2014]. As previous studies have emphasized, this elastic signature provides one of the few ways to assess middeep crustal temperatures in active orogenic belts (Figure 1). In spite of this potential, the elastic properties of quartz have not been measured at high P and high T, such that making a concrete link between seismic velocities and the α - β transition is somewhat speculative.

The α - β transition in quartz is a displacive transformation that is reversible at laboratory time scales [Buerger, 1951; Keith and Tuttle, 1952; Ghiorso et al., 1979; Raz et al., 2002; Zappone and Benson, 2013]; it is not a reconstructive transformation or net-transfer reaction that requires significant catalysis to operate. Structural changes—in atomic positions, amplitudes of atomic vibration, bond angles, and the development of Dauphiné twins—occur over tens of Kelvin below the transition [Young, 1962] and are mirrored by changes in volume, heat capacity, and elastic behavior [Ghiorso et al., 1979; Carpenter et al., 1998]. The transformation temperature is affected by impurities, but typically by not more than a few Kelvin [Keith and Tuttle, 1952]. In summary, the α - β transition is expected to occur in Earth under near-equilibrium conditions. For these reasons, the toolbox does not allow the user to specify the quartz polymorph, but calculates which polymorph is stable at the specified pressure and temperature.

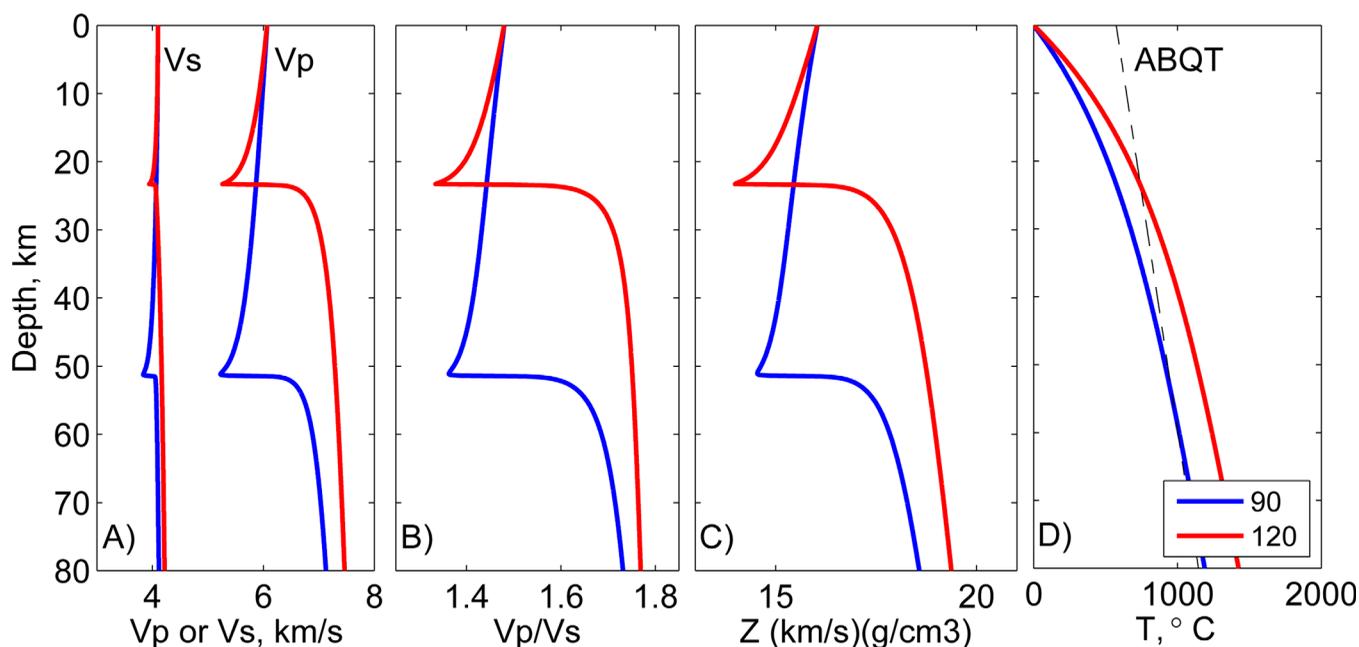


Figure 1. Predicted quartz properties across the α - β quartz transition along a hot (red) and moderate (blue) continental geotherm. Geotherms calculated for exponentially decaying crustal heat production with depth [Turcotte and Schubert, 2002] for a 20 km e -folding production depth, mantle heat input of 20 mW/m², thermal conductivity of 2.5 W m⁻¹ K⁻¹, and surface heat flow of 90 or 120 mW m⁻². (a) V_p or V_s velocity as labeled. (b) V_p/V_s ratio; $V_p/V_s = 1.414$ corresponds to a Poisson's ratio of zero. (c) Impedance as product of V_p and density, changes in which scale to reflection amplitude. (d) Geotherms used for the two models, labeled with surface heat flow (mW m⁻²) along with α - β quartz transition (dashed).

The stiffness tensor, C_{ij} , of quartz has been measured at elevated T and 1 atm, and at elevated P and 25°C; V_p and V_s have also been measured in quartzite at elevated P and T . It is uncertain, however, how the values of C_{ij} change with increasing P and T —for example, does the temperature dependence of the C_{ij} simply scale with ΔT from the α - β equilibrium boundary as the boundary shifts to higher temperature with increasing pressure? Below we summarize what is known.

3.1. Effect of Temperature on Quartz Elasticity

The stiffness tensor, C_{ij} , of quartz single crystals has been measured in detail at 1 atm under increasing temperature, most recently using rectangular parallelepiped resonance [Ohno *et al.*, 2006] and Brillouin spectroscopy [Lakshatanov *et al.*, 2007]. At standard temperature and pressure (STP), the bulk and shear moduli are $K = 37.9$ – 38.2 GPa and $G = 44.9$ GPa, corresponding to $V_p = 6.1$ km/s [Ohno *et al.*, 2006; Lakshatanov *et al.*, 2007]; note that $K < G$, which is quite unusual. The calculated values of the bulk and shear moduli as a function of temperature differ by <1% between the two techniques—except for a narrow, <25°C, interval just above the α - β transition, where the derived bulk moduli differ by up to 8%.

In quartz single crystals, the first 300°C of heating beyond STP induces a 3% decrease in V_p —similar to some other minerals. In the next 200°C—approaching the 1 atm α - β transition temperature of 575°C— V_p plummets an additional 14% to reach a minimum of 5.0 km/s [Ohno *et al.*, 2006; Lakshatanov *et al.*, 2007]. Inside the β quartz stability field, V_p rebounds rapidly with temperature, reaching 7 km/s at 700°C, and then—in contrast to nearly all other minerals—continues to increase up to at least 1050°C [Ohno *et al.*, 2006; Lakshatanov *et al.*, 2007], partly because the thermal expansivity of β quartz is weakly negative [Welche *et al.*, 1998].

This unusual elastic behavior is also evident in Poisson's ratio. The calculated Poisson's ratio for an α quartz crystal is very unusual at STP—0.08 ($V_p/V_s = 1.48$)—but gets even stranger with increasing temperature, reaching a minimum of -0.27 ($V_p/V_s = 1.27$) at $\sim 570^\circ\text{C}$, just below the α - β transition. At temperatures above the α - β transition, quartz starts to behave more normally, and by 700°C at 1 atm, β quartz approaches a typical Poisson solid ($V_p/V_s = 1.72$). Novaculites (fine-grained quartzose rocks) display similarly unusual behavior across the α - β transition, indicating that the behavior is not unique to single crystals [McKnight

et al., 2008]; in novaculite and quartzite, the magnitude of the changes is muted (relative to single crystals) by the different orientations of the grains.

3.2. Effect of Pressure on Quartz Elasticity

The pressure dependence of the bulk modulus has been measured in quartz single crystals compressed in a diamond-anvil cell using X-ray diffraction [Angel *et al.*, 1997], and the complete stiffness tensor, C_{ij} , of quartz has been measured in a hydraulic press to 1 GPa using ultrasonic travel times [Calderon *et al.*, 2007] and by Brillouin spectroscopy along with the pressure derivatives [Wang *et al.*, 2014]. C_{ij} have also been calculated at high pressure using density functional theory [Kimizuka *et al.*, 2007]. These methods obtained slightly different results, but the 1 GPa values for the bulk modulus for all the studies are relatively similar—40.4 [Calderon *et al.*, 2007], 41.3 GPa [Angel *et al.*, 1997; Kimizuka *et al.*, 2007], and 43.4 GPa [Wang *et al.*, 2014].

Experiments have also been conducted on quartzite at 25°C and pressures to 1 GPa using the pulse-transmission technique [Christensen, 1965, 1966, 1996; Musacchio *et al.*, 1997]. The application of modest pressure is required to close cracks in polycrystalline materials; measured elastic properties above ~200 MPa show the expected linear dependence on pressure [Christensen, 1965; Kern *et al.*, 2008].

3.3. Effect of Pressure and Temperature on Quartz Elasticity

There has been minimal investigation of the elastic properties of quartz at high pressure and temperature—in fact, 0.2 GPa is the highest pressure at which elevated-temperature measurements have been done, and only on quartzite [Fielitz, 1971; Christensen, 1979; Kern, 1979; Lu and Jackson, 1998]. At 0.2 GPa, thermally induced cracks in quartzite are closed [e.g., Lu and Jackson, 1998], and the α - β transition induces a reduction in V_p [Fielitz, 1971; Christensen, 1979; Kern, 1979] identical to that seen in quartz single crystals. One set of experiments on a metasedimentary rock with 36% quartz demonstrated that the acoustic changes associated with the α - β transition at 1 atm are also seen at temperatures appropriate for the α - β transition pressures of 200–400 MPa [Zappone and Benson, 2013].

3.4. Summary

None of this unusual elastic behavior of quartz is well fit by the standard thermal expansion models used for other minerals. For these reasons, the algorithm included in this toolbox handles the elastic properties of α and β quartz independently from the primary calculation framework used for other minerals [Hacker and Abers, 2004], through a series of functional regressions on density, bulk, and shear modulus data (Figure 1). We assume, after Zappone and Benson [2013], that the elastic behavior of the α - β transition at elevated pressure is identical to that at 1 atm. Specifically, we assume that the temperature dependences of the elastic properties scale with the difference in temperature from the α - β transition, matching Ohno *et al.* [2006] at zero pressure and shifting to higher temperatures as the transition temperature increases with pressure [Shen *et al.*, 1993]. The elastic moduli also increase with pressure as indicated by variable-pressure studies at room temperature [Angel *et al.*, 1997; Calderon *et al.*, 2007; Kimizuka *et al.*, 2007; Wang *et al.*, 2014]; we assume that the pressure variations are independent of temperature except in defining the temperature of the α - β transition. These assumptions remain to be tested by experiments—beyond Zappone and Benson [2013]—that measure the elastic properties of quartz at elevated P and T.

4. Excel Workbook

The Excel workbook is similar to the 2004 version, with the following changes: (a) the mineral-physics data in the “database” sheet has been updated, (b) the bulk-rock major element composition is now calculated and reported in the “rocks” page, and (c) more accurate elastic properties of quartz are now calculated in the code. Supporting information Table S1 describes codes for all references from which properties are derived, and supporting information Table S2 lists notes on database parameters not described previously [Hacker and Abers, 2004]. The workbook was tested under Microsoft Excel 2003 and 2010 for Windows.

5. Using the MATLAB Toolbox

To use the MATLAB toolbox, place the directory containing all.m code files and.txt database tables on your MATLAB search path, e.g., via the “addpath” function. In the compressed supporting information file

Table 1. Functions, Files, and Databases

File	Description
ah16_loaddb.m	Loads database files into MATLAB structures
ah16_minervel.m	Calculates properties for all minerals at P, T
ah16_rockvel.m	Calculates physical properties for composites (rocks)
ah16_rockcomp.m	Major element compositions for rocks
ah16_hsvbounds.m	Hashin-Shtrikman-Walpole bounds on elastic moduli
ah16_guidriver.m	Creates graphical user interface
rockvelcalculate.m	Example script demonstrating calculations
test_quartz.m	Example script that created Figure 1
AbersHackerMacroJan2016.xls	Excel spreadsheet
AbersHackerMacroJan2016.txt	Thermal-elastic database
mindict_AbersHackerMacroJan2016.txt	Mineral names and rock compositions

distributed with this paper, this directory is called "ABERSHACKER16." All of the files are described below and summarized in Table 1. The codes were tested under MATLAB 2014a.

5.1. Data Files

The distribution file includes the following data tables in plain-text format:

- A. AbersHackerMacroJan2016.txt
- B. mindict_AbersHackerMacroJan2016.txt

The first file compiles the elasticity and thermodynamic data for each mineral, whereas the second includes a dictionary of mineral names and compositions, and a suite of model rock compositions. Both can be regenerated from the Excel spreadsheets if the user changes the primary values in the spreadsheets. To do so, open Excel and save (i) the "database" worksheet and (ii) the "rock mineral modes" worksheet, as "separate files of Windows Formatted Text (.txt)." The filenames can be changed, although the second filename must be the same as the first with "mindict_" prepended. As a caution, we found that Excel only exports numerical values to text files at the precision shown on the screen, so that severe roundoff errors can occur during generation of text files with insufficient precision. To generate the.txt tables provided here, we saved tables with six digits after the decimal for elastic moduli and oxide weights and with four digits for most other parameters, leading to consistency between Excel and MATLAB calculations better than one part in 10^{-6} .

5.2. MATLAB Function Files

The MATLAB code distributed in the supporting information data includes the following MATLAB functions. The exact syntax for each can be obtained from standard help commands, and the comments at the start of each file.

- A. `ah16_loaddb.m`: this function reads the two data files and creates MATLAB structures for use elsewhere. The input parameter is the filename of the primary thermoelastic database. Files are first searched for in the user's current directory, and then in the directory where this routine is located (e.g., ABERSHACKER16). Output includes a structure "minpropar" with physical properties for each mineral and a structure "compar" with compositional data for each mineral; both are keyed to a 2–5 letter code for each mineral. Optional output includes "mindict" a dictionary providing an explanation of the mineral code (full name, composition, and mineral family), and tables of model rock compositions "rocknames" and "rockmodes" providing a short name and mineral modes for those compositions. Unless otherwise stated, these rock names and modes correspond to the mafic and ultramafic compositions described in *Hacker et al.* [2003].
- B. `ah16_minervel.m`: calculates elastic properties for a single mineral at elevated T and P. Input parameters are T, P, and a MATLAB structure of mineral properties of the same form as minpropar above, but for one mineral. Quartz is handled by an internal function in this file. Outputs include scalar density, elastic moduli, and velocities for the mineral at the specified P and T.
- C. `ah16_rockvel.m`: calculates physical properties for a mineral composite (rock) at elevated temperature and pressure. Input parameters are T, P, the minpropar structure, and a list of minerals and their modal abundances in the rock of interest. Creates a structure with the elastic moduli, velocities, and

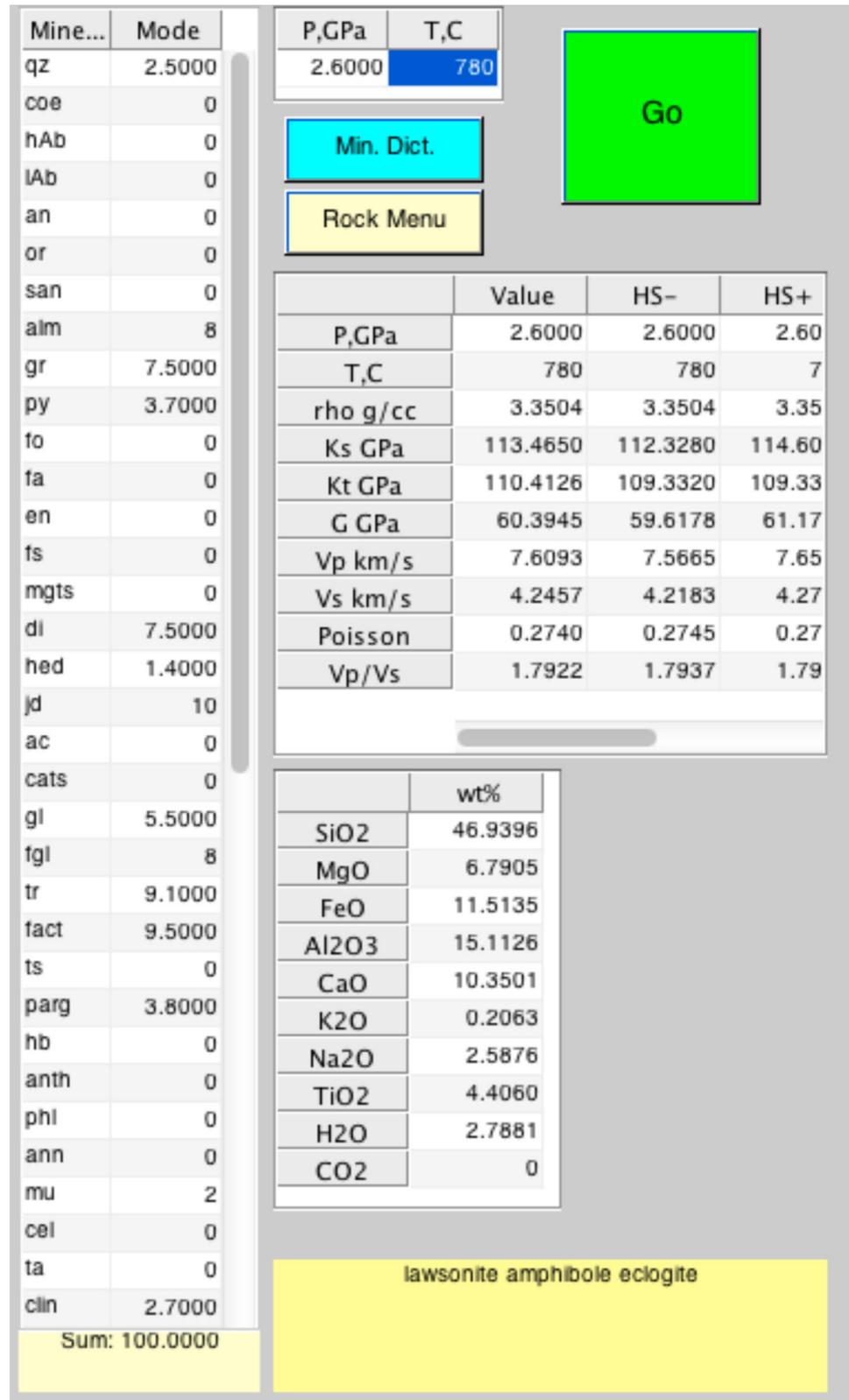


Figure 2. Snapshot of the GUI.

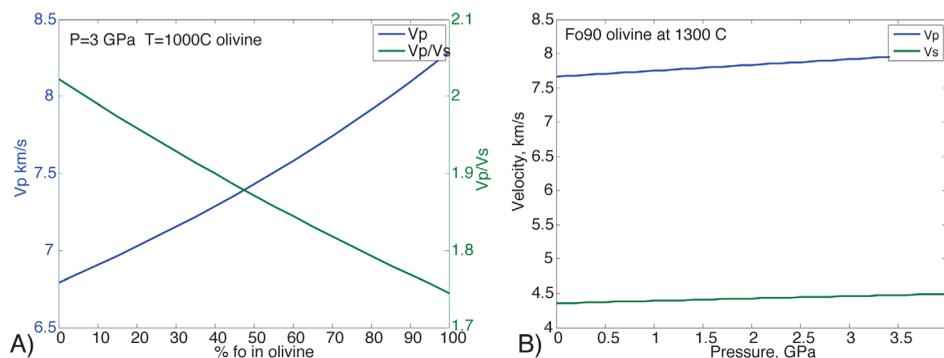


Figure 3. Velocities in olivine generated by the test script. (a) V_p and V_p/V_s varying with Mg/(Mg + Fe) or mol % fo in olivine, at 3 GPa and 1000°C. (b) V_p and V_s varying with pressure for fo₉₀ olivine, at 1000°C.

densities for the rock at the specified P and T, as well as structures with Hashin-Shtrikman bounds and Voigt-Reuss bounds on elasticity. Optionally, this routine also calculates major element oxide abundances (wt %).

- D. `ah16_rockcomp.m`: calculates the major element compositions for a rock. The input is an array of mineral compositions (i.e., `compar` from `ah16_loaddb`) and an array of mineral modal abundances in vol %. Output is a structure like `compar` with aggregate rock composition as wt % oxides. Primarily used through calls to `ah16_rockvel`.
- E. `ah16_hswbounds.m`: calculates the Hashin-Shtrikman-Walpole bounds on the elastic moduli of a composite material [Berryman, 1995]. Primarily used through calls to `ah16_rockvel`.

5.3. MATLAB GUI

The function “`ah16_guidriver.m`” generates a simple graphical user interface (GUI) to allow quick calculation for a single rock (Figure 2). To use the calculator, enter P (GPa) and T (°C), enter the volume-fraction mode of each mineral in the “Mode” column, and press the “Go” button. The calculated physical properties (density, moduli, wave speeds, Poisson’s ratio, and major element composition) appear in tables. Clicking on a mineral code in the left column of the “Mineral Mode” table generates a popup showing the full mineral name, chemical formula, and mineral family. The “Min. Dict.” button provides the same information for all minerals. The “Sum:” textbox at the bottom of the “Mineral Mode” table shows the sum of the mineral modes; these are renormalized to 100% prior to calculation. The “Rock Menu” button allowing users to select mineral modes for a predefined rock composition from the “mindict” table; users can add frequently used rocks as columns to this table. Data in the output tables can be copied and pasted into other windows or applications.

5.4. MATLAB Example Scripts

`rockvelcalculate.m`: this example script generates two plots (Figure 3). The first shows V_p and V_p/V_s as a function of the Mg/(Mg + Fe) content in olivine, at constant P and T. The second shows the pressure dependence of V_p and V_s at constant temperature for fo₉₀ olivine.

`test_quartz.m`: this script generates Figure 1, showing how velocities and impedances can be calculated over a range of conditions, in this case corresponding to two example geotherms. It illustrates the behavior of quartz across the α - β transition.

6. Summary

Updated data on mineral elastic and thermodynamic properties, along with increased development of elaborate calculations with high-level scripting languages, motivate the release of a new MATLAB toolbox and updated Excel workbook for rock velocity calculations. The unusual behavior of quartz, particularly as it passes through the α - β transition, receives special treatment. The MATLAB toolbox enables a wide variety of applications that predict velocities and other properties of rocks at elevated pressures and temperatures. The ease of its use, the inclusion of major element data, and a basic graphical user interface enable a wide variety of educational applications.

Acknowledgments

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References

- Angel, R. J., D. R. Allan, R. Miletich, and L. W. Finger (1997), The use of quartz as an internal pressure standard in high-pressure crystallography, *J. Appl. Crystallogr.*, *30*, 461–466.
- Berryman, J. G. (1995), Mixture theories for rock properties, in *Rock Physics and Phase Relations: AGU Reference Shelf*, vol. 3, edited by T. J. Ahrens, pp. 205–228, AGU, Washington, D. C.
- Bina, C. R., and G. R. Helffrich (1992), Calculation of elastic properties from thermodynamic equation of state principles, *Annu. Rev. Earth Planet. Sci.*, *20*, 527–552.
- Buerger, M. J. (1951), Crystallographic aspects of phase transformations, in *Phase Transformations in Solids*, edited by R. Smoluchowski, J. E. Mayer and W. A. Weyl, pp. 183–211, Wiley, N. Y.
- Calderon, E., M. Gauthier, F. Decremps, G. Hamel, G. Syfosse, and A. Polian (2007), Complete determination of the elastic moduli of α -quartz under hydrostatic pressure up to 1 GPa: An ultrasonic study, *J. Phys. Condens. Matter*, *19*, 436228, doi:10.1088/0953-8984/19/43/436228.
- Carlson, R. L. (2014), The effects of alteration and porosity on seismic velocities in oceanic basalts and diabbases, *Geochem. Geophys. Geosyst.*, *15*, 4589–4598, doi:10.1002/2014GC005537.
- Carpenter, M. A., E. K. H. Salje, A. Graeme-Barber, B. Wruck, M. T. Dove, and K. S. Knight (1998), Calibration of excess thermodynamic properties and elastic constant variations associated with the $\alpha \leftrightarrow \beta$ phase transition in quartz, *Am. Mineral.*, *83*, 2–22.
- Christensen, N. I. (1965), Compressional wave velocities in metamorphic rocks at pressures to 10 kilobars, *J. Geophys. Res.*, *70*, 6147–6164.
- Christensen, N. I. (1966), Shear wave velocities in metamorphic rocks at pressures to 10 kilobars, *J. Geophys. Res.*, *71*, 3549–3556.
- Christensen, N. I. (1979), Compressional wave velocities in rocks at high temperatures and pressures, critical thermal gradients, and crustal low-velocity zones, *J. Geophys. Res.*, *84*, 407–412.
- Christensen, N. I. (1996), Poisson's ratio and crustal seismology, *J. Geophys. Res.*, *101*, 3139–3156.
- Fielitz, K. (1971), Elastic wave velocities in different rocks at high pressure and temperature up to 750°C, *Z. Geophys.*, *37*, 943–956.
- Ghiorso, M. S., I. S. E. Carmichael, and L. K. Moret (1979), Inverted high-temperature quartz unit cell parameters and properties of the α - β inversion, *Contrib. Mineral. Petrol.*, *68*, 307–323.
- Hacker, B. R., and G. A. Abers (2004), Subduction factory 3. An Excel worksheet and macro for calculating the densities, seismic wave speeds, and H₂O contents of minerals and rocks at pressure and temperature, *Geochem. Geophys. Geosyst.*, *5*, Q01005, doi:10.1029/2003GC000614.
- Hacker, B. R., G. A. Abers, and S. M. Peacock (2003), Subduction factory 1: Theoretical mineralogy, density, seismic wavespeeds, and H₂O content, *J. Geophys. Res.*, *108*(B1), 2029, doi:10.1029/2001JB001127.
- Jackson, I., and U. H. Faul (2010), Grainsize-sensitive viscoelastic relaxation in olivine: Toward a robust laboratory-based model for seismological application, *Phys. Earth Planet. Inter.*, *183*, 151–163.
- Karato, S. (1993), Importance of anelasticity in the interpretation of seismic tomography, *Geophys. Res. Lett.*, *20*, 1623–1626.
- Keith, M. L., and O. F. Tuttle (1952), Significance of variation in the high-low inversion of quartz, *Am. J. Sci., Bowen Volume*, 203–280.
- Kern, H. (1979), Effect of high-low quartz transition on compressional and shear wave velocities in rocks under high pressure, *Phys. Chem. Miner.*, *4*, 161–171.
- Kern, H., T. I. Ivankina, A. N. Nikitin, T. Lokajčićek, and Z. Pros (2008), The effect of oriented microcracks and crystallographic and shape preferred orientation on bulk elastic anisotropy of a foliated biotite gneiss from Outokumpu, *Tectonophysics*, *457*, 143–149.
- Kimizuka, H., S. Ogata, J. Li, and Y. Shibutani (2007), Complete set of elastic constants of α -quartz at high pressure: A first-principles study, *Phys. Rev. B*, *75*, 054109.
- Kuo-Chen, H., F. T. Wu, D. M. Jenkins, J. Mechie, S. W. Roecker, C.-Y. Wang, and B.-S. Huang (2012), Seismic evidence for the α - β quartz transition beneath Taiwan from Vp/Vs tomography, *Geophys. Res. Lett.*, *39*, L22302, doi:10.1029/2012GL053649.
- Lakshmanov, D. L., S. V. Sinogeikin, and J. D. Bass (2007), High-temperature phase transitions and elasticity of silica polymorphs, *Phys. Chem. Miner.*, *34*(1), 11–22.
- Lu, C., and I. Jackson (1998), Seismic-frequency laboratory measurements of shear mode viscoelasticity in crustal rocks II: Thermally stressed quartzite and granite, *Pure Appl. Geophys.*, *153*, 441–473.
- Mainprice, D. (1990), A FORTRAN program to calculate seismic anisotropy from the lattice preferred orientation of minerals, *Comput. Geosci.*, *16*, 385–393.
- Mainprice, D., and M. Casey (1990), The calculated seismic properties of quartz mylonites with typical fabrics: Relationship to kinematics and temperature, *Geophys. J. Int.*, *103*, 599–608.
- Mavko, G., T. Mukerji, and J. Dvorkin (2009), *The Rock Physics Handbook: Tools for Seismic Analysis of Porous Media*, 2nd ed., Cambridge Univ. Press, N. Y.
- McCarthy, C., Y. Takei, and T. Hiraga (2011), Experimental study of attenuation and dispersion over a broad frequency range: 2. The universal scaling of polycrystalline materials, *J. Geophys. Res.*, *116*, B09207, doi:10.1029/2011JB008384.
- McKnight, R. E. A., T. Moxon, A. Buckley, P. A. Taylor, T. W. Darling, and M. A. Carpenter (2008), Grain size dependence of elastic anomalies accompanying the α - β phase transition in polycrystalline quartz, *J. Phys. Condens. Matter*, *20*, 075229, doi:10.1088/0953-8984/20/7/075229.
- Mechie, J., S. V. Sobolev, L. Ratschbacher, A. Y. Babeyko, G. Bock, A. G. Jones, K. D. Nelson, K. D. Solon, L. D. Brown, and W. Zhao (2004), Precise temperature estimation in the Tibetan crust from seismic detection of the alpha-beta quartz transition, *Geology*, *32*(7), 601–604, doi:10.1130/g20367.1.
- Muscacchio, G., W. D. Mooney, J. H. Luetgert, and N. I. Christensen (1997), Composition of the crust in the Grenville and Appalachian Provinces of North America inferred from Vp/Vs ratios, *J. Geophys. Res.*, *102*, 15,225–15,241.
- Ohno, I. (1995), Temperature variation of elastic properties of α -quartz up to the α - β transition, *J. Phys. Earth*, *43*, 157–169.
- Ohno, I., K. Harada, and C. Yoshitomi (2006), Temperature variation of elastic constants of quartz across the α - β transition, *Phys. Chem. Miner.*, *33*, 1–9.
- Raz, U., S. Girsperger, and A. B. Thompson (2002), Thermal expansion, compressibility and volumetric changes of quartz obtained by single crystal dilatometry to 700°C and 3.5 kilobars (0.35 GPa), *Schweiz. Mineral. Petrogr. Mitt.*, *82*, 561–574.
- Schmeling, H., J. P. Kruse, and G. Richard (2012), Effective shear and bulk viscosity of partially molten rock based on elastic moduli theory of a fluid filled poroelastic medium, *Geophys. J. Int.*, *190*, 1571–1578, doi:10.1111/j.1365-246X.2012.05596.x.
- Sheehan, A. F., T. L. de la Torre, G. Monsalve, G. A. Abers, and B. R. Hacker (2014), Physical state of Himalayan crust and uppermost mantle: Constraints from seismic attenuation and velocity tomography, *J. Geophys. Res. Solid Earth*, *119*, 567–580, doi:10.1002/2013JB010601.

- Shen, A. H., W. A. Bassett, and I. M. Chou (1993), The alpha-beta quartz transition at high temperatures and pressures in a diamond-anvil cell by laser interferometry, *Am. Mineral.*, *78*(7–8), 694–698.
- Turcotte, D., and G. Schubert (2002), *Geodynamics*, 456 pp., edited, Cambridge Univ. Press, N. Y.
- Walker, A. M., and J. Wookey (2012), MSAT—A new toolbox for the analysis of elastic and seismic anisotropy, *Comput. Geosci.*, *49*, 81–90.
- Wang, J., Z. Mao, F. Jiang, and T. S. Duffy (2014), Elasticity of single-crystal quartz to 10 GPa, *Phys. Chem. Miner.*, *42*, 203–212.
- Welche, P. R. L., V. Heine, and M. T. Dove (1998), Negative thermal expansion in beta-quartz, *Phys. Chem. Miner.*, *26*, 63–77.
- Young, R. A. (1962), *Mechanism of the Phase Transition in Quartz*, final report, 156 pp., Report No. AD276235, Air Force Off. Sci. Res., Washington, D. C.
- Zappone, A. S., and P. M. Benson (2013), Effect of phase transitions on seismic properties of metapelites: A new high-temperature laboratory calibration, *Geology*, *41*, 463–466.