Subduction Factory 3: An Excel worksheet and macro for calculating the densities, seismic wave speeds, and H_2O contents of minerals and rocks at pressure and temperature

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[1] An Excel macro to calculate mineral and rock physical properties at elevated pressure and temperature is presented. The workbook includes an expandable database of physical parameters for 52 rock-forming minerals stable at high pressures and temperatures. For these minerals the elastic moduli, densities, seismic velocities, and H_2O contents are calculated at any specified P and T conditions, using basic thermodynamic relationships and third-order finite strain theory. The mineral modes of suites of rocks are also specifiable, so that their predicted aggregate properties can be calculated using standard solid mixing theories. A suite of sample rock modes taken from the literature provides a useful starting point. The results of these calculations can be applied to a wide variety of geophysical questions including estimating the alteration of the oceanic crust and mantle; predicting the seismic velocities of lower-crustal xenoliths; estimating the effects of changes in mineralogy, pressure and temperature on buoyancy; and assessing the H_2O content and mineralogy of subducted lithosphere from seismic observations.

1. Introduction

[2] Addressing many geodynamic problems requires calculating the densities and wave speeds of rocks at elevated pressure and temperature. *Hacker et al.* [2003] presented a database of mineral physical properties and a

formalism for such calculations. Here we present an Excel workbook that includes that database of mineral physical properties and a macro[1] that uses that formalism to calculate mineral and

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[1]Auxiliary material is available at ftp://ftp.agu.org/apend/gc/2003GC000614.

rock physical properties at elevated pressure and temperature.

2. Database

[3] The mineral physical properties database comprises the "database" worksheet of the workbook. It includes the formula weight ("gfw" column), molar volume ("V"), H_2O content ("H2O"), expansivity α ("a0") parameterized to vary with temperature [*Holland and Powell*, 1998], isothermal bulk modulus K_T ("KT"), $K'_T = \partial K_T/\partial P$ ("KT prime"), shear modulus G ("G"), $G' = \partial G/\partial P$ ("G prime"), $\Gamma = (\partial lnG/\partial ln\rho)_P$ ("gamma"), the first thermodynamic Grüneisen parameter $\gamma_{th} = (\partial lnT/\partial ln\rho)_S$ ("gth"), and second Grüneisen parameter $\delta_T = (\partial lnK_T/\partial ln\rho)_P$ ("dT") for common minerals [e.g., *Anderson et al.*, 1992; *Bina and Helffrich*, 1992]. (Here, P = pressure, T = temperature, and S = entropy.) See *Hacker et al.* [2003] for a brief discussion of uncertainties in these data. Explanations of the mineral abbreviations as well as mineral formulae can be found in the "rock mineral modes" worksheet.

[4] Many of these parameters have not been measured directly for all the minerals in the database, and have been approximated from a variety of scaling relationships [see also *Helffrich*, 1996]. The most critical approximations are of the shear moduli (G) of hydrous phases, which have been measured directly for few hydrous minerals. Where G has not been measured, we estimate it from K_T by assuming that the Poisson ratio matches that of a mineral of similar structure for which G is known. A variety of observed relations among Γ, δ_T, γ_{th}, K'_T, and G' [*Anderson et al.*, 1992] allow some of the other needed parameters to be estimated from others, or we make other standard assumptions (e.g., $K'_T = 4$). If no derivative terms are available, they are scaled from those of similar minerals. All of these approximations are specified on a case-by-case basis in the Notes on Parameter Values section below, which are keyed to notes next to each parameter value in the "database" worksheet.

3. Mineral Properties at Pressure and Temperature

[5] The "minerals" worksheet contains single-crystal physical properties calculated at elevated temperature and pressure (T, P). To calculate properties at elevated temperature and pressure, individual properties are first extrapolated from STP (standard temperature and pressure) in temperature and then in pressure. The specific values calculated are: the thermal expansivity at temperature ("alpha(T, 0)" column), density at temperature ("rho(T, 0)"), isothermal bulk modulus at temperature ("Kt(T, 0)"), shear modulus at temperature ("G(T, 0)"), isothermal bulk modulus at temperature and pressure ("Kt(T, P)"), thermal expansivity at temperature and pressure ("alpha(T, P)"), adiabatic bulk modulus at temperature and pressure ("Ks(T, P)"), shear modulus at temperature and pressure ("G(T, P)"), density at temperature and pressure ("rho(T, P)"), bulk wave speed at temperature and pressure ("V bulk"), P wave speed at temperature and pressure ("Vp"), S-wave speed at temperature and pressure ("Vs"), and Poisson's ratio ("Poisson's ratio"). The methodology, based on that of *Bina and Helffrich* [1992], was described by *Hacker et al.* [2003] and is repeated below with minor modification (principally, we now uniformly apply a third-order approximation for finite strain, producing negligible changes to velocities for the upper-mantle pressures, as discussed previously).

[6] *Holland and Powell* [1998] advocated a relationship between expansivity α and temperature $T(K)$, defined by a single constant a° for each mineral:

$$\alpha(T) = a^\circ\left(1 - 10/\sqrt{T}\right) \tag{1}$$

which gives

$$\partial\alpha/\partial T = 5a^o/T^{3/2} \tag{2}$$

and

$$\Phi \equiv \ln(V(T)/V_o) = \int_{T_o}^{T} \alpha(T)dT$$
$$= a^o\left\{(T - T_o) - 20\left(\sqrt{T} - \sqrt{T_o}\right)\right\} \tag{3}$$

where $V(T)$ is the molar volume at temperature, V_o is the molar volume at STP, and $T_o = 298$ K.

[7] The density at elevated temperature $\rho(T)$ is related to the density at STP ρ_o by:

$$\rho(T) = \rho_o e^{-\Phi} \qquad (4)$$

The isothermal bulk modulus at elevated temperature $K_T(T)$ is related to the isothermal bulk modulus at STP K_{T_o} by:

$$K_T(T) = K_{T_o} e^{-\delta_T \Phi} \qquad (5)$$

where δ_T is the second Grüneisen parameter. We assume that δ_T is invariant with respect to temperature and pressure, and for most minerals δ_T was approximated as $\delta_T \approx \gamma_{th} + K'_T$ [Anderson et al., 1992]; as explained below, γ_{th} was calculated using Bina and Helffrich's [1992] equation (16) at 1000 K. The shear modulus at elevated temperature $G(T)$ follows in similar fashion from the shear modulus at STP G_o:

$$G(T) = G_o e^{-\Gamma \Phi} \qquad (6)$$

where

$$\Gamma = (\partial \ln G / \partial \ln \rho)_P = -(1/G\alpha)(\partial G / \partial T) \qquad (7)$$

[Duffy and Anderson, 1989]. We assume that Γ is independent of T and P. This parameter has been measured directly for only a few minerals, mostly by Anderson and Isaak [1995], from whom we take their highest temperature values. For other minerals, we approximate $\Gamma = \delta_T$ [Anderson et al., 1992].

[8] The finite Eulerian strain f is calculated from pressure P and the material parameters by assuming the third-order finite strain equation [Birch, 1978]

$$P/K_T = 3f(1 + 2f)^{5/2}(1 - 2\zeta f) \qquad (8)$$

where

$$\zeta = \frac{3}{4}(4 - K') \qquad (9)$$

and

$$K' = (dK_T/dP)_T \qquad (10)$$

typically evaluated at T_o. The finite-strain relationship is monotonic over the range of strains encountered in the Earth but is implicit in f, so must

be solved numerically. The spreadsheet determines f such that the difference between the left- and right-hand sides of equation (8) is zero, within some tolerance, using Brent's zero-finding method [Press et al., 1992]. We set a tolerance in f of 10^{-8}, equivalent to five significant digits precision for f at typical pressures. This precision far exceeds the accuracy of any material parameters.

[9] The density at elevated pressure $\rho(P)$ is then

$$\rho(P) = \rho_o(1 + 2f)^{3/2} \qquad (11)$$

and the isothermal bulk modulus at elevated pressure and temperature $K_T(T, P)$ is

$$K_T(T,P) = K_T(T)\{1 - f(5 - 3K')\}(1 + 2f)^{5/2} \qquad (12)$$

The expansivity at elevated pressure and temperature $\alpha(T, P)$ is

$$\alpha(T,P) = \alpha(T)[\rho(P)/\rho_o]^{-\delta_T} \qquad (13)$$

[10] The isentropic bulk modulus K_S is

$$K_S = K_T(T,P)[1 + T\gamma_{th}\alpha(T,P)] \qquad (14)$$

where γ_{th} is the first Grüneisen parameter. For most minerals γ_{th} was calculated using Bina and Helffrich's [1992] equation (16) at 1000 K, using Holland and Powell's [1998] values and $\delta = 4$. The shear modulus at elevated pressure and temperature $G(T, P)$ is

$$G(T,P) = G(T)(1 + 2f)^{5/2}\{1 - f[5 - 3G'K_T(T)/G(T)]\} \qquad (15)$$

The density at elevated pressure and temperature $\rho(P, T)$ is

$$\rho(T,P) = [\rho(P)/\rho_o]\rho(T) \qquad (16)$$

from which the P wave velocity V_P, shear wave velocity V_S, and Poisson's ratio ν are calculated as [Birch, 1978]:

$$V_P = \sqrt{(K_S + 4/3G)/\rho} \qquad (17)$$

$$V_S = \sqrt{G/\rho} \qquad (18)$$

$$\nu = (3K_S - 2G)/(6K_S + 2G) \qquad (19)$$

[11] See *Hacker et al.* [2003] for a brief discussion of the limitations and uncertainties inherent in such calculations.

4. Rock Properties at Pressure and Temperature

[12] The "rocks" worksheet contains (1) the modal or volume proportions of minerals in rocks, and (2) the physical properties of those rocks calculated at elevated pressure and temperature. The density of a mineral aggregate is calculated from the densities ρ_i of n constituent minerals as:

$$\rho = \left(\sum_{i=1}^{n} \rho_i \nu_i\right)/n \qquad (20)$$

where ν_ι is the volume proportion of each mineral. The bulk modulus is calculated, following *Hashin and Shtrikman* [1962], as

$$K = (K_1 + [A_1/(1 + \alpha_1 A_1)] + K_n + [A_n/(1 + \alpha_n A_n)])/2 \qquad (21)$$

where K_1 is the smallest modulus, K_n is the largest modulus, and

$$\alpha_1 = -3/(3K_1 + 4G_1) \ , \ \alpha_n = -3/(3K_n + 4G_n) \qquad (22)$$

$$A_1 = \sum_{i=2}^{n} \nu_i/[1/(K_i - K_1) - \alpha_1],$$
$$A_n = \sum_{i=1}^{n-1} \nu_i/[1/(K_i - K_n) - \alpha_n] \qquad (23)$$

The shear modulus is analogous:

$$G = (G_1 + [B_1/(1 + \beta_1 B_1]/2 + G_n + [B_n/(1 + \beta_n B_n]/2)/2 \qquad (24)$$

where G_1 and G_n are the smallest and largest moduli, respectively, and

$$\beta_1 = \alpha_1(K_1 + 2G_1)/5/G_1 \ , \beta_n = \alpha_n(K_n + 2G_n)/5/G_n \qquad (25)$$

$$B_1 = \sum_{i=2}^{n} \nu_i/[2/(G_i - G_1) - \beta_1] \ ,$$
$$B_n = \sum_{i=2}^{n} \nu_i/[2/(G_i - G_n) - \beta_n] \qquad (26)$$

Voigt and Reuss [*Hill*, 1952] bounds on the moduli and velocities are also reported.

5. Using the Workbook

[13] To calculate the physical properties of rocks at pressure and temperature, follow these steps.

[14] 1. Select the "rocks" worksheet.

[15] 2. Enter the names of individual rocks in the "vol%" row or copy them from the "rock mineral modes" worksheet.

[16] 3. Enter the volume percentages of the minerals that make up the individual rocks in separate yellow columns. If the percentages do not sum to 100%, they will be renormalized.

[17] 4. Enter the pressure and temperature for each of these rocks in the yellow "P(GPa)" and "T(°C)" rows.

[18] 5. Run the "HackerandAbers03" macro by pressing the "Click to Run" button on the "rocks" worksheet or selecting the macro from the Tools menu.

[19] After the macro has finished executing, the calculated values for each rock can be found in the green "H₂O wt%"…"Poissons" rows of the "rocks" worksheet; the Hashin-Shtrikman averages are listed above the "Click to Run" button and the Voigt bounds, Reuss bounds, and Voigt-Reuss-Hill averages [*Hill*, 1952] are listed below. The "minerals" worksheet contains the calculated physical properties of minerals for the last pressure and temperature used in the "rocks" worksheet. To calculate the physical properties of minerals at pressure and temperature, follow the steps above and then select the "minerals" worksheet.

[20] Note that the macro does not make any determinations about which minerals are stable at specific pressures and temperatures, e.g., be sure to specify the correct SiO_2 polymorph (alpha quartz, beta quartz, coesite) that is stable at the conditions of interest.

5.1. Worksheet Explanations

[21] Mineral abbreviations in all worksheets follow *Holland and Powell* [1998], except for: lab, low

albite; hab, high albite; hb, hornblende; aqz, α quartz; bqz, β quartz; or, orthoclase.

5.2. Explanation for "Database" Worksheet

[22] The "database" worksheet contains values that we consider to be optimal as of the date stamped in the upper left corner. Where possible, the parameters are direct measurements, but where unavailable they are derived using a variety of assumptions, as discussed above and detailed in the Notes on Parameter Values below. The user can change these values as desired to explore the effects of different mineral properties. The authors would appreciate being apprised of new or improved values to be incorporated in future versions of the database.

[23] New minerals can also be added to the database with the following steps:

[24] 1. Insert new rows in the "database" worksheet for each of the new minerals. The "END" marker in the first column must immediately follow the list of minerals.

[25] 2. Insert the same number of rows into the "rocks" worksheet.

[26] 3. Run the macro.

[27] Values in the "database" worksheet are from *Holland and Powell* [1998], except: A01, *Angel et al.* [2001]; A88, *Angel et al.* [1988]; A97, *Angel et al.* [1997]; AA97, *Allan and Angel* [1997]; AI95, *Anderson and Isaak* [1995]; AJ02, *Angel and Jackson* [2002]; A04, *Angel* [2004]; B95, *Bass* [1995]; BA03, *Boffa Ballaran and Angel* [2003]; BH00, *Bailey and Holloway* [2000]; C91, *Comodi et al.* [1991]; C95, *Comodi and Zanazzi* [1995]; C96, *Christensen* [1996]; C97, *Comodi et al.* [1997]; C00, *Chinnery et al.* [2000]; CR02, *Crichton and Ross* [2002]; F95, *Fei* [1995]; G00, *Grevel et al.* [2000]; H00, *Haavik et al.* [2000]; H96, *Helffrich* [1996]; HF78, *Hazen and Finger* [1978]; HP98, *Holland and Powell* [1998]; J99, *Jackson et al.* [1999]; K95, *Knittle* [1995]; L80, *Levien et al.* [1980]; O95, *Ohno* [1995]; P02, *Pawley et al.* [2002]; P03, *Pavese et al.* [2003]; PW96, *Pawley and Wood* [1996]; RA99, *Redfern and Angel* [1999]; RC01, *Ross and Crichton*

[2001]; S00, *Smyth et al.* [2000]; SOA00, *Suzuki et al.* [2000]; SB02, *Sinogeikin and Bass* [2002]; T03, *Theye et al.* [2003]; T91, *Tyburczy* [1991]; WJ01, *Wang and Ji* [2001]; X98, *Xia et al.* [1998].

5.3. Notes on Parameter Values

[28] The following explanations correspond to the enumerated notes on the "database" worksheet: note 1, adjusted to fit STP Poisson's ratio measured by *Tyburczy* [1991]; note 2, assumed that low albite and high albite have equivalent elastic moduli; note 3, adjusted to fit STP Poisson's ratio in *Christensen* [1982, 1996]; note 4, assumed no compositional dependence of bulk modulus; note 5, *Theye et al.* [2003] show no dependence of bulk modulus on Mg# for chlorite; note 6, calculated using Poisson's ratio for forsterite and scaled against bulk modulus of forsterite (structures are similar); note 7, calculated using Poisson's ratio for muscovite and scaled against bulk modulus of muscovite (all are phyllosilicates); note 8, hornblendite data [*Christensen*, 1996] were used instead of hornblende data [*Alexandrov and Ryzhova*, 1961]; note 9, calculated from regression fit to Poisson's ratios of intermediate-composition plagioclase measured by *Ryzhova* [1964]; note 10, calculated using Poisson's ratio for hornblende and scaled against bulk modulus of hornblende (structures are similar); note 11, calculated using Poisson's ratio for sillimanite and scaled against bulk modulus of sillimanite (structures are similar); note 12, calculated using Poisson's ratio for orthoclase and scaled against bulk modulus of orthoclase (structures are similar); note 13, assumed, common value [*Anderson*, 1989]; note 14, calculated at high T using *Anderson and Isaak*'s [1995] highest temperatures where $\partial G/\partial T$ is nearly constant; note 15, adjusted from *Bass* [1995], using $K_T = K_S/(1 + \alpha\gamma_{th}T)$ [*Anderson et al.*, 1992]; note 16, approximated as $\Gamma \approx \delta_T$ [*Anderson et al.*, 1992]; note 17, approximated as $G' \approx (5*G)/(3*K_T)$ [*Anderson et al.*, 1992]; note 18, approximated as $\delta_T \approx \gamma_{th} + K_T'$ [*Anderson et al.*, 1992]; note 19, we used *Holland and Powell*'s [1998] values and expansion for thermal expansivity: $a(T) = a^o(1 - 10/\text{SQRT}(T))$, giving $\ln(V(T)/V_o) = a^o*((T - 298 + \text{SQRT}(T) - \text{SQRT}(298))$; note 20, γ_{th} was calculated using *Bina and Helffrich*'s [1992] equation (16) at

1000 K, using *Holland and Powell*'s [1998] values and δ = 4; note 21, mass, density, and H_2O content were calculated from mineral formula in *Holland and Powell* [1998]; note 22, zoisite K_T and K_T' were used for clinozoisite, following *Grevel et al.* [2000]. The user should be aware that some of these approximations, while required to supplement an incomplete data set, must necessarily lead to uncertainties that can only be resolved with further physical measurements.

5.4. Explanation for "Minerals" Worksheet

[29] This worksheet holds intermediate calculation results. The pressure and temperature shown in the upper left corner of the "minerals" worksheet reflect the most recent pressure and temperature read by the macro (typically the rightmost values in the "P (GPa)" and "T (°C)" rows of the "rocks" worksheet). All of the remaining values in this worksheet are calculated based on that pressure and temperature. Nothing in the "minerals" worksheet should be modified by the user.

5.5. Explanation for "Rocks" Worksheet

[30] The user can add as many rocks, in separate columns, as will fit in the "rocks" worksheet. The composition of each rock is defined by the modal percentages of the various minerals. The pressure and temperature for each rock must be specified.

5.6. Explanation for "Rock Mineral Modes" Worksheet

[31] This worksheet provides several examples of rock descriptions, from *Hacker et al.* [2003] or elsewhere in the literature, for many common rock types. Individual columns can be copied and pasted into the appropriate part of the "rocks" worksheet.

Acknowledgments

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