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Planetary Seismology Simulants

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Abstract

A simple procedure is developed for simulating elastic compositions of substances as may occur in exogeologic bodies. It is based on a mixing law using acoustic slownesses obtained by averaging elasticities of crystallite aggregate components. The method applies to materials having an arbitrary number of constituents; illustrative examples are given for two-component solid solutions in the olivine and pyroxene families. The averaging algorithm is also applied to perovskite, post-perovskite, and alumina elasticities. Linear temperature and pressure coefficients are estimated for the perovskites; higher-order temperature coefficients are computed for alumina. Debye temperatures are given for the various simulants.

INTRODUCTION

Aspera ad astra had, for millenia, been cited only metaphorically. [1]No longer [1-14]. The exertions of still-nascent space programs have already yielded an abundance of results revealing properties of planetary [15-29], cometary [30-35], and stellar bodies [4]. In the near and in the farther future, probes will continue to amass information permitting inferences to be drawn about the constitution and evolution of the cosmos. At present, most of the data have been harvested by means of remote sensing modalities from proximate spacecraft orbits and fly-bys. Valuable as these are, a much fuller picture is to be had by supplementing these with information gleaned from on-site samplings of material constituents, and their relations to acoustic and seismic properties. This approach has proven its value in geology by allowing models of the Earth's directly inaccessible interior to be constructed from, *inter alia*, a knowledge of the elastic properties of minerals, and acoustic wave propagation therein [36-43].

Seismology provides a direct probe of solid environments. Acoustic wave speeds and transit times yield data of material extent, composition, and gradation. These data, in turn, permit formulation of specific models (simulants) for interpreting physical features of exogeologic bodies, such as elastic coefficients determining lithospheric bending; these features are not immediately accessible to remote sensing methods. Such models do not by themselves yield unique characterizations of planetary, meteoric, or cometary interiors, yet they are an invaluable adjunct to other measurement modalities.

In this paper, a simple homogenization procedure is applied to convert single crystal elastic constants to isotropic elastic stiffnesses of microcrystalline aggregates, such as those commonly occurring in planetary bodies. These coefficients, for each mineral, are then combined with those of all other constituents in an algorithm yielding effective elastic parameters that characterize both seismic wave propagation and quasi-static deformations in the mineral composite. [2]Using data from the literature, example simulants are provided for olivines: forsterite–fayalite, and pyroxenes: enstatite–ferrosilite. These are known constituents of solid planetary bodies.

Models for acoustic wave propagation in geologic-type media (e.g., inhomogeneous, stratified, porous, non-linear, etc.) are quite well developed [44-51], and will not be discussed, nor will be reviewed the various modes of acoustic propagation. Considered only are the two canonical, non-dispersive, plane body wave types that propagate in homogeneous, linear media: shear (S) and pressure (P). [3]Other wave types and parameters may be considered to be admixtures of these. As examples, the seismic parameter $\Phi = V_P^2 - (4/3) \cdot V_S^2$ is a combination of P and S wavespeeds [52,53], as is the the velocity of a wave localized near the free surface of an isotropic elastic half-space (Rayleigh wave) [54].

The main thrust of this paper is presentation of a simple

model of acoustic properties of mineralogical compositions that is generally applicable to many of the material systems likely to be encountered in exogeology. The WSD model, described subsequently, makes direct use of the S and P wave speeds, and is a means of computing velocities in mineral species as function of mole fractions of the constituents.

Inasmuch as realistic macroscopic mineralogical deposits are found to be composed largely of randomly oriented polycrystalline aggregates, the starting point of the model is reduction of the elasticities of each crystal constituent to equivalent isotropic values by means of a simple extension of the Voigt-Reuss-Hill (VRH) procedure [55-58]. The extension (VRHx) yields a single set of relaxed quantities for each material, rather than a range of values. The VRHx values are then "mixed," for specified mole fractions, by a time-of-flight assignment applied separately to the S and P wave slownesses. The results provide simulants [19] of various mineral combinations for comparison with experimental seismic data, thereby enabling inferences of internal composition and structure to be made. It is understood that, whereas a knowledge of material composition may permit computation of wave velocities, the reverse is generally not possible. Useful inferences about composition may, however, be drawn from a knowledge of wavespeeds when combined with ancillary data, and a more complete theoretical treatment.

MATERIALS AND METHODS

While the WSD mixing algorithm may be applied to an arbitrary number of components, for didactic purposes two-component, solid-solution, examples are provided in the section on olivine (forsterite-fayalite) and pyroxene (enstatite-ferrosilite) [59-67]. These families are prominent constituents of the Earth's mantle; moreover, forsterite has been found in cometary dust of probable supernova ejecta origin [4]. The model does not depend on the constituents being members of a solid-solution family, only that the material assemblage be considered "isotropic" on the scale of the acoustic wavelengths used. General references to material properties, and methods of their determination are found in [68-86].

In view of their geological and planetary importance, VRHx values are included here for perovskite [87,88], post-perovskite [89-95], (both rhombic class mmm), and for α-alumina (trigonal class $\bar{3}$m) [96,97]. Least-squares fits are also provided for critical properties of α-alumina versus temperature. These enable rapid and accurate estimates of elasticities and velocities, etc., as function of temperature in a wide range.

Footnote: [1]The reader may perhaps forgive the classical illusion to "reaching for the stars." It seems not out of place to juxtapose the metaphorical dream of the ancients with the reality of the present.

[2]See Supplemental Information.

[3]By Helmholtz's Theorem, the elastic displacement vector may be decomposed into a divergenceless portion, derivable from a vector potential, and an irrotational part, derivable from a scalar potential. Some synonymous terms for plane bulk acoustic waves in solids of the vector type are: shear (S), transverse, equivoluminal, distortional, rotational, and solenoidal. Synonymous terms for those of the scalar type are: pressure (P), longitudinal, dilatational, compressional, extensional, and curl-free.

We anticipate that future applications of the WSD procedure will include other prominent mineral constituents such as:

(a) Garnets [98-101], a major component of Earth's mantle. The two main families, $Ca_3(Cr, A\ell, Fe)_2(SiO_4)_3$, and $(Mg, Mn, Fe)_3A\ell_2(SiO_4)_3$, crystallize in cubic point group m$\bar{3}$m.

(b) Periclase (MgO, m$\bar{3}$m), another abundant planetary mantle constituent [102-104].

(c) Spinel ($MgA\ell_2O_4$, m$\bar{3}$m), and m$\bar{3}$m analogs, such as peridotite $(Mg, Fe)(A\ell, Cr)_2O_4$ and pleonaste $(Mg, Fe)A\ell_2O_4$ [105].

(d) Topaz ($A\ell_2SiO_4F_2$, rhombic mmm) and $A\ell_2SiO_5$ analogs such as andalusite (mmm), sillimanite (mmm), and kyanite (triclinic $\bar{1}$) [106,107].

(e) Merrillite ($Ca_9NaMg(PO_4)_7$), which occurs prominently in extraterrestrial rocks, and whitlockite ($Ca_9Mg(PO_4)_6(PO_3OH)$. These are members of trigonal, acentric class 3m, rendering them both piezoelectric and pyroelectric [108-115].

Many mineral species of interest presently lack precision determinations of elastic constant values, not only at standard pressure and temperature, but particularly for those values existing at the ambient conditions where the minerals occur.

Crystal elasticities reduced to isotropy:

The Voigt-Reuss-Hill procedures [55-58] for space-averaging crystal elastic stiffnesses (Voigt) and compliances (Reuss) are not discussed in detail here.

In brief, stiffness ($c_{\lambda\mu}$) and compliance ($s_{\lambda\mu}$) = $(c_{\lambda\mu})^{-1}$ matrices are converted to isotropic matrix averages $\langle c_V \rangle$ and $\langle s_R \rangle$ via the relations (valid for the most general triclinic crystal):

Voigt:

$$\langle c_{11V} \rangle = [3\cdot(c_{11} + c_{22} + c_{33}) + 2\cdot(c_{12} + c_{13} + c_{23}) + 4\cdot(c_{44} + c_{55} + c_{66})]/15$$
$$\langle c_{44V} \rangle = [(c_{11} + c_{22} + c_{33}) - (c_{12} + c_{13} + c_{23}) + 3\cdot(c_{44} + c_{55} + c_{66})]/15$$
$$\langle c_{12V} \rangle = \langle c_{11V} \rangle - 2\cdot\langle c_{44V} \rangle$$

Reuss:

$$\langle s_{11R} \rangle = [3\cdot(s_{11} + s_{22} + s_{33}) + 2\cdot(s_{12} + s_{13} + s_{23}) + (s_{44} + s_{55} + s_{66})]/15$$
$$\langle s_{44R} \rangle = [4\cdot(s_{11} + s_{22} + s_{33}) - 4\cdot(s_{12} + s_{13} + s_{23}) + 3\cdot(s_{44} + s_{55} + s_{66})]/15$$
$$\langle s_{12R} \rangle = \langle s_{11R} \rangle - \langle s_{44R} \rangle/2$$

A self-consistent relaxation method (VRHx):

The Voigt and Reuss formulas produce upper and lower bounds on the elasticities of a given crystal of any anisotropy. Hill [57] found that an arithmetic average of the bounds agreed better with experiment in many cases. The VRH homogenization procedure has been augmented over the years by many variants; these improve on the VRH method, producing closer bounds, ability to incorporate measures of texture and inclusions, treatment of multiphase materials, etc. [116-145]. Any of these

advanced methods may be applied in the WSD model discussed in the next section. For the purpose of illustrating the WSD model here, a simple homogenization scheme, referred to as the self-consistent relaxation (VRHx) method [58] is applied to the Voigt and Reuss matrices c_V and s_R. It employs "interleaved averaging," iteratively relaxing the Voigt-Reuss extremes, to arrive at matrices such that $\langle s^x \rangle = \langle c^x \rangle^{-1}$, replacing bounds with consistent mean values.

The VRHx method begins with the Voigt stiffness matrix: $c_V = c_V^{(0)}$ and the Reuss compliance matrix: $s_R = s_R^{(0)}$. Each is then inverted to give $s_V^{(0)} = (c_V^{(0)})^{-1}$ and $c_R^{(0)} = (s_R^{(0)})^{-1}$. From these, the arithmetic (Hill) averages are formed: $c_{VR}^{(1)} = (c_V^{(0)} + c_R^{(0)})/2$ and $s_{RV}^{(1)} = (s_R^{(0)} + s_V^{(0)})/2$.

These are again inverted to yield: $s_{VR}^{(1)} = (c_{VR}^{(1)})^{-1}$ and $c_{RV}^{(1)} = (s_{RV}^{(1)})^{-1}$, and are further averaged via the inversions:
$s_{VR}^{(n)} = (c_{VR}^{(n)})^{-1}$ and $c_{RV}^{(n)} = (s_{RV}^{(n)})^{-1}$

and recursions:
$c_{VR}^{(n+1)} = (c_{VR}^{(n)} + c_{RV}^{(n)})/2$ and $s_{RV}^{(n+1)} = (s_{RV}^{(n)} + s_{VR}^{(n)})/2$.

The numerical process is doubly convergent, and rapidly yields "best" isotropic matrices, $\langle c^x \rangle$ and $\langle s^x \rangle = \langle c^x \rangle^{-1}$. From these coefficients and mass density, the S and P wave speeds for substance k are found:

$$V_{Pk} = \sqrt{(\langle c_{11k}{}^x \rangle / \rho_k)} \; V_{Sk} = \sqrt{(\langle c_{44k}{}^x \rangle / \rho_k)}.$$

The WSD additivity model

The model proposed here has its genesis in the Winkelmann-Schott work that was originally applied to glass mixtures [146]. The modern version is due to Dragic, who refined it, and successfully applied it to germanium doping of silica glass [147]. The Winkelmann-Schott-Dragic (WSD) model proceeds as follows: Given the mole fraction ($f_k^{(mol)}$), mass density (ρ_k), and molecular mass (M_k) of each constituent k, the corresponding volume fraction ($f_k^{(vol)}$), and weighted average mass density ($\rho^{(mix)}$) are first determined. For the simple two-component case the relations are:

$$(1/f_1^{(vol)} - 1) \cdot (\rho_2 / \rho_1) = (1/f_1^{(mol)} - 1).(M_2/M_1)$$
$$(f_1^{(vol)} + f_2^{(vol)}) = 1$$
$$\rho^{(mix)} = (\rho_1 . f_1^{(vol)} + \rho_2 . f_2^{(vol)}).$$

From the volume fraction of each isotropic constituent and its corresponding inverse wave speed [38,42], i.e., "slowness" ($1/V_{Sk}$, $1/V_{Pk}$), the transit time for an S or P wave traversing its fraction of a unit distance is determined; the sum over all components yields the total slowness associated with the S or P wave in the composite. Continuing the two-component example, the relations are:

$$1/V_P^{(mix)} = (1/V_{P1}).f_1^{(vol)} + (1/V_{P2}).f_2^{(vol)}$$
$$1/V_S^{(mix)} = (1/V_{S1}).f_1^{(vol)} + (1/V_{S2}).f_2^{(vol)}$$

Using both the S and P wavespeeds so determined, one finds the isotropic elastic constants of the mixture. Key here is the use of slownesses in determining average elasticities. Slowness is proportional to transit-time, and has a direct physical meaning, whereas the meanings of velocity averaging, or other criteria [52,53], are less obvious.

The elasticities of the composite, (introducing the Lamé constants λ, μ [37-39] that characterize isotropic media), are then

Isotropic stiffnesses:

$$\langle c_{11} \rangle = \rho^{(mix)} . (V_P^{(mix)})^2 = \lambda + 2\mu$$
$$\langle c_{44} \rangle = \rho^{(mix)} . (V_S^{(mix)})^2 = \mu$$
$$\langle c_{12} \rangle = \langle c_{11} \rangle - 2 . \langle c_{44} \rangle = \lambda$$

Young's modulus, $\langle Y \rangle = \mu(3\lambda + 2\mu)/(\lambda + \mu)$
Bulk modulus, $\langle K \rangle = \lambda + (2/3)\mu$
Poisson's ratio, $\langle \nu \rangle = \lambda/(3\langle K \rangle - \lambda)$

Isotropic compliances:

$$\langle s_{11} \rangle = 1/Y$$
$$\langle s_{44} \rangle = 1/\mu$$
$$\langle s_{12} \rangle = \langle s_{11} \rangle - \langle s_{44} \rangle /2 = - \langle s_{11} \rangle . \langle \nu \rangle.$$

The WSD procedure is given here only in schematic outline; as with the VRHx method, it can be generalized in various ways to accommodate texture, etc.

Application: Olivines and pyroxenes

The olivine series [59-66] consists of solid solutions between the end members forsterite (Mg_2SiO_4) and fayalite (Fe_2SiO_4). These crystalize in centric, rhombic point group mmm. Table 1 presents the WSD model results for 0(10)100 mole % of fayalite in fosterite. The pyroxene silicate solid solution series [67] extends from enstatite ($MgSiO_3$) to ferrosilite ($FeSiO_3$); all members also have mmm symmetry. Table 2, for ferrosilite in enstatite, is the complement to Table 1. In Table 1 and Table 2, the experimental data appearing in [83] have been used. Columns labeled "$\langle c_{mix} \rangle$" and "Θ_{Dmix}" in Tables 1 & 2, and subsequently in Table 7, are pertinent to the section on perovskite and post-perovskite, and are discussed there.

Reasonable agreement is seen in Table 3 (olivine) and Table 4 (pyroxene) between the WSD model predictions and experimental results. A more comprehensive comparison could not be made because of the paucity of experimental data; these results are from naturally occurring specimens containing admixtures of other substances [83]. In all cases the agreement is within < 5% (olivine) and < 8% (pyroxene). Given the vagaries of the natural samples, the agreement with the WSD model is encouraging, although an unqualified justification of the procedure cannot be adduced from these results.

Values reported in Tables 1-4 are for room temperature (RT), and zero applied pressure. The WSD procedure generalizes for conditions of spatially varying temperature and pressure. This requires a knowledge of the first- and higher-order temperature and pressure coefficients of the elasticities of the constituents.

Table 1: Room temperature WSD model predictions as function of mole % of fayalite in forsterite

Mole	Vol	ρ	M	V_S	V_P	$<c_{11}>$	$<c_{12}>$	$<c_{44}>$	$<c_{mix}>$	<K>	<Y>	<ν>	Θ_{Dmix}
%		Mg/m³	g/mole	km/s		GPa							K
fosterite	0	3.221	140.69	5.016	8.587	237.5	75.4	81.1	99.7	129.4	759.7	0.241	759.7
10	10.55	3.345	147	4.776	8.349	233.2	80.6	76.3	94.2	131.5	723.1	0.257	723.1
20	20.98	3.467	153.31	4.56	8.127	229	84.8	72.1	89.3	132.9	690.2	0.270	690.2
30	31.28	3.588	159.62	4.365	7.918	225	88.3	68.4	84.9	133.8	660.2	0.282	660.2
40	41.45	3.707	165.92	4.188	7.723	221.1	91	65	81	134.4	633	0.292	633
50	51.5	3.825	172.23	4.027	7.539	217.4	93.3	62	77.4	134.7	608.1	0.300	608.1
60	61.43	3.941	178.54	3.879	7.365	213.8	95.2	59.3	74.2	134.7	585.2	0.308	585.2
70	71.25	4.056	184.85	3.744	7.202	210.4	96.7	56.9	71.2	134.6	564.1	0.315	564.1
80	80.94	4.17	191.16	3.619	7.047	207.1	97.9	54.6	68.5	134.3	544.6	0.321	544.6
90	90.53	4.282	197.46	3.503	6.901	203.9	98.8	52.6	66	133.8	526.6	0.326	526.6
fayalite	100	4.393	203.77	3.396	6.762	200.8	99.5	50.7	63.7	133.3	509.8	0.331	509.8

Input values: [83]

Abbreviations: ρ: mass density; M: molecular mass; V_S, V_P: S and P wave speeds; $<c_{ij}>$: VRHx isotropic stiffnesses; $<c_{mix}>$: equivalent Debye stiffness; <K>, <Y>, <ν>: VRHx isotropic compressibility, Young's modulus, and Poisson's ratio; Θ_{Dmix}: equivalent Debye temperature

Table 2: Room temperature WSD model predictions as function of mole % of ferrosilite in enstatite

Mole	Vol	ρ	M	V_S	V_P	$<c_{11}>$	$<c_{12}>$	$<c_{44}>$	$<c_{mix}>$	<K>	<Y>	<ν>	Θ_{Dmix}
%		Mg/m³	g/mole	km/s		GPa							K
enstatite	0	3.198	100.39	4.864	8.078	733.1	57.3	75.7	92.5	107.8	184	0.216	733.1
10	10.45	3.282	103.54	4.694	7.884	707.1	59.3	72.3	88.6	107.6	177.2	0.225	707.1
20	20.8	3.365	106.7	4.537	7.7	683	61	69.3	85.1	107.2	171	0.234	683
30	31.04	3.448	109.85	4.392	7.527	660.6	62.3	66.5	81.8	106.6	165.2	0.242	660.6
40	41.18	3.529	113	4.257	7.363	639.7	63.4	64	78.8	106	159.7	0.249	639.7
50	51.22	3.61	116.16	4.131	7.207	620.3	64.3	61.6	76	105.4	154.7	0.255	620.3
60	61.17	3.69	119.31	4.014	7.059	602.1	65	59.4	73.5	104.6	149.9	0.261	602.1
70	71.02	3.769	122.47	3.904	6.919	585	65.6	57.4	71.1	103.8	145.5	0.267	585
80	80.77	3.847	125.62	3.801	6.785	569	66	55.6	68.8	103	141.3	0.271	569
90	90.43	3.925	128.77	3.704	6.658	553	66.3	53.8	66.8	102.2	137.4	0.276	553
ferrosilite	100	4.002	131.93	3.613	6.536	539.7	66.5	52.2	64.8	101.3	133.7	0.28	539.7

Input values: [83]

Abbreviations: ρ: mass density; M: molecular mass; V_S, V_P: S and P wave speeds; $<c_{ij}>$: VRHx isotropic stiffnesses; $<c_{mix}>$: equivalent Debye stiffness; <K>, <Y>, <ν>: VRHx isotropic compressibility, Young's modulus, and Poisson's ratio; Θ_{Dmix}: equivalent Debye temperature

Table 3: Comparison of WSD model predictions with experimental values reported in [83]

Mole	ρ	V_S	V_P	$<c_{11}>$	$<c_{44}>$	$<c_{mix}>$	<K>	<Y>
%	Mg/m³	km/s		GPa				
7.0 a	3.308	4.845	8.419	234.4	77.7	95.88	130.9	194.5
7.0 b	3.311	4.883	8.418	234.6	79	97.2	129.4	196.8
7.5 a	3.314	4.833	8.407	234.2	77.4	95.5	131	194
7.5 b	3.299	4.892	8.385	232	78.9	97.1	126.7	196.1
8.1 a	3.321	4.819	8.393	234	77.1	95.2	131.1	193.5
8.1 b	3.316	4.871	8.382	233	78.7	96.8	128.1	195.9
9.0 a	3.332	4.799	8.372	233.6	76.7	94.7	131.3	192.7
9.0 b	3.325	4.832	8.371	233	77.6	95.7	129.53	194.1

Mole % fayalite in forsterite.

Abbreviations: ρ: mass density; V_S, V_P: S and P wave speeds; $<c_{ij}>$: VRHx isotropic stiffnesses; $<c_{mix}>$: equivalent Debye stiffness; <K>, <Y>, < ν>: VRHx isotropic compressibility, Young's modulus, and Poisson's ratio. a: WSD prediction; b: experimental value (natural specimens)

Many of the requisite data are not yet available, but an example is provided in Table 5 for naturally occurring forsterite and olivine, using the data in [83].

Application: Perovskite and post-perovskite

Because it is considered a significant component of telluric bodies, [16-29], the VRHx procedure is applied to perovskite ($MgSiO_3$), with the results reported in Table 6. This table provides VRHx computations from the data of [87], and the simulations of [88,93,94], including those of the post-perovskite phase. Pressure- and temperature-coefficient estimations derived from [88,93,94] are also given.

Alumina

Another important geological and planetary constituent is alumina ($A\ell_2O_3$) in its various phases. The careful and accurate measurements of stiffnesses of α-alumina, (point group symmetry $\bar{3}$m), in an extended temperature range [96] have been used to compute the VRHx elasticities, and associated quantities, as a function of temperature in the range 300 to 1800K. The results are expressed here as coefficients of power series expansions in temperature. The coefficients $T^{(n)}$ are derived from least-squares fits of values tabulated at 50K intervals in the cited range.

Table 4: Comparison of WSD model predictions with experimental values reported in [83]

Mole	ρ	V_S	V_P	$<c_{11}>$	$<c_{44}>$	$<c_{mix}>$	<K>	<Y>
%	Mg/m^3	km/s		GPa				
06 a	3.249	4.761	7.96	205.8	73.6	90.2	107.7	179.9
06 b	3.272	4.753	7.834	200.8	73.9	90.3	102.3	178.7
15.2 a	3.325	4.611	7.787	201.6	70.7	86.7	107.4	173.9
15.2 b	3.335	4.749	7.845	205.2	75.2	91.9	105	182.1
20 a	3.365	4.537	7.7	199.5	69.3	85.1	107.2	171
20 b	3.354	4.72	7.781	203.1	74.7	91.2	103.5	180.7
Mole % ferrosilite in enstatite								

Abbreviations: ρ: mass density; V_S, V_P: S and P wave speeds; $<c_{ij}>$: VRHx isotropic stiffnesses; $<c_{mix}>$: equivalent Debye stiffness; <K>, <Y>, <v>: VRHx isotropic compressibility, Young's modulus, and Poisson's ratio. a: WSD prediction; b: experimental value (natural specimens)

Table 5: First-order temperature ($Tc^{(1)}$) and pressure ($Pc^{(1)}$) coefficients of elastic stiffnesses ($c_{\lambda\mu}$) of naturally occurring forsterite and olivine; input data: [83]

forsterite	$(Mg_2SiO_4)_{99.9}(Mn_2SiO_4)_{0.01}$; ρ = 3,224 [kg/m³]								
λμ ⟶	11	22	33	44	55	66	23	31	12
$Tc^{(1)}$	100.8	140.6	120.3	199.5	162.6	186.7	62.3	119.2	162.8
$Pc^{(1)}$	25.8	32.8	27.9	32.5	20.4	29.3	55.7	70.3	73.1
olivine	$(Mg_2SiO_4)_{92.72}(Fe_2SiO_4)_{7.24}(Mn_2SiO_4)_{0.04}$; ρ = 3,311 [kg/m³]								
λμ ⟶	11	22	33	44	55	66	23	31	12
$Tc^{(1)}$	105	144.2	121.7	198.1	166.6	198.6	67.5	131.3	158.1
$Pc^{(1)}$	24.7	32.2	27.1	33.6	21	29.2	49.7	62.6	71.4

Abbreviations:
ρ: mass density
First-order temperature coefficient of elastic stiffness: $Tc^{(1)} = (\Delta c/\Delta T)/c$ in [ppm/K]
First-order pressure coefficient of elastic stiffness: $Pc^{(1)} = (\Delta c/\Delta P)/c$ in [1/TPa]

Table 6: VRHx algorithm applied to measured [87] and simulated [88,93,94] stiffness values at 120 GPa for perovskite and post-perovskite

perovskite $MgSiO_3$ (M = 100.39 g/mole)							
ρ	V_S	V_P	$<c_{11}>$	$<c_{12}>$	$<c_{44}>$	$<c_{mix}>$	Ref.
Mg/m^3	km/s		GPa				
5.332 [94]	7.682	13.981	1042.3	413	314.7	391	[88]
5.332 [94]	7.45	13.63	990.6	398.8	295.9	368	[93]
5.332 [94]	7.675	14.186	1073	444.8	314.1	391.2	[93]
5.332 [94]	7.942	14.579	1133.3	460.7	336.3	418.5	[88]
5.332 [94]	7.635	14.115	1062.4	440.7	310.8	387.1	[94]
4.108 [87]	6.692	10.937	491.4	123.5	184	224.2	[87]
$Tc^{(1)}$ (10^{-6}/K) ⟶			-3.29	-3.08	-3.44		[94]
$Pc^{(1)}$ (1/TPa) ⟶			4.16	5.78	3.07		[93]
post-perovskite $MgSiO_3$ (M = 100.39 g/mole)							
ρ	V_S	V_P	$<c_{11}>$	$<c_{12}>$	$<c_{44}>$	$<c_{mix}>$	Ref.
Mg/m^3	km/s		GPa				
5.407 [94]	7.525	13.62	1003	390.7	306.2	380.1	[93]
5.407 [94]	7.835	14.279	1102.4	438.6	331.9	412.5	[93]
5.407 [94]	7.781	14.157	1083.7	428.9	327.4	406.8	[94]
$Tc^{(1)}$ (10^{-6}/K) ⟶			-5.67	-7.36	-4.56		[94]
$Pc^{(1)}$ (1/TPa) ⟶			4.95	6.13	4.2		[93]

Abbreviations:
First-order temperature coefficient of elastic stiffness: $Tc^{(1)} = (\Delta c/\Delta T)/c$
First-order pressure coefficient of elastic stiffness: $Pc^{(1)} = (\Delta c/\Delta P)/c$
ρ: mass density; M: molecular mass; V_S, V_P: S and P wave speeds; $<c_{ij}>$: VRHx isotropic stiffnesses; $<c_{mix}>$: equivalent Debye stiffness.

Each quantity y(T), appearing in Tables 8, 9, and 10, is computed as follows:

$$\Delta y(T)/y_0 = T_y^{(0)} + T_y^{(1)}\,\Delta T + T_y^{(2)}\,(\Delta T)^2 + T_y^{(3)}\,(\Delta T)^3 + T_y^{(4)}\,(\Delta T)^4,$$

where $\Delta y(T) = (y(T) - y_0)$, $\Delta T = (T - T_0)$, and $y_0 = y(T_0)$.

In Tables 9 and 10, T_0 = 296K; superscript "x" refers to values obtained from the VRHx procedure. The units of the temperature coefficients $T^{(n)}$ are $10^{-3(n+1)}/K^n$; the correlations of the curve-fits with the tabulated values in each instance yields a goodness-of-fit $R^2 > 99.9\%$.

Debye temperature

The Debye temperature (Θ_D) [148] is used in considerations of specific heats of elastic solids. It provides a quantitative estimate demarcating classical (Dulong-Petit) and quantum regimes. For our purposes, it affords a simple indication that the VRHx results agree with a more accurate computation [149]. The Debye procedure globally averages the three plane acoustic wave speeds in a crystal over all propagation directions. In terms of the space-averaged elastic stiffness (c_m) characterizing wave m, the requisite Debye expression is:

Table 7: VRHx algorithm applied to measured [87] and simulated [88,93,94] elastic values for perovskite and post-perovskite

perovskite $MgSiO_3$ (M = 100.39 g/mole)										
ρ	$<s_{11}>$	$<s_{12}>$	$<s_{44}>$	<K>	<Y>	< ν >	Θ_{Dmix}	T	P	Ref.
Mg/m^3	1/TPa			GPa			K		GPa	
5.332 [94]	1.238	-0.351	3.178	622.7	807.9	0.284		0	100	[88]
5.332 [94]	1.313	-0.377	3.38	596	761.7	0.287	1347	0	100	[93]
5.332 [94]	1.231	-0.361	3.184	654.2	812.2	0.293	1389	0	120	[93]
5.332 [94]	1.153	-0.333	2.973	684.9	867	0.289		0	120	[88]
5.332 [94]	1.244	-0.365	3.217	647.9	803.9	0.293	1380	3,000	120	[94]
4.108 [87]	2.264	-0.455	5.436	246.1	441.8	0.201	1091	300	0	[87]
post-perovskite $MgSiO_3$ (M = 100.39 g/mole)										
ρ	$<s_{11}>$	$<s_{12}>$	$<s_{44}>$	<K>	<Y>	<ν>	Θ_{Dmix}	T	P	Ref.
Mg/m^3	1/TPa			GPa			K		GPa	
5.407 [94]	1.275	-0.358	3.266	594.8	784	0.280	1325	0	100	[93]
5.407 [94]	1.173	-0.334	3.013	659.9	852.8	0.285	1383	0	120	[93]
5.407 [94]	1.19	-0.337	3.055	647.2	840.4	0.284	1371	3,000	120	[94]

Abbreviations:
First-order temperature coefficient of elastic stiffness: $Tc^{(1)} = (\Delta c/\Delta T)/c$
First-order pressure coefficient of elastic stiffness: $Pc^{(1)} = (\Delta c/\Delta P)/c$
ρ: mass density; $<s_{ij}>$, <K>, <Y>, <ν>: VRHx isotropic compliances, compressibility, Young's modulus, and Poisson's ratio; Θ_{Dmix}: equivalent Debye temperature; T: temperature; P: pressure.

Table 8: Higher-order temperature coefficients of elastic stiffnesses and compliances of α-$A\ell_2O_3$

GPa	$c_{\lambda\mu}$ (RT)	$T^{(0)}$	$T^{(1)}$	$T^{(2)}$	$T^{(3)}$	$T^{(4)}$
c_{11}	497.3	+1.198488	−64.460817	−50.110218	+28.337272	−5.501432
c_{33}	500.9	+0.176642	−71.486857	−15.490214	−9.699813	+7.521084
c_{44}	146.8	+0.717945	−165.017400	−28.311180	−15.398713	−1.804866
c_{12}	163.8	+0.170563	−4.211675	−21.881483	−0.862603	+4.668163
c_{13}	116	+1.530500	−86.598114	+17.459421	−72.519021	+37.063488
c_{14}	-21.9	+9.442588	+238.788360	−252.815870	+166.215030	−47.879821
c_{66}	166.75	+1.703358	−94.052449	−63.974887	+42.678919	−10.496273
1/TPa	$s_{\lambda\mu}$ (RT)	$T^{(0)}$	$T^{(1)}$	$T^{(2)}$	$T^{(3)}$	$T^{(4)}$
s_{11}	2.3524297	-1.128903	+85.615147	+67.357057	-30.874116	8.297397
s_{33}	2.1730056	-0.018508	+67.276682	+26.211000	+2.906003	-3.215423
s_{44}	6.9481222	-0.350667	+179.500980	+53.505900	+5.694479	-2.355433
s_{12}	-0.7059941	-2.053974	+182.558470	+92.611856	-23.083560	+5.874893
s_{13}	-0.3812867	+0.811997	+24.693309	+107.382030	-124.548690	+49.903673
s_{14}	0.4562635	+7.396371	+515.499870	-57.316463	+152.578980	-46.226595
s_{66}	6.1168476	-1.342452	+107.993250	+73.186583	-29.075665	+7.738180

Input data: [96]

Abbreviations:
Nth-order temperature coefficient of elastic stiffness: $Tc^{(n)} = (\Delta c/\Delta T)/(n!\ c)$
Nth-order temperature coefficient of elastic compliance: $Ts^{(n)} = (\Delta s/\Delta T)/(n!\ s)$

$c_D = [(c_a^{-3/2} + c_b^{-3/2} + c_c^{-3/2})/3]^{-2/3}$.

The VRHx algorithm also produces a global space averaging; the resultant equivalent elastic stiffness corresponding to c_D is:

$<c^x> = <c_{mix}> = [(<c_{11}>^{-3/2} + 2\ .\ <c_{44}>^{-3/2})/3]^{-2/3}$.

For the VRHx (and consequently the WSD) procedures to render accurate results it is necessary that $c^x \approx c_D$. The Debye temperature of a single component, linearly elastic solid is given by:

$\Theta_D = (h/k)\ .\ V\ .\ [(3qN\rho)/(4\ \pi M)]^{1/3}$,

where h is Planck's constant, k is Boltzmann's constant, q is the number of atoms in the molecule, ρ is the mass density, N is

Table 9: Higher-order temperature coefficients of elastic stiffnesses, compliances and mass density of α-$A\ell_2O_3$ reduced to isotropy by the VRHx procedure

GPa	c^x(RT)	$T^{(0)}$	$T^{(1)}$	$T^{(2)}$	$T^{(3)}$	$T^{(4)}$
c_{11}^x	471.210551	0.865804	-89.332734	-32.859794	9.143476	1.555329
c_{12}^x	145.306373	0.918558	-18.785851	-9.431711	-29.923438	18.090020
c_{44}^x	162.952089	0.842297	-120.786410	-43.305726	26.562106	-5.816879
Y^x	402.716269	0.842664	-110.330780	-41.182737	21.843169	-3.811046
K^x	253.941099	0.885934	-62.421180	-23.922837	-5.759213	7.862764
ν^x	0.235689	0.152056	51.411132	31.223218	-37.961271	15.609018
1/TPa	**s^x(RT)**	**$T^{(0)}$**	**$T^{(1)}$**	**$T^{(2)}$**	**$T^{(3)}$**	**$T^{(4)}$**
s_{11}^x	2.483138	-0.824258	109.806000	54.521691	-12.786087	2.196537
s_{12}^x	-0.585249	-0.691949	161.489570	91.890974	-49.250966	18.943261
s_{44}^x	6.1367731	-0.799026	119.663740	61.649617	-19.741494	5.390812
Mg/m³	**ρ(RT)**	**$T^{(0)}$**	**$T^{(1)}$**	**$T^{(2)}$**	**$T^{(3)}$**	**$T^{(4)}$**
ρ	3.982	0.053034	-17.093205	-15.079869	10.240228	-2.549397
Input data: [96]						
Abbreviations: Nth-order temperature coefficient of elastic stiffness: $Tc^{(n)} = (\Delta c/\Delta T)/(n!\ c)$ Nth-order temperature coefficient of elastic compliance: $Ts^{(n)} = (\Delta s/\Delta T)/(n!\ s)$						

Table 10: Higher-order temperature coefficients of acoustic longitudinal and shear velocities and Debye temperatures of α-$A\ell_2O_3$ reduced to isotropy by the VRHx procedure

km/s	V_P^x, V_S^x(RT)	$T^{(0)}$	$T^{(1)}$	$T^{(2)}$	$T^{(3)}$	$T^{(4)}$
V_P^x	10.8781959	0.409514	-36.177269	-9.759152	-2.308254	2.633480
V_S^x	6.397044	0.388270	-51.670599	-16.983074	7.264243	-1.462067
K	**Θ_D, Θ_x**	**$T^{(0)}$**	**$T^{(1)}$**	**$T^{(2)}$**	**$T^{(3)}$**	**$T^{(4)}$**
Θ_D	1026.4758	0.349702	-59.713768	-18.890236	8.128135	-1.394143
Θ_x	1034.1824	0.408064	-55.945675	-21.109861	10.016589	-2.001376
Input data: [96]; Θ_D computed using procedure in [150]						
Abbreviations: V_S^x, V_P^x: S and P wave speeds; K: isotropic compressibility; Θ_D and Θ_x: equivalent Debye temperatures						

Avogadro's number, and M is the molecular mass. V is the average acoustic wave speed: $V = (C/\rho)^{1/2}$, where C is either c_D, ($\Theta = \Theta_D$), the true average elastic stiffness, or $<c_{mix}>$, ($\Theta = \Theta_{Dmix}$), the VRHx approximate average elastic stiffness. For mixtures, appropriate average values of ρ, q, and M are used.

The classical Debye procedure averages each of the three elastic plane wave velocities over all space directions. As a practical computational matter, this necessitates covering a sphere with a grid of finite patches, computing the velocities at a convenient point within each patch, then summing the result over all patches to approximate the true values that would be obtained in the limit as the patch sizes diminish to zero. Depending on the grid size and shape, this has, in the past, resulted in either a loss of accuracy, or excessive computational effort. The essential difficulty is the impossibility of uniformly tessellating a sphere, familiar as the "dimples on a golf ball" situation. However, an accurate and efficient algorithm based on Fibonacci sequences [150] has been used to arrive quickly at accurate results for c_D to compare with $<c_{mix}>$. Using F_{20} = 6,765 averaging points, Table 10 gives an example for α-$A\ell_2O_3$; Θ_D and Θ_x agree within 0.75%. This is a representative value; the agreement in all cases is within a few percent.

SUMMARY

A simple computational procedure (VRHx) relaxing single crystal elastic constants in a self-consistent manner has been used to obtain equivalent isotropic elastic stiffnesses of microcrystalline aggregates, such as those that commonly occur in exogeologic bodies. These coefficients, for each mineral, are then combined with those of all other constituents in a "mixing" algorithm to yield effective elastic parameters characterizing both seismic wave propagation and quasi-static deformations in the mineral composite.

Data from the literature are used to compute simulants for olivines: forsterite- fayalite, and for the pyroxenes: enstatite-ferrosilite, as examples of the WSD mixing procedure. The VRHx algorithm is further applied to other geological constituents: perovskite, post-perovskite, and alumina. Variations with pressure and temperature are also considered.

SUPPLEMENTAL INFORMATION

The thrusts of this paper are introduction of a simple homogenization procedure converting crystal elasticity data to

isotropic values, and use thereof in a physically realistic mixing formula that provides a rapid estimate of acoustic properties.

It is suitable for use with much more sophisticated and elegant programs, such as BurnMan [A1-A3] and Perplex [A4-A8], that are available for producing detailed and accurate phase diagrams, phase equilibria, and extensive thermodynamic data of mineral mixtures.

Elastic nonlinearities, whose treatment in its modern form began with Francis Murnaghan [A9], is also incorporated in the advanced programs. Tables 5 to 10 of the present paper contain some pressure and temperature derivatives of elasticities of selected minerals. These are illustrative of what may be gleaned from the present procedure, and can be used with the advanced algorithms [A1, A4].

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DISCLOSURE

The authors declare no conflicts of interest.

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