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Key Points:

- First report of high pressure elasticity of chlorite
- Unusual shear wave anisotropy for chlorite
- Shear elastic anisotropy explains seismological observations in subduction zones

Supporting Information:

- Text S1
- Figure S1

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Unusually large shear wave anisotropy for chlorite in subduction zone settings

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Abstract Using first principle simulations we calculated the elasticity of chlorite. At a density $\rho \sim 2.60 \text{ g cm}^{-3}$, the elastic constant tensor reveals significant elastic anisotropy: $V_p \sim 27\%$, $V_{S1} \sim 56\%$, and $V_{S2} \sim 43\%$. The shear anisotropy is exceptionally large for chlorite and enhances upon compression. Upon compression, the shear elastic constant component C_{44} and C_{55} decreases, whereas C_{66} shear component stiffens. The softening in C_{44} and C_{55} is reflected in shear modulus, G , and the shear wave velocity, V_S . Our results on elastic anisotropy at conditions relevant to the mantle wedge indicates that a 10–20 km layer of hydrated peridotite with serpentine and chlorite could account for the observed shear polarization anisotropy and associated large delay times of 1–2 s observed in some subduction zone settings. In addition, chlorite could also explain the low V_p/V_S ratios that have been observed in recent high-resolution seismological studies.

1. Introduction

Chlorite, $\text{Mg}_5\text{Al}(\text{Si}_3\text{Al})\text{O}_{10}(\text{OH})_8$, is a layered hydrous silicate mineral with $\sim 13 \text{ wt } \%$ water stored in its crystallographic sites. It is an alteration product that is stabilized in the hydrated oceanic lithosphere, metasomatized mantle rocks, and hydrated mantle wedge. Phase equilibria studies indicate that chlorite is stable up to a temperature of 800–820°C and pressures of 2.0–3.6 GPa [Pawley, 2003; Fumagalli and Poli, 2005; Grove et al., 2006; Dvir et al., 2011; Till et al., 2012]. Upon subduction, the hydrous phases stable in the hydrated lithosphere become thermodynamically unstable and undergo dehydration [Ulmer and Trommsdorff, 1995; Schmidt and Poli, 1998; Iwamori, 1998, 2007; Pawley, 2003; Grove et al., 2006]. Dehydration of these hydrous phases, including chlorite has been related with the *seismogenic* activities along the double Benioff zones [Burdzinski et al., 2007]. In addition fluids are also released by the dehydration of the subducting sediments. The released fluid migrates upward, rehydrates cooler and shallow parts of the slab-wedge interface where hydrous minerals such as serpentine and chlorite are stabilized [Till et al., 2012; Grove et al., 2012]. A fertile peridotite has sufficient Al_2O_3 to stabilize 6 to 7 wt % chlorite in the hydrated lithosphere and in the basal region of the upper mantle wedge [Grove et al., 2012]. Low-velocity layers, observed in seismic images of Honshu subduction zone system [Kawakatsu and Watada, 2007], have been interpreted to indicate the presence of hydrous phases such as chlorite and serpentine in the shallow mantle wedge. Despite the importance of chlorite for our understanding of upper mantle structure and dynamics, little is known of its atomic structure and elasticity at high pressure. What is the effect of pressure on the elastic anisotropy of chlorite? Could elasticity and anisotropy of chlorite explain the (a) observed large delay time ($\sim 1\text{--}2 \text{ s}$) between arrival of the two shear waves V_{S1} and V_{S2} , in certain subduction zones [Long and van der Hilst, 2006; Long and Silver, 2008], (b) the range of V_p/V_S ratios observed in the mantle wedge [Hacker and Abers, 2012]? To address these fundamental questions, we explore the full elastic constant tensor and anisotropy of chlorite at conditions relevant to mantle wedge.

2. Method

Static, density functional theory (DFT) calculations [Hohenberg and Kohn, 1964; Kohn and Sham, 1965] were performed with Vienna ab initio simulation package [Kresse and Hafner, 1993; Kresse and Furthmüller, 1996a, 1996b; Kresse and Joubert, 1999]. The generalized gradient approximation (GGA) [Perdew et al., 1996] and highly accurate projector augmented wave method [Kresse and Joubert, 1999] were used for all calculations. We investigated chlorite, with 72 atoms in a formula unit with $\text{Mg}_5\text{Al}(\text{Si}_3\text{Al})\text{O}_{10}(\text{OH})_8$ stoichiometry. We used an energy cutoff $E_{\text{cut}} = 600 \text{ eV}$, and a Monkhorst-Pack [Monkhorst and Pack, 1976] $2 \times 2 \times 2$ k -point mesh. A series of convergence tests demonstrated that these computational parameters

Table 1. Equation-of-State Parameters for Chlorite

${}^a E_0$ (eV)	${}^b \sigma_{E0}$	V_0 (\AA^3)	σ_{V0}	K_0 (GPa)	σ_{K0}	K'	$\sigma_{K'}$	P_{\max} (GPa)	Method
-461.22	0.005	715.1	0.313	74.7	1.7	6.6	0.6	15.0	GGA ^c
		703.5	0.160	72.3	2.4	5.4	1.0	6.5	NPD ^d
		703.4	0.400	71.0	0.9	8.0	0.5	5.5	SCXRD ^e
		701.3	0.190	83.4	0.7			3.6	SXRPD ^f
		702.6	0.400	55.0	10.0			4.0	SCXRD ^g

^a E_0 refers to the ground state energy from first principles.

^b σ refers to the error associated with the parameters.

^cGGA: Generalized Gradient Approximation (this study).

^dNPD: neutron powder diffraction [Welch and Marshall, 2001].

^eSCXRD: Single-Crystal X-ray diffraction [Zanazzi et al., 2007].

^fSXRPD: Synchrotron X-ray powder diffraction [Pawley et al., 2002].

^gSCXRD: Single-Crystal X-ray diffraction [Hazen and Finger, 1978].

yield total energies that are converged to within 0.2 meV. We analyze bulk compression behavior using the third-order Birch Murnaghan equation of state [Birch, 1978]. Full elastic constant tensor was determined by straining the lattice by 1%, the details of the methods are described in Karki et al. [2001]. Finite strain fits to the elasticity data, computation of isotropic bulk (K) and shear (G) moduli were made using the finite strain formulations as in Karki et al. [2001]. Previous studies have shown that DFT captures the relevant physics of hydrous minerals [Mookherjee and Stixrude, 2006, 2009; Mainprice et al., 2007; Tsuchiya and Tsuchiya, 2009; Chantel et al., 2012; Mookherjee and Bezacier, 2012] with varying bond strengths from strong hydroxyl to weak interlayer forces [Mainprice et al., 2008; Mookherjee and Capitani, 2011; Militzer et al., 2011]. We computed the single-crystal azimuthal anisotropy for P and S waves in chlorite using the formulation for maximum polarization anisotropy [Mainprice, 1990].

3. Results

Previously reported equation-of-state parameters for chlorite exhibit large variations (Table 1). In particular, the zero pressure value of the bulk modulus ranges from 55.0 (± 10.0) GPa [Hazen and Finger, 1978] to 83.4 (± 0.7) GPa [Pawley et al., 2002]. This is likely to translate to more than 50% difference in the bulk sound velocity, since the variation in the zero pressure volume between these different sets of experiments is less than 0.3%. The pressure-volume relation and the variation of lattice parameters under compression for chlorite determined using DFT provides tighter constraints on the equation-of-state parameter. The pressure-volume results from DFT for chlorite are well represented by a finite strain formulation, with $K_0 = 74.7$ (± 1.7) GPa and $K'_0 = 6.6$ (± 0.6). The equation-of-state parameter based on DFT within GGA is in good agreement with recent experimental studies [Welch and Marshall, 2001; Zanazzi et al., 2007] (Figure 1 and Table 1). The static zero pressure volume within GGA is 1.7% greater and the zero pressure value of the bulk modulus within GGA is 5.2% greater than the room temperature single-crystal X-ray diffraction experimental value [Zanazzi et al., 2007]. We used a Cartesian reference frame for the elastic tensor of $X = a$, $Y = b$, and $Z = c^*$. The linear moduli along a , b , and c^* axis directions are $K_a = 258$ (± 6.8), $K_b = 280.2$ (± 4.7), and $K_{c^*} = 155.4$ (± 6.4) GPa, respectively, in good agreement with a recent single-crystal X-ray diffraction study [Zanazzi et al., 2007] (Table 2). The calculated elastic constants show substantially softer elasticity along the stacking direction (c^*) (Table 3 and Figure 2). The elastic constants also exhibit striking anisotropy at ambient pressures. At ambient pressures, $C_{11} \sim C_{22}$ is 1.4 times greater than C_{33} , reflecting weaker bonding along [001] direction. The principle elastic moduli, C_{33} , increases

Table 2. Lattice Parameters and Linear Moduli for Chlorite

a_0 (\AA)	σ_{a0} ^a	K_a (GPa)	σ_{K_a}	b_0 (\AA)	σ_{b0}	K_b (GPa)	σ_{K_b}	c_0 (\AA)	σ_{c0}	K_c (GPa)	σ_{K_c}	Method
5.3624	0.0001	258.00	6.8	9.292	0.001	280.2	4.7	14.367	0.01	155.4	67.4	GGA ^b
5.3363	0.0009	263.15	0.3	9.240	0.001	277.8	0.3	14.265	0.03	185.2	0.9	SCXRD ^c

^a σ refers to the error associated with the parameters.

^bGGA: Generalized Gradient Approximation (this study).

^cSCXRD: Single-Crystal X-ray diffraction [Zanazzi et al., 2007].

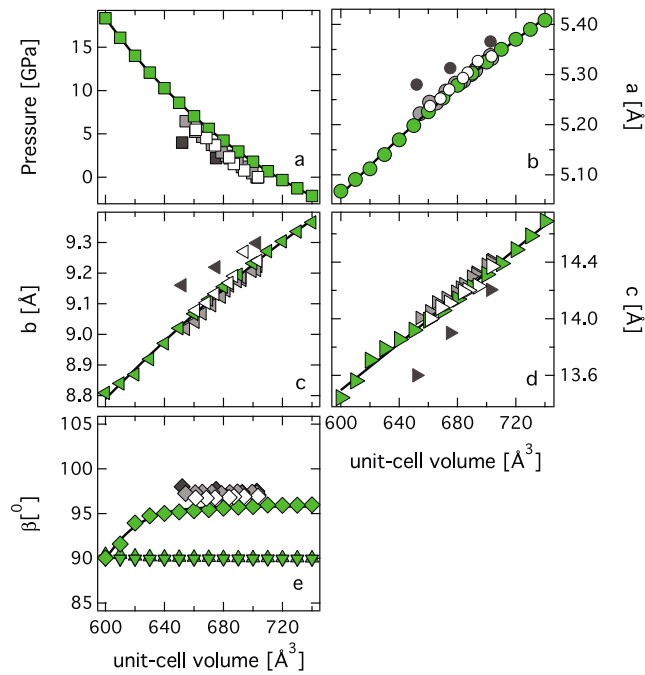


Figure 1. Plot of (a) pressure, (b) *a* axis, (c) *b* axis, (d) *c* axis, and (e) lattice parameter β versus unit-cell volume. Result from the simulations (GGA) (this study) is denoted with “light green filled symbols” and compared with previous X-ray diffraction results denoted by “dark grey” [Hazen and Finger, 1978], “light grey symbols” [Welch and Marshall, 2001], and “white” symbols [Zanazzi et al., 2003]. The black lines denote finite strain fits.

rapidly upon compression, with $\partial C_{33}/\partial P \sim 14$ (Table 3). This is similar to other layered hydrous phases including serpentine and talc [Mookherjee and Stixrude, 2009; Mookherjee and Capitani, 2011; Bezacier et al., 2013]. The strong anisotropy is also reflected in shear elastic constants via the ratio C_{66}/C_{44} , where C_{66} governs shear deformation of the T-O sheets, and C_{44} shear sliding of sheets across each other. The C_{66}/C_{44} ratio increases from 2.8 at ambient conditions to 4.2 at 7 GPa. The principal elastic constants of chlorite increase monotonically with pressure until ~ 10 GPa. Above 10 GPa, the pressure dependence of the elastic constants exhibits anomalous behavior (Figure 2). Previous experimental studies have given some indications of anomalous compressional behavior in chlorite related to the behavior of protons upon compression [Kleppe et al., 2003; Welch et al., 2004]. In agreement with the experiments, we do observe reorientation of the protons upon compression (Figure S1 in the supporting information). Orientation-averaged isotropic bulk and shear moduli, and the compressional and shear wave velocities are in good agreement with our computed equation of state, and with experimental measurements (Figure 2).

Table 3. Pressure Dependence of the Full Elastic Constant Tensor (C_{ij}), Bulk (K), and Shear (G) Modulus for Chlorite Using *First Principles* Simulations^a

V	ρ	P	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{23}	C_{15}	C_{25}	C_{35}	C_{46}	K	G
(\AA^3)	(g/cm^3)		(GPa)														
720	2.53	-0.3	197.8	202.3	135.1	24.5	24.4	70.3	60.7	21.1	34.1	3.3	0.2	0.4	0.1	82.6	45.7
700	2.60	1.8	202.0	199.7	152.7	23.9	23.9	72.0	58.0	22.4	27.3	3.4	-0.3	0.7	0.5	83.9	46.8
680	2.67	4.2	199.4	204.7	198.2	23.0	20.9	73.8	56.6	34.5	40.3	3.9	0.0	1.4	0.1	95.9	46.5
660	2.75	7.0	209.8	207.1	233.4	17.9	16.5	74.8	60.3	45.2	49.5	4.4	-0.5	2.7	-0.2	106.5	43.5
640	2.84	10.3	220.5	216.1	284.5	11.8	11.8	76.6	66.7	66.2	70.0	6.1	1.2	5.0	0.2	123.6	39.3
620	2.93	14.0	236.2	229.8	316.3	6.7	11.6	77.7	77.1	77.0	78.8	10.5	4.1	10.0	2.0	134.6	36.9
600	3.03	18.4	251.0	240.6	299.8	21.8	32.4	79.6	84.5	77.3	73.1	20.0	4.6	22.0	3.8	136.2	53.7
<i>Finite Strain Fit</i>																	
715	2.54	0	198.4	197.7	138.1	25.9	24.6	71.0	57.3	14.0	19.6	3.0	-0.5	0.1	0.1	79.2	47.4
			(2.0)	(1.6)	(14.2)	(-1.2)	(-1.2)	(0.5)	(0.4)	(4.7)	(4.9)	(0.2)	(0.1)	(0.4)	(0.01)	(3.7)	(-0.3)

^aIn addition, the finite strain fit results are also tabulated. The values in the bracket () denote the pressure derivatives dC_{ij}/dP .

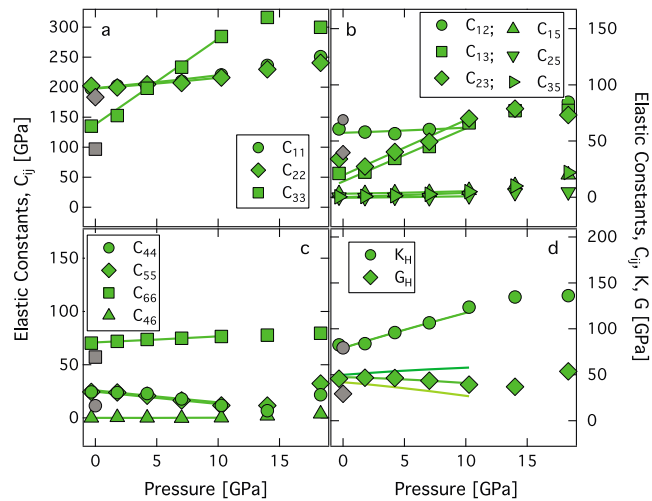


Figure 2. Elastic constants (C_{ij}) as a function of pressure, (a) compressional components, C_{11} , C_{22} , and C_{33} ; (b) off-diagonal components, C_{12} , C_{13} , C_{23} , C_{15} , C_{25} , and C_{35} ; (c) shear components, C_{44} , C_{55} , C_{66} , and C_{46} ; and (d) plot of bulk (K) and shear (G) modulus versus pressure. The “green” symbols refer to the predictions from simulation (this study), the grey symbols refer to the room pressure data [Alexandrov and Ryzhova, 1961]. In Figure 2d, subscript “H” refers to the Hill average. Finite strain fits for Voigt, Hill, and Ruess limits are plotted. For the bulk (K) modulus, the Voigt and Ruess bounds are tighter, for the shear (G) modulus, the bounds are divergent with Voigt bounds shown in “dark green” line and the Ruess bounds are shown in “light green” line. The lines refer to the finite strain fit up to 10 GPa beyond which the pressure dependence of elasticity exhibits anomalous behavior.

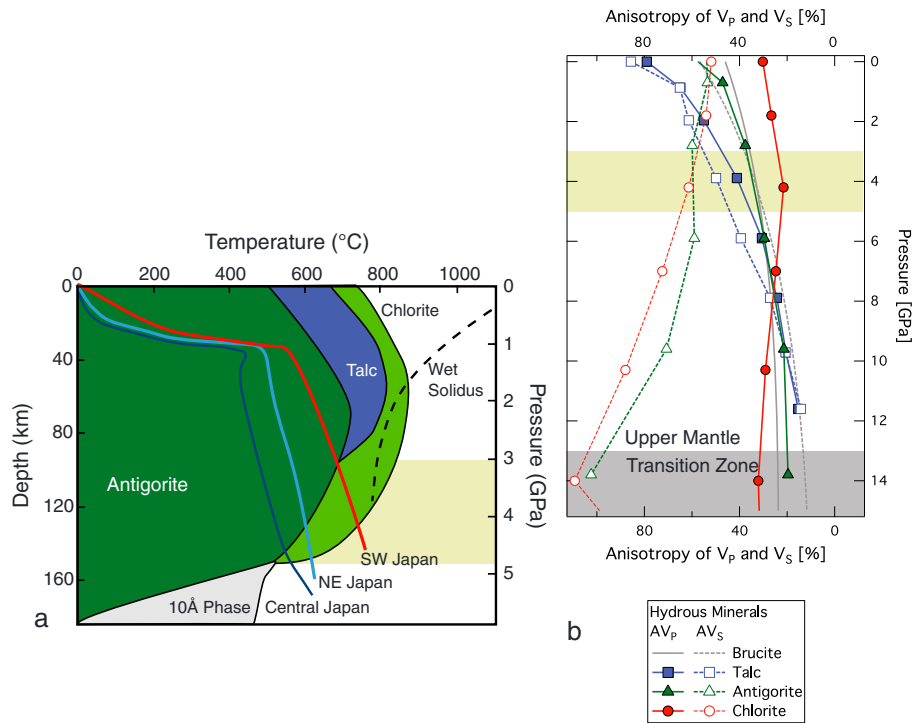


Figure 3. (a) Thermodynamic stability of hydrous phases including, antigorite [Ulmer and Trommsdorff, 1995], chlorite [Grove et al., 2006], talc [Pawley and Wood, 1995], and 10 Å phase [Fumagalli and Poli, 2005]. Also shown are the subduction geotherms [Iwamori, 2007], the “light green” band indicates the depth range of stability of chlorite and (b) plot of seismic anisotropy of various hydrous phases including, brucite [Jiang et al., 2006], antigorite [Mookherjee and Capitani, 2011], talc [Mainprice et al., 2008], and chlorite (this study). We note that the S wave anisotropy for antigorite and chlorite increases dramatically under compression. The depth range of stability for chlorite is indicated with the light green band.

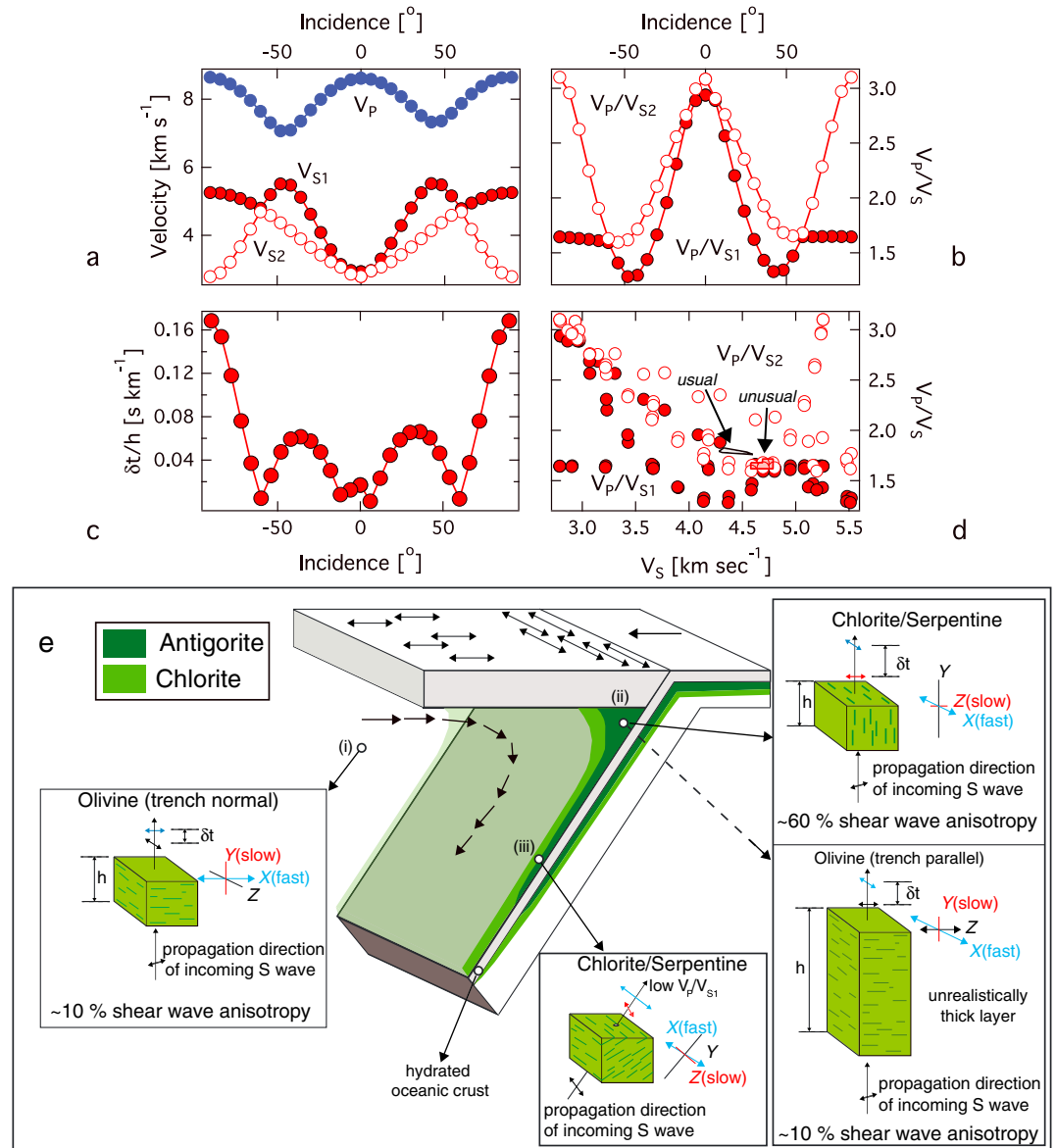


Figure 4. Anisotropy of chlorite variation of (a) V_P , V_{S1} , and V_{S2} ; (b) V_P/V_{S1} and V_P/V_{S2} ; (c) delay time/layer thickness, $\delta t/V_S/(V_{S1} \times V_{S2})$, as a function of the angle of incidence with respect to [001] plane of chlorite at condition relevant to subduction zone (density $\sim 2.67 \text{ g/cm}^3$), 0° refers to the seismic ray parallel to the [001] direction and 90° refers to the seismic rays oriented perpendicular to the [001] direction; and (d) plot of V_P/V_S versus V_S . Two regions marked with black and red lines refer to the "usual" ($4.28 < V_S < 4.59 \text{ km s}^{-1}$ and $1.76 < V_P/V_S < 1.82$) and "unusual" ($4.58 < V_S < 4.79 \text{ km s}^{-1}$ and $1.62 < V_P/V_S < 1.72$) [Hacker and Abers, 2012] velocity ratios observed from the mantle wedges in subduction zone settings [Hacker and Abers, 2012]. Note: filled and open symbols refer to V_{S1} and V_{S2} , respectively, (e) a schematic diagram of subduction zone indicating the stability fields of antigorite and chlorite, following recent work [Till et al., 2012]. Also shown are the schematic representations of the CPO and the incident rays in different regions (i) mantle overlying the subducting slab, region where the fabric is dominated by olivine and produces trench normal shear wave polarization (ii) hydrated mantle wedge is likely to be dominated by antigorite and chlorite and the near vertical teleseismic rays are likely to generate large delay time, and low V_P/V_{S1} velocity ratios. If this region were to be dominated by olivine, an unrealistically thick layer would have been required to produce large delay time owing to lower shear wave anisotropy of olivine [Kumazawa and Anderson, 1969] (iii) above the subducting slabs, the (001) planes are likely to be aligned parallel to the foliation and seismic rays from the local earthquakes are likely to traverse these hydrated assemblages of rock to produce low V_P/V_{S1} .

4. Discussion

The subduction of hydrated lithosphere leads to dehydration and subsequent rehydration of the parts of the overlying mantle wedge. Mantle wedges are often characterized by various geophysical observations including anomalous shear wave velocity [Bostock *et al.*, 2002; Kawakatsu and Watada, 2007], large delay times and trench parallel anisotropy [Long and Silver, 2008], and large P to S wave velocity ratios [Hacker and Abers, 2012, and references therein]. All these observations have been attributed to presence of hydrous phases [Faccenda *et al.*, 2008; Katayama *et al.*, 2009; Mainprice and Ildefonse, 2009; Kim *et al.*, 2012, 2013; Jung, 2011; Reynard, 2012; Wagner *et al.*, 2013; Faccenda, 2014]. In a hydrated fertile peridotite, chlorite is likely to be stable in addition to serpentine. Thermodynamic stability of chlorite is likely to exceed beyond the stability limits of antigorite along warmer slab geotherms [Fumagalli and Poli, 2005; Grove *et al.*, 2006; Till *et al.*, 2012]. Based on the subduction zone geotherms of Iwamori [2007] for central, NE, and SW Japan, it is estimated that a stable chlorite layer thickness between 5, 20, and 40 km, respectively, at depths between 100 and 150 km, corresponding to 3–5 GPa and 550–750°C.

Based on our study, the most striking feature of the elasticity of chlorite is the pressure dependence of P and S wave anisotropy (Figure 3). In a warm subduction zone geotherm such as Cascadia or southwest Japan, chlorite is likely to be stable between a depth range of 100–130 km, whereas antigorite followed by chlorite is likely to be stable between 120 and 150 km in a relatively cold subduction zone such as northeast Japan (Figure 3). For other layered hydrous minerals relevant for subduction zone settings, such as brucite and talc, both P and S wave anisotropy decrease with increasing pressure [Mainprice and Ildefonse, 2009]. In contrast, the S wave anisotropy of antigorite and chlorite increases in the depth range 100–150 km (3–5 GPa), so that the anisotropy of antigorite and chlorite are ~60% higher than that of brucite (~35%) and talc (50%), whereas P wave anisotropy of chlorite (~20%) is lower than brucite (~35%), antigorite (~40%), and talc (~40%). As the slab reaches greater depth, dense hydrous phases, such as phase D, are likely candidates for transporting the water into the deeper parts of the mantle. A sharp contrast in shear wave anisotropy is to be expected as the subducting slabs reach greater depths since the dense hydrous phases such as phase D have significantly lower shear wave anisotropy (18–19%) [Mainprice *et al.*, 2007; Rosa *et al.*, 2012].

The full elastic stiffness tensor, elastic anisotropy, and its pressure dependence suggests that a conservative estimate of 10–20 km layer thickness of hydrated peridotite with chlorite and serpentine could account for a large delay time of around 1.4–2.8 s, assuming perfect crystal alignment (Figure 4). Chlorite is stable to higher temperatures and pressures than antigorite; therefore, a wider range of depth will be characterized by an S wave anisotropy similar to antigorite. Intergrowths of antigorite and chlorite [Morales *et al.*, 2013] result in the crystal preferred orientation (CPO) of antigorite and chlorite being similar to other layered silicates with pole of (001) plane oriented normal to the foliation [Morales *et al.*, 2013; Padron-Navarta *et al.*, 2012; Puelles *et al.*, 2012]. The combined stability range of antigorite and chlorite increases the potential anisotropic zone thickness to 2 to 3 times the chlorite stability field. In addition, elastic anisotropy of chlorite could explain a wide range of V_P/V_{S1} and V_P/V_{S2} ratios. For instance, the rays traversing parallel to the (001) basal planes of chlorite, the V_P/V_{S1} ratio could be as low as 1.30–1.60, whereas rays traversing perpendicular to the (001) basal planes has $V_P/V_{S1} \sim 3.14$ (Figure 3). Such low V_P/V_S could account for recent high-resolution seismological observations [Wagner *et al.*, 2005, 2006; Rossi *et al.*, 2006; Eberhart-Phillips *et al.*, 2006; Hacker and Abers, 2012].

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