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Elasticity of serpentines and extensive serpentinization in subduction zones

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[1] Elastic constants of lizardite [Mg₃Si₂O₅(OH)₄] were computed using first-principles quantum mechanical calculations within the density functional theory. The predicted c-axis compressibility is much larger than measured. Modeling of the weak O-H···O interactions between layers must be improved in order to better predict layered hydrated mineral elastic properties. The large computed bulk modulus range is consistent with equation of state and seismic velocities in chrysotile-lizardite serpentinites, but shear wave velocities are lower than the lowest theoretical estimate. The low seismic velocities measured for chrysotile serpentinites can be attributed to specific contribution of the nanotube-textured chrysotile. For antigorite, the data from acoustic and EoS measurements are consistent. If used for interpreting seismic velocities, the inferred degrees of serpentinization of the mantle wedge are higher than with the commonly used calibrations using chrysotile-serpentinite properties. Serpentine is likely a dominant phase in low velocity areas of the mantle wedge at 30-50 km depths. Citation: Reynard, B., N. Hilairet, E. Balan, and M. Lazzeri (2007), Elasticity of serpentines and extensive serpentinization in subduction zones, Geophys. Res. Lett., 34, L13307, doi:10.1029/2007GL030176.

1. Introduction

[2] Serpentine minerals are hydrous phyllosilicates $(\sim 13 \text{ wt\% water})$ among which lizardite and antigorite are stable at temperatures and pressures achieved during hydrothermal alteration of ultrabasic and basic rocks of the oceanic lithosphere, antigorite is stable at greater depths in subduction zones, and chrysotile or fibrous varieties are metastable forms appearing at low temperatures and pressures [Evans, 2004]. They are major water carriers in subduction zones [Schmidt and Poli, 1998; Ulmer and Trommsdorff, 1995]. The increasing accuracy of seismic tomography allows detecting local seismic velocity anomalies in subducting slabs or in the mantle wedge just above the subducting slabs [DeShon and Schwartz, 2004; Park et al., 2004; Wang and Zhao, 2005]. These low velocities, high Poisson ratio and high anisotropy zones are often interpreted as regions of serpentinization and serpentinites play an important role in the localization of seismic activity [Yamasaki and Seno, 2003].

[3] The degree of serpentinization is inferred by comparison of seismic velocities from tomography with available seismic velocities measured on bulk peridotites with various degrees of hydration, including chrysotile-lizardite- and antigorite-dominated serpentinites. These two types of serpentinite have very different elastic properties [*Christensen*, 2004]. In order to calibrate the effect of serpentinization on the sound velocities of ultrabasic rocks [*Carlson and Miller*, 2003], the properties of chrysotile-lizardite serpentinized peridotites were used [*Christensen*, 1966]. *Christensen* [2004] showed that the data for antigorite-dominated serpentinite define a very different calibration, yielding much larger estimates for the proportion of serpentine in the mantle wedge of subduction zones.

[4] Detailed modeling of seismic properties of serpentinites requires the knowledge of single-crystal elastic constants. These are difficult to obtain on natural samples because of difficulties in preparation of phyllosilicates for techniques such as Brillouin spectroscopy. As an alternative approach, atomistic simulations using empirical potentials have been used to calculate elastic properties of lizardite [Auzende et al., 2006]. Although antigorite is the stable form at high temperatures and pressures [Evans, 2004; Ulmer and Trommsdorff, 1995; Wunder and Schreyer, 1997], its first-principles modeling cannot be achieved at a reasonable computational cost because of its structural complexity and related large cell-size. On the other hand, lizardite has a much smaller unit cell and its vibrational properties have been successfully reproduced using Density Functional Theory (DFT) [Balan et al., 2002a]. Here we use the same first-principle methods to calculate its elastic properties. The results are compared with available EoS and acoustic measurements of lattice and bulk elastic properties of serpentine and serpentinites. Implications for interpreting the seismic properties of the mantle wedge in subduction zones are discussed.

2. Ab Initio Calculations

[5] The calculations were performed by using DFT and the generalized gradient approximation (GGA) to the exchangecorrelation functional as proposed by Perdew, Burke, and Ernzerhof (PBE) [*Perdew et al.*, 1996]. The ionic cores were described by norm-conserving pseudo-potentials [*Troullier and Martins*, 1991] in the Kleinman-Bylander form [*Kleinman and Bylander*, 1982]. The wave functions and the charge density were expanded in plane-waves with 100 and 400 Ry cutoffs, respectively. The Brillouin zone was sampled using a $2 \times 2 \times 2$ *k*-point grid according to the Monkhorst-Pack scheme [*Monkhorst and Pack*, 1976]. Convergence of energies with respect to the basis set size and to the Brillouin zone sampling was tested with

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Table 1. Elastic Constants (C_{ii}) of Lizardite From DFT

| C _{ii} (GPa) | 1 | 2 | 3 | 4 | 5 | 6 |
|-----------------------|-----|-----|----|------|------|------|
| 1 | 245 | 50 | 31 | | | |
| 2 | | 245 | 31 | | | |
| 3 | | | 23 | | | |
| 4 | | | | 11.6 | | |
| 5 | | | | | 11.6 | |
| 6 | | | | | | 97.5 |
| | | | | | | |

calculations using a 120 Ry cutoff on wave-functions and a $3 \times 3 \times 3$ *k*-point grid, respectively.

[6] The five independent elastic constants of hexagonal lizardite were obtained by applying a set of five deformation matrices [Fast et al., 1995] to the experimental geometry with a = 5.3267 Å, and c = 7.2539 Å [Gregorkiewitz et al., 1996] and calculating the lattice energy for three negative and three positive increments of deformation. Applying the strains on the experimental geometry improves the estimation of the compressibility along the c-axis, with respect to the use of the DFT equilibrium geometry. In this direction, the compressibility is indeed dominated by the properties of weak H-bonds, difficult to describe at the DFT level. For every cell geometry, the atomic positions were relaxed until the residual forces on atoms were less than 10^{-3} Ry/Å. Energy curves as a function of the applied deformation were fitted using a parabola whose second derivative at null deformation constrain five linear combinations of the independent elastic constants. Convergence of elastic constants with respect to the basis set size and to the Brillouin zone sampling was tested by calculating the C₃₃ constant using a 120 Ry cutoff on wave-functions and a 3 \times 3 \times 3 k-point grid, respectively. The related variations of the C_{33} constant are of the order of 1%. Calculations were performed with the PWSCF code (Baroni et al.; http://www.pwscf.org).

3. Elastic Constants of Lizardite

[7] Elastic constants and compliances of lizardite are reported in Table 1. They are in reasonable agreement with those determined from atomistic calculations on lizardite [*Auzende et al.*, 2006]. There is no complete experimental determination of single-crystal elastic modulus to which they can be compared, only compressibilities of lizardite [*Hilairet et al.*, 2006a, 2006b] and bulk serpentinite sound velocities have been determined [*Christensen*, 2004]. For the sake of comparison with EoS data, acoustic measurements of compressional and shear waves velocities, V_P and V_S , are translated into adiabatic bulk and shear modulus (K_S and G) using the measured bulk rock density through the relations:

$$\rho V_p^2 = K_S + 4/3G \tag{1}$$

$$\rho V_s^2 = G. \tag{2}$$

Equations of state measurements give crystallographic lattice volumes and isothermal linear compressibilities and bulk modulus (K_T), the latter being related to the adiabatic bulk modulus through:

$$\mathbf{K}_{\mathbf{S}} = \mathbf{K}_{\mathbf{T}} (1 + \alpha \gamma \mathbf{T}), \tag{3}$$

where α is the thermal expansivity with typical values around 3 10⁻⁵ K⁻¹, γ is the Grüneisen parameter, usually in the range 1–1.5 for silicates, and T the temperature in K. At 300K, this yields a correction of 1–1.5% between adiabatic and isothermal moduli, which is well within the variability or uncertainties of measurements. A correction of 1.5% (i.e. \approx 1 GPa) was however applied to EoS isothermal values for comparison purposes in Table 2.

[8] A large elastic anisotropy is predicted, with the *c*-axis compressibility five times greater than the experimental one [*Hilairet et al.*, 2006b]. Atomistic calculations [*Auzende et al.*, 2006] yielded axial compressibilities in better agreement with experimental values, although the c-axis compressibility was also overestimated with respect to experiments. Thus the predicted elastic constants are too low, with most of the inconsistency between theory and experiment coming

| | , I | 1 | | | | |
|-----------------|----------------------------|------------------------------------|------------------------------------|------------------------------|-------------------------------|-------------------------------|
| | Lizardite DFT ^a | Chrysotile Ultrasonic ^b | Antigorite Ultrasonic ^b | Lizardite (EoS) ^c | Antigorite (EoS) ^d | Chrysotile (EoS) ^c |
| VP | 4460-7710 | 4700 | 6520 | 6500 ^e | <i>6400</i> ^e | <i>6260</i> ^e |
| Vs | 2770 - 4490 | 2260 | 3570 | 3540 ^e | 3480 ^e | <i>3410</i> ^e |
| V _o | 3120-5700 | 3910 | 5160 | 5140 | 5060 | 4950 |
| σ^{T} | 0.19 - 0.24 | 0.34 | 0.29 | $(0.29)^{\rm e}$ | $(0.29)^{\rm e}$ | $(0.29)^{\rm e}$ |
| ρ | 2.61 | 2.52 | 2.665 | 2.61 | 2.62 | 2.57 |
| K _S | 25 - 82 | 39 | 69 | 68 ± 1 | 66 ± 1 | 62 ± 2 |
| μ^{-} | 19-51 | 13 | 34 | nd | nd | nd |
| β_a | -0.0017 | | | 0.0027(3) | 0.0037(3) | 0.0027(4) |
| $\beta_{\rm h}$ | | | | | 0.0033(3) | 0.0027(4) |
| $\beta_{\rm c}$ | 0.0479 | | | 0.0097(5) | 0.0082(5) | 0.011(1) |

Table 2. Comparison of Computed Single-Crystal Elastic Properties, Measured Bulk Mineral Aggregate Sound Velocities, Bulk Sound Velocities, and Incompressibilities From Equation of State Measurements

^aThis study, for seismic velocities and elastic moduli, K_s and μ , the Reuss and Voigt averages are given, respectively; the Hill average is their arithmetic mean.

^bSeismic velocities of bulk serpentinites from *Christensen* [2004] are extrapolated to ambient pressure, uncertainties are 0.5 and 1% for V_P and V_S , respectively.

^c*Hilairet et al.* [2006b].

^dHilairet et al. [2006a].

^eSound velocities recalculated from EoS bulk modulus assuming the Poisson ratio from acoustic measurements. V_P, V_S, V_{ϕ}; compressional wave, shear wave and bulk sound velocities (m.s⁻¹); σ : Poisson ratio; ρ : density from bulk rock measurements or from lattice volume (EoS); K, μ , bulk and shear moduli (GPa).



Figure 1. Comparison of compressional wave velocities from acoustic and EoS measurements plotted against rock or crystallographic density. Filled circles: acoustic measurements from Christensen [2004] for peridodites dominated by olivine properties (Fo), brucite dominated rock (Br), chrysotile-lizardite dominated serpentinite (Chr-Liz) and antigorite-dominated serpentinite (Atg). Open circles: acoustic measurements on various partially to totally serpentinized peridotites [Christensen, 1989]. Squares: P wave velocities of serpentine varieties (italic abbreviations) from EoS [Hilairet et al., 2006b] assuming a Poisson ratio of 0.29. These lie close to the point defined by acoustic measurements on antigorite-dominated serpentinites even for the less dense chrysotile variety. Most acoustic measurements on serpentinites or altered peridotites lie below the trend defined olivine-dominated peridotite and antigorite-dominated serpentinite, and by EoS values. This indicates a specific contribution of chrysotile, which causes a strong reduction in wave velocities and in some cases in bulk rock density that can reach values well below the limit of crystallographic density. Lowering of bulk density and sound velocity is attributed to the specific texture of chrysotile nanotubes that accounts for large porosities and possible damping of acoustic waves. For mantle conditions, chrysotile is not stable, and the trend defined by the acoustic measurements on antigorite-dominated serpentinite and by EoS measurements must be used in order to assess the degree of serpentinization from seismic wave velocities.

from a large underestimation of the stiffness of the structure perpendicular to the layer in the DFT calculation. A similar and large anisotropy was predicted in kaolinite from DFT calculations [*Sato et al.*, 2005]. In these minerals, the compressibility along the *c*-axis is dominated by weak bonding interactions between hydroxyl groups of adjacent layers, which are notoriously difficult to describe at the DFT level. Their weakness is attested by the high frequency of the OH stretching vibrational modes in serpentine group minerals [*Auzende et al.*, 2004; *Balan et al.*, 2002a; *Reynard and Wunder*, 2006].

[9] Predicted bulk (K) and shear (G) moduli are calculated from elastic constants and compliances as $K^{Voigt} = 81.9$ GPa, $K^{Reuss} = 24.5$ GPa, $G^{Voigt} = 50.9$ GPa, and

 $G^{Reuss} = 19.3$ GPa. The range of values defined by the Voigt and Reuss limits is large because of the large predicted anisotropy (Table 1). The bulk modulus obtained from the experimental equation of state is 68 GPa, close to the Voigt limit and significantly above the predicted Voigt-Reuss-Hill (VRH) average of 53 GPa. This discrepancy would slightly increase if the effect of temperature was taken into account to correct between the static DFT calculation and the experimental value at 295 K. The discrepancy cannot be attributed to stress and grain-grain interactions as in talc [Stixrude, 2002] because the EoS measurements were performed on dispersed powders in a hydrostatic medium [Hilairet et al., 2006b]. Bulk compressional and shear velocities of chrysotile-lizardite dominated serpentinite are 4700 and 2260 m/s as extrapolated to ambient pressure from ultrasonic measurements up to 1 GPa [Christensen, 2004]. Bulk and shear moduli of 39 and 13 GPa are obtained using the bulk rock density of 2.52. Measured values of bulk modulus from EoS and acoustic measurements for lizardite are within the predicted range defined by the Voigt and Reuss limits from ab initio calculations, but EoS and acoustic measurements are not consistent with each other. Ultrasonic values are lower than the predicted VRH averages, which are already underestimated due to inaccurate prediction of elasticity along the *c*-axis. The ultrasonic shear modulus is extremely low, and below the lowest predicted Reuss limit. Discrepancies between calculated and experimental values, and between experimental values from different types of measurements are discussed below.

4. Elastic Properties of Serpentines and Serpentinites

[10] The comparison of the predicted properties of lizardite with the available experimental data reveals a large discrepancy between the bulk elastic properties derived from EoS and acoustic measurements. Such a discrepancy can be explained either by an effect specific to the type of measurements or by a difference in the material studied. In order to evaluate these possibilities, elastic properties measured for different varieties of serpentines or serpentinites dominated by a single variety of serpentine are compared in Table 2. The acoustic velocities and bulk and shear moduli for chrysotile-lizardite serpentinite and antigorite serpentinite are very different [*Christensen*, 2004]. EoS-derived densities and compressibilities of lizardite and antigorite are very similar, and chrysotile is slightly less dense (1.5%) and more compressible (7%) than other serpentines.

[11] Bulk moduli of lizardite and antigorite from EoS are very consistent with that for antigorite serpentinite from acoustic measurements, while the EoS bulk modulus of chrysotile is much higher than that derived from acoustic measurements for chrysotile-lizardite serpentinite. Thus most of the inconsistency between experimental values lies in the determination of acoustic velocities in chrysotilelizardite serpentinites. Actually, compressional wave velocities of many serpentinites do not lie in the field defined by peridotite, antigorite- and chrysotile-lizardite-serpentinite end-members (Figure 1). A similar plot can be drawn for shear wave velocities. Some serpentinites have very low densities, below the crystallographic limit, and low velocities. Others have densities above 3, indicating no more than



Figure 2. Pressure dependence of seismic velocities in antigorite serpentinite [*Christensen*, 2004]. Line is (a) a fit giving $G' = 0.5 \pm 0.1$ and (b) a calculation assuming G' = 0.5 and K' = 4. Standard deviation from the fits is 4.5 m.s^{-1} for V_S and 12.5 m.s^{-1} for V_P , below the experimental uncertainties of 35 m.s⁻¹.

30% serpentine, yet their velocities are well below the line for simple mixture of single component properties. Lowest densities are easily explained by the porosity of chrysotile nanotube packing. Nanotube exterior and interior diameters are usually around 25 nm and 5 nm, respectively [Yada, 1971]. Assuming close packing of perfectly circular nanotubes, it yield porosities of 13%, allowing bulk density down to about 2.2 that account for the observed range of densities down to 2.3 in some serpentinites. The specific texture of chrysotile samples can also significantly affect other macroscopic properties. For example, specific features have been observed in the infrared spectrum of chrysotile. These features are related to the peculiar electrostatic properties of the nanotubes, whereas changes in the microscopic structure (e.g. bond lengths) between lizardite and chrysotile only have a much weaker effect on their vibrational properties [Balan et al., 2002b]. We propose that the low velocities observed in these rocks is also due to the particular texture of chrysotile nanotubes that allows damping of ultrasonic waves of a few hundred μm wavelength.

5. Implications for Serpentinization of the Mantle Wedge

[12] Because chrysotile is a metastable variety of serpentine that forms only at low pressures in the oceanic lithosphere and antigorite is the stable form at the pressures and temperatures of subduction, serpentinization of mantle rocks can be constrained from seismic velocities by assuming that sound velocities of partially serpentinized peridotites will lie along the line connecting measured velocities for antigorite serpentinite and peridotite (Figure 1). This differs strongly from the commonly used calibration between peridotite and chrysotile-dominated serpentinites [Carlson and Miller, 2003] and should increase the calculated degree of serpentinization [Christensen, 2004]. The extent of serpentinization is usually derived from V_P tomographic models, which requires extrapolation of experimental data to the corresponding pressures and temperatures. Using the measured shear velocities for antigorite serpentinite at high pressures [Christensen, 2004], the pressure dependence of the shear modulus G' is tightly constrained to a value of 0.5 ± 0.1 (Figure 2a). Constraining the pressure

derivative of the bulk modulus K' from the pressure dependence of V_P is more difficult because of a larger scatter of data (Figure 2b). If instead we use the above value of G' and combine it with K' = 4 from EoS [*Hilairet et al.*, 2006a], to calculate $V_{P}(P)$, we obtain a very good agreement with measured sound velocities with $V_{P0} = 6550 \pm 40$ $m.s^{-1}$ (Figure 2b). In the absence of relevant data, the temperature dependence of V_P is more difficult to estimate, and we used a $\partial ln V_{P} / \partial T$ value similar to olivine. At a maximum temperature around 600°C, this assumption has little contribution to uncertainties, and has a negligible effect when compared with the difference between commonly assumed chrysotile elastic properties [Carlson and Miller, 2003] and antigorite elastic properties used here. For peridotite, we use $V_{P0} = 8250 \pm 150 \text{ m.s}^{-1}$, $\partial V_P / \partial P = 150 \text{ m.s}^{-1}$. GPa⁻¹ and $\partial ln V_P / \partial T = -0.03 \text{ K}^{-1}$. Taking V_P value of 7.2–7.6 km.s⁻¹ for the mantle wedge at depths of 40–60 km in the tomographic model of Costa Rica subduction [DeShon and Schwartz, 2004], this yields estimate of serpentinization between 40 and 80% including uncertainties, more than twice those originally estimated. Other estimates of 15-25% serpentinization from tomographic models in the subduction zone of Japan [Wang and Zhao, 2005] should be revised by a similar factor. Another important consequence is that compressional wave velocities in serpentinites are similar to those of the oceanic crust, making their high Poisson ratio (0.29) the only criterion for their detection [Christensen, 2004]. Modeling of the seismic properties of an anisotropic layer of a few km thickness in subduction zone below Oregon [Park et al., 2004] yields Pwave velocities as low as 6.5 km.s⁻¹. If interpreted as serpentinite, it suggests complete serpentinization. Thus seismic tomography is consistent with high serpentinization of the mantle wedge, in agreement with field observations of a few km-thick sequences of serpentinites in fossil subduction zones [Hermann et al., 2000; Sedlock, 2003]. The presence and thickness of a serpentinite layer control the mechanical coupling and advection pattern above the subducted slab, recorded through the exhumation of highpressure rocks [Gerya et al., 2002; Schwartz et al., 2001].

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References

- Auzende, A. L., I. Daniel, B. Reynard, C. Lemaire, and F. Guyot (2004), High-pressure behaviour of serpentine minerals: A Raman spectroscopic study, *Phys. Chem. Miner.*, 31, 269–277.
- Auzende, A. L., R. Pellenc, B. Devouard, A. Baronnet, and O. Grauby (2006), Atomistic calculations of structural and elastic properties of serpentine minerals: The case of lizardite, *Phys. Chem. Miner.*, 33, 266– 275.
- Balan, E., A. Marco Saitta, F. Mauri, C. Lemaire, and F. Guyot (2002a), First-principles calculation of the infrared spectrum of lizardite, *Am. Miner.*, 87, 1286–1290.
- Balan, E., F. Mauri, C. Lemaire, C. Brouder, F. Guyot, A. M. Saitta, and B. Devouard (2002b), Multiple ionic-plasmon resonances in naturally occurring multiwall nanotubes: Infrared spectra of chrysotile asbestos, *Phys. Rev. Lett.*, 89(17), 177401.
- Carlson, R. L., and D. J. Miller (2003), Mantle wedge water contents estimated from seismic velocities in partially serpentinized peridotites, *Geophys. Res. Lett.*, 30(5), 1250, doi:10.1029/2002GL016600.
- Christensen, N. I. (1966), Elasticity of ultrabasic rocks, J. Geophys. Res., 71(24), 5921-5931.
- Christensen, N. I. (1989), Seismic velocities, in *Practical Handbook of Physical Properties of Rocks and Minerals*, edited by R. S. Carmichael, pp. 429–546, CRC Press, Boca Raton, Fla.
- Christensen, N. I. (2004), Serpentine, peridotites and seismology, *Int. Geol. Rev.*, 46, 795–816.
- DeShon, H. R., and S. Y. Schwartz (2004), Evidence for serpentinization of the forearc mantle wedge along the Nicoya Peninsula, Costa Rica, *Geophys. Res. Lett.*, 31, L21611, doi:10.1029/2004GL021179.
- Evans, B. (2004), The serpentinite multisystem revisited: Chrysotile is metastable, *Int. Geol. Rev.*, 46, 479–506.
- Fast, L., J. M. Wills, B. Johansson, and O. Eriksonn (1995), Elastic constants of hexagonal transition metals: Theory, *Phys. Rev. B Condens. Matter*, 51, 17,431–17,438.
- Gerya, T. V., B. Stockhert, and A. L. Perchuk (2002), Exhumation of highpressure metamorphic rocks in a subduction channel: A numerical simulation, *Tectonics*, 21(6), 1056, doi:10.1029/2002TC001406.
- Gregorkiewitz, M., B. Lebech, M. Mellini, and C. Viti (1996), Hydrogen positions and thermal expansion in lizardite-1T from Elba: A low-temperature study using Rietveld refinement of neutron diffraction data, *Am. Miner.*, *81*, 1111–1116.
- Hermann, J., O. Muntener, and M. Scambelluri (2000), The importance of serpentinite mylonites for subduction and exhumation of oceanic crust, *Tectonophysics*, 327, 225–238.
- Hilairet, N., I. Daniel, and B. Reynard (2006a), Equation of state of antigorite, stability field of serpentines, and seismicity in subduction zones, *Geophys. Res. Lett.*, 33, L02302, doi:10.1029/2005GL024728.
- Hilairet, N., I. Daniel, and B. Reynard (2006b), P–V equations of state and the relative stabilities of serpentine varieties, *Phys. Chem. Miner.*, *33*, 629–637.

- Kleinman, L., and D. M. Bylander (1982), Efficacious form for model pseudopotentials, *Phys. Rev. Lett.*, 48, 1425–1428.
- Monkhorst, H. J., and J. D. Pack (1976), Special points for Brillouin-zone integrations, *Phys. Rev. B Condens. Matter*, 13, 5188–5192.
- Park, J., H. Yuan, and V. Levin (2004), Subduction zone anisotropy beneath Corvallis, Oregon: A serpentinite skid mark of trench-parallel terrane migration?, J. Geophys. Res., 109, B10306, doi:10.1029/2003JB002718.
- Perdew, J. P., K. Burke, and M. Ernzerhof (1996), Generalized gradient approximation made simple, *Phys. Rev. Lett.*, 77, 3865–3868.
- Reynard, B., and B. Wunder (2006), High-pressure behavior of synthetic antigorite in the MgO-SiO2-H2O system from Raman spectroscopy, *Am. Miner.*, 91, 459–462.
- Sato, H., K. Ono, C. T. Johnston, and A. Yamagishi (2005), First-principles studies on the elastic constants of a 1/1 layered kaolinite mineral, Am. Miner., 990, 1824–1826.
- Schmidt, M., and S. Poli (1998), Experimentally based water budgets for dehydrating slabs and consequences for arc magma generation, *Earth Planet. Sci. Lett.*, 163, 361–379.
- Schwartz, S., P. Allemand, and S. Guillot (2001), Numerical model of the effect of serpentinites on the exhumation of eclogitic rocks: Insights from the Monviso ophiolitic massif (Western Alps), *Tectonophysics*, 342, 193–206.
- Sedlock, R. L. (2003), Four phases of Mesozoic deformation in the Sierra de San Andres ophiolite, Vizcaíno Peninsula, west-central Baja California, México, in *Tectonic Evolution of Northwestern México and the Southwestern USA*, edited by S. E. Johnson et al., *Spec. Pap. Geol. Soc. Am.*, 374, 73–92.
- Stixrude, L. (2002), Talc under tension and compression: Spinodal instability, elasticity, and structure, J. Geophys. Res., 107(B12), 2327 doi:10.1029/ 2001JB001684.
- Troullier, N., and J. L. Martins (1991), Efficient pseudopotentials for planewave calculations, *Phys. Rev. B Condens. Matter*, 43, 1993–2006.
- Ulmer, P., and V. Trommsdorff (1995), Serpentine stability to mantle depths and subduction-related magmatism, *Science*, 268, 858-861.
- Wang, Z., and D. P. Zhao (2005), Seismic imaging of the entire arc of Tohoku and Hokkaido in Japan using P-wave, S-wave and sP depthphase data, *Phys. Earth Planet. Inter.*, 152(3), 144–162.
- Wunder, B., and W. Schreyer (1997), Antigorite: high-pressure stability in the system MgO-SiO2-H2O, *Lithos*, *41*, 213–227.
- Yada, K. (1971), Study of microstructure of chrysotile asbestos by high resolution electron microscopy, *Acta Crystallogr., Sect. A Found. Crystallogr.*, 27, 659–664.
- Yamasaki, T., and T. Seno (2003), Double seismic zone and dehydration embrittlement of the subducting slab, J. Geophys. Res., 108(B4), 2212, doi:10.1029/2002JB001918.

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