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High-pressure phase of brucite stable at Earth’s mantle transition zone and lower mantle conditions

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We investigate the high-pressure phase diagram of the hydrous mineral brucite, Mg(OH)2, using structure search algorithms and ab initio simulations. We predict a new high-pressure phase stable at pressure and temperature conditions found in cold subducting slabs in Earth’s mantle transition zone and lower mantle. This implies that brucite can play a much more important role in water transport and storage in Earth’s interior than hitherto thought. The predicted high-pressure phase, stable in calculations between 20-35 GPa and up to 800 K, features MgO6 octahedral units arranged in the anatase-TiO2 structure. This suggests that brucite will transform from a layered to a compact three-dimensional network structure before eventual decomposition into periclase and ice. We show that the new phase has unique spectroscopic fingerprints that should allow for straightforward detection in experiments. The new phase also has distinct elastic properties that might make its direct detection in the deep Earth with geophysical methods possible.

Introduction

Water plays an important role in sustaining geological activity. For instance, water helps in lowering the mantle’s melting temperature, enhancing diffusion and creep thus affecting rheology of rocks, and also influences mineral phase boundaries. Current estimates suggest that the Earth’s mantle is likely to contain a mass of water equivalent to the mass of the world’s oceans.1, 2 The exchange of water between the surface and deep mantle reservoirs is vital for the sustenance of surface water over geological time scales.3 Hydrous minerals stable in the hydrated oceanic crust and mantle play an important role in transporting water into the Earth’s interior. Hydrated peridotite, the major mantle rock type, can be understood by considering mineral phases stable in the ternary system of MgO-SiO2-H2O (MASH). Brucite, Mg(OH)2, is arguably the simplest hydrous mineral in the MASH system. Brucite is also the most important MgO-H2O binary and the most water-rich phase within the MSH ternary system.

The crystal structure of brucite consists of Mg2+ cations and OH anions arranged in layers, in an overall trigonal structure (space group symmetry p3m1), see Figure 1. The common ionic compound CdI2 is the archetype crystal structure for brucite as well as for portlandite (Ca(OH)2) and several other transition metal hydroxides M(OH)2, where M= Mn, Ni, Co, Fe, Cd etc.(4–10) In brucite, the crystal structure comprises layers of edge-sharing MgO6 polyhedra. The interaction between the layers is weak at ambient conditions, where each upward pointing OH group is surrounded by three downward pointing OH groups in the adjacent layer and vice-versa. Under compression the H—H repulsive interactions lead to positional disordering of the protons, which are displaced from the 2d Wyckoff site into one of three equivalent 6i sites as documented from neutron diffraction studies.(11, 12) Vibrational spectroscopic studies including infrared and Raman spectroscopy show a broad νOH stretching band with appearance of additional bands upon compression. The appearance of additional bands hints at the pressure induced frustrations of the proton.(13, 14) First principles molecular dynamics simulations also demonstrated the proton frustrations in brucite and portlandite at high pressure.(15) A first principles study at static conditions indicated that the pressure-induced hydrogen bonding in brucite is weak or unlikely to occur within the thermodynamic stability field of brucite.(16) In addition, the study also predicted that upon compression, protons may transition from a dynamic positional disorder to a static positional disorder, leading to a lowering of the trigonal symmetry to p2.

Layered structures similar to that of brucite are also common in group-I (alkali) hydroxides. Under pressure, the alkali hydroxides tend not only to form hydrogen bonds between the layers, but undergo transitions to three-dimensional network structures, with 0-, 1-, or 2-dimensional hydrogen bonded sublattices.(17–20) The rationale from the high-pressure behavior of those systems is that layered phases are ultimately too loosely packed to survive under pressure. The important question relevant for deep Earth geophysics is whether brucite will undergo a similar transition and densification at high pressures, and significantly deviate from a layered structure, before decomposition into MgO and H2O occurs. The presence of such a phase would have a significant impact on whether brucite itself could be stable in the mantle transition zone and lower mantle (potentially with quite different properties than those of the known phase), as well as the relative stability of competing MSH phases. We address this question here using structure prediction methods and first-principles total energy calculations, which enable us to bypass potential difficulties in high-pressure experiments such as sample preparation or kinetic reaction barriers. In recent years, such calculations have been crucial in making important predictions of high-pressure phases relevant for solid Earth geophysics.(21, 22) These have been very

Significance

Hydrous minerals help transporting water deep into Earth’s mantle, and form part of a cycle that regulates the sustained presence of surface water on Earth. To understand the deep water cycle, it is crucial to study the properties of hydrous minerals under the conditions present in Earth’s mantle. Brucite is one of the simplest hydrous minerals and stores significant amounts of water as hydroxyl groups. It is assumed to decompose in the mantle transition zone, but we show here that a more compact high-pressure phase is stabilized instead that pushes the stability region of brucite into the lower mantle. Brucite might be present in much larger quantities, and play a larger role in water transport and storage, than previously thought.

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helpful for experimental discoveries. Here, we suggest that brucite transforms to a new high-pressure phase at conditions relevant to subducting slabs in the mantle transition zone and lower mantle, i.e., pressures of ~20 GPa and temperatures of ~800 K.

Results

Our density functional calculations give excellent agreement for the structural parameters of brucite ($P\bar{6}m\bar{1}$) with experimental data at $P$=1atm, see Table 1. They also correctly reproduce the pressure-induced stabilization of hydrogen bond formation and static proton disorder, in the form of the $P\bar{6}$ phase,(16) see the upper panel of Figure 1. For those two known brucite phases, decomposition into periclase (MgO) and ice-VIII is then calculated to occur at 18 and 21 GPa, respectively, i.e., in the Earth mantle transition zone. This agreesreasonably well with thermodynamic modeling based on measured $P-V-T$ equation of state for brucite, which estimated a decomposition pressure of 27 GPa at $T=300K$.(24) Note that brucite has been compressed significantly higher pressures: by 8 GPa in the ground state, from (towards decomposition into MgO and ice-VIII) is shifted to significantly beyond this pressure, likely due to kinetic barriers in the decomposition reaction.(24, 25)

Our crystal structure prediction runs, however, revealed a candidate for a high-pressure phase of Mg(OH)$_2$: with tetragonal space group symmetry ($P4_2\bar{1}2_1$), which is energetically more stable than both known modifications above 17 GPa, see the upper panel of Figure 2. With the appearance of a new high-pressure phase, the thermodynamic stability limit of Mg(OH)$_2$ (towards decomposition into MgO and ice) is shifted to significantly higher pressures: by 8 GPa in the ground state, from 21 GPa to 29 GPa. This delays the decomposition of Mg(OH)$_2$ from the lower part of the mantle transition zone (the pressure region 13–21 GPa) into the lower mantle. The stability of the tetragonal Mg(OH)$_2$ phase is unaffected by the choice of exchange-correlation functional or the inclusion of zero-point effects (ZPE). For instance, using the vdW-DF approach with the optB88 functional(27–30) which includes dispersion interactions based on the electronic density, instead of the PBE functional, we find tetragonal Mg(OH)$_2$ to be stable from 18 to 27 GPa. When ZPE are included with the PBE functional, tetragonal Mg(OH)$_2$ is stable from 19 to 33 GPa.

We used the quasi-harmonic approximation to estimate the Gibbs free energies of the relevant phases and construct the finite-temperature phase diagram of Mg(OH)$_2$. To that end, we included the vibrational contribution to the entropy of each phase, which results in

$$F(T, P) = E(V, P) + kT \sum g(\omega) \ln \left[ \cosh \left( \frac{\hbar \omega}{kT} \right) \right]$$

where $g(\omega)$ is the phonon density of states obtained from finite displacement calculations. As shown in the lower panel of Figure 2, this results in a large stability field for the tetragonal Mg(OH)$_2$ phase, up to $T=800$ K at 30 GPa, where it forms a triple point with brucite (in the $P\bar{6}$ model) and the decomposition into MgO + Ice-VII. This triple point corresponds to a depth of about 800 km, in the upper reaches of the lower mantle, and approaches cold geothermal gradients estimated for subducting slabs(23, 31, 32) and the melting line of ice.(33, 34) We included in this phase diagram the calculated geotherm for old and rapidly descending slabs as solid blue line.(32) This should serve as a low-temperature boundary for mantle slab geotherms (we extrapolated the data from ref. (32) beyond 20 GPa in a power expansion). We did not consider nuclear quantum effects in the construction of the phase diagram. Those can play an important role in aqueous systems(35) and might affect the phase transitions pressures in the low-temperature region—in particular if the protons’ chemical environment differs significantly across the respective phases. There is some indication (see below) that the hydrogen bonds in tetragonal Mg(OH)$_2$ are stronger than in brucite.

The tetragonal Mg(OH)$_2$ phase ($P4_2\bar{1}2_1$) is very different from the low-pressure layered phase (see Figure 1, and Table 1 for structural data). The high-pressure phase forms a three-dimensional network of edge-sharing MgO$_6$ octahedral units. In fact, the phase (when ignoring protons) is isostructural with the anatase-TiO$_2$ crystal structure, but with MgO$_6$ octahedral units that are less distorted compared to the TiO$_6$ octahedral units in anatase (see inset in lower panel of Figure 2). The protons are located in channels in between the MgO$_6$ polyhedral units. Alternatively, the crystal structure can be characterized by zig-zag hydrogen-bonded O-H...O-H chains running along the a and b directions, and which are lying in the bc and ac planes, respectively. In the ground state, the O-H vectors order antiferroelectrically (see Figure 1), but it is very likely that proton disorder sets in at finite temperatures. The major structural differences compared to the low-pressure phase of brucite suggest that there are significant kinetic barriers to transform from the layered phase into the tetragonal phase (just as for the decomposition), which would explain why the transition has not been observed in room-temperature experiments to pressures well into the predicted pressure stability region of the tetragonal phase.

The pressure-volume relation for brucite ($P\bar{6}$) can be described by a Birch Murnaghan equation of state with equilibrium volume $v_0 = 41.68 (± 0.09) \AA^3$, bulk modulus $K_0 = 43.4 (± 1.1)$ GPa, and its pressure derivative $\frac{dK_0}{dP} = 5.39 (± 0.10)$. In contrast to brucite, the three-dimensional network of MgO$_6$ polyhedra in tetragonal Mg(OH)$_2$ allows for a substantially more compact packing with $v_{0}^{2/3} = 38.06 (± 0.07) \AA^3$, $\sigma_{0}^{2/3} = 67.3 (± 1.6)$ GPa, and $\frac{d\sigma_{0}^{2/3}}{dP} = 4.91 (± 0.09)$. At 1 bar the tetragonal phase is 6.8% smaller than brucite, and stiffer by ~55%. At 20 GPa, where tetragonal Mg(OH)$_2$ has the lower enthalpy, it is 3.8% more compact than the brucite ($P\bar{6}$) phase.

Although the tetragonal phase is denser compared to the brucite phase, at 1 bar, the full elastic stiffness tensor reveals significant anisotropy. The principal stiffness components are related as $c_{11} = 1.5 c_{12}$, $c_{22} = 1.5 c_{12}$, $c_{33} = 1.5 c_{12}$, and the shear stiffness components are related as $c_{44} = 2 c_{12}$ (see Figure 3). At zero pressure (i.e., 1 bar), the Hill-averaged bulk ($\sigma_{0}^{2/3}$) and shear ($c_{44}^{2/3}$) moduli are 69.5 and 55.4 GPa respectively for the tetragonal Mg(OH)$_2$ phase. This is significantly stiffer than the bulk $\sigma_{0}^{2/3}$ and shear $c_{44}^{2/3}$ moduli for the trigonal phase, 46.7 and 36.4 GPa(36) The compressional ($V_P$) and shear ($V_S$) sound velocity for the tetragonal phase are also faster compared to the trigonal phase (see Figure 3).
Phase Pressure Lattice constants Atomic positions
(Exp) 1 atm a= b= 3.150 Å, c= 4.770 Å α= β=90°, γ=120° Mg(0,0,0) ... -0.370, 0.016) H1(-0.126, -0.477, 0.404)
H2(0.381, 0.227, 0.404) H3(0.227, 0.129, 0.154)
H4(-0.477, -0.378, 0.154)

(a) Ground state energies of various Mg(OH)₂ phases, from ground state DFT-PBE calculations.

Table 1. Optimized crystal structures of various brucite phases, from ground state DFT-PBE calculations.

<table>
<thead>
<tr>
<th>Phase</th>
<th>Pressure</th>
<th>Lattice constants</th>
<th>Atomic positions</th>
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</table>
| p3m1 (Exp) | 1 atm | a= b= 3.150 Å, c= 4.770 Å α= β=90°, γ=120° | Mg(0,0,0) ... -0.370, 0.016) H1(-0.126, -0.477, 0.404)
H2(0.381, 0.227, 0.404) H3(0.227, 0.129, 0.154)
H4(-0.477, -0.378, 0.154) |
| p3m1 (DFT) | 1 atm | a= b= 3.182 Å, c= 4.801 Å α= β=90°, γ=120° | Mg(0, 0, 0) O(1/3, 2/3, 0.220) H(1/3, 2/3, 0.413) |
| P3 | 10 GPa | a= b= 5.310 Å, c= 4.383 Å α= β=90°, γ=120° | Mg(10, 0, 0) Mg2(1/3, 2/3, -0.018) O(0-0.06, -0.336, -0.239) H(-0.070, -0.365, -0.451) |
| P4212 | 20 GPa | a= b= 8.178 Å, c= 7.549 Å α= β= γ=90° | Mg(10, 380, 0, 380) Mg(2-0.130, -0.130, 0) |

The changes in the hydrogen bonding lead to significant differences in the vibrational properties, which should make detection of the high-pressure phase quite straightforward. In Figure 5, we show calculated O-H stretch modes of the different phases as a function of distance, compared to an empirical functional relation established from experimental spectroscopic data on hydrous minerals. Calculated frequencies for the p3m1 and p2 phases, as has been noted before,(39, 40) good accounts of existing experimental data: in p3m1, the O-H stretch...
Fig. 3. Equation of state, elasticity and sound velocity of Mg(OH)$_2$. (a) Plot of volume as a function of pressure. Green symbols and thin dotted line refer to the - and -Mg(OH)$_2$ phases, respectively. The dashed line gives the finite strain fit to the phase. Experimental results are shown in filled light grey (single crystal X-ray diffraction), dark grey (powder neutron diffraction), black, and white symbols (synchrotron based powder X-ray diffraction), from Refs. (12, 14, 24, 25). (b) The full elastic stiffness tensor and the Hill-averaged Bulk ($K_H$) and Shear ($G_H$) moduli for tetragonal Mg(OH)$_2$ as function of pressure. (c) Calculated compressional/shear sound wave velocities (circles/squares) for tetragonal brucite (light green symbol). Grey symbols refer to the experimentally determined sound velocity of brucite.(36) Experimental data are given for the decomposition products periclase (MgO) (filled blue symbols)(63) and ice-VII (filled light blue symbols-compression, white symbols-decompression). (50)

Fig. 4. Elastic anisotropy of Mg(OH)$_2$. (a) Plot of P-wave anisotropy ($AV_P$, blue) and S-wave anisotropy ($AV_S$, red) as a function of pressure. The light and dark color symbols correspond to trigonal (brucite) and tetragonal Mg(OH)$_2$, respectively. (b) and (d) show the stereographic projection of the P-wave velocity variations across the orthogonal directions for both phases. (c) and (e) shows the stereographic projection of the S-wave anisotropy variations across the orthogonal directions for both phases. The orthogonal coordinates $X_1$ and $X_2$ are shown in the stereographic projections. The $X_3$ axis is perpendicular to both $X_1$ and $X_2$ axes. The color shadings are in inverse logarithmic scales. The minimum and maximum velocity directions for tetragonal Mg(OH)$_2$ along the $X_3$ and $X_1$ axes coincide with the extremal $C_{33}$ and $C_{11}$ elastic constants, respectively.

frequency is almost independent of pressure (i.e., independent of the $d_{O…O}$ distance), whereas the $p_{\overline{3}}$ phase reproduces the softening of the O-H stretch modes due to increased hydrogen bonding under pressure. Note that in Figure 5 we have shifted the axes of computed against experimental frequencies by 100 cm$^{-1}$ to account for the anharmonicity of the O-H stretch.(40) The hydrogen bonding is much more pronounced in the tetragonal phase, and as a consequence its O-H stretch frequencies are significantly redshifted, about 400 cm$^{-1}$ relative to the $p_{\overline{3}}$ phase, and also show a more rapid decrease upon compression. At 20 GPa, where tetragonal Mg(OH)$_2$ should become stable at low temperatures, $\nu_{O-H}=2840...3140$ cm$^{-1}$ in our calculations, while the $p_{\overline{3}}$ phase at the same pressure has $\nu_{O-H}=3540...3670$ cm$^{-1}$. The stretch mode frequencies of tetragonal Mg(OH)$_2$ at low pressures (large $d_{O…O}$ distance) are significantly lower than the correlation from Ref. (38) suggests; however, under compression, in the region of its stability, the calculated modes are in quite good agreement with the empirical relation.
In the low- and high-pressure phases of Mg(OH)₂, as function of hydrogen-bonded distance $d_{OH}$. Also shown is a correlation curve based on ambient pressure data for various hydrous phases including minerals. The red and green shaded region indicates the complete range of modes for the and phases respectively. The inset shows a plot of $d_{OH}$ vs $d_{OH}$ for tetragonal Mg(OH)₂. The hydrogen bond symmetrization ($d_{OH}=1/2d_{OH}$) occurs at 100 GPa. Note calculated frequencies are red-shifted by 100 cm⁻¹ with respect to the functional fit.

Discussion

Our first-principles calculations suggest that upon compression, the hydrous mineral brucite will transform to a dense phase with a three-dimensional network structure, before eventual decomposition into periclase (MgO) and ice-VII (H₂O). The new phase is found to be stable at pressure-temperature conditions that correspond to cold subducting slabs in Earth's mantle transition zone and lower mantle. It is possible that configurational disorder, on the proton and/or cation sites (for instance by forming (Mg, Fe, Ca)(OH)₂), stabilizes tetragonal Mg(OH)₂ at higher temperatures. It is also known that brucite and gibbsite (Al(OH)₃) have similar structures and can form mixed layered double hydroxides. A high-pressure phase of gibbsite exists, δ-Al(OH)₃, that comprises a three-dimensional structure of corner-sharing AlO₆ octahedra. It is thus conceivable that elevated temperatures stabilize a high-pressure solid solution (Mg₆Al₂(OH)₁₆)₁₆⁺ with a more complex three-dimensional network structure, or a tetragonal structure $[Mg₆(Al)₃]$(OH)₁₆⁺ balanced by an appropriate anion presence, e.g. (A³⁻). Any incorporation of Al³⁺ in high-pressure Mg(OH)₂ is also likely to enhance its thermal stability: recent studies on aluminium incorporation in phase-D (Al₂SiO₄(OH)₂) have shown that it enhances its thermal stability significantly. Thus, dense tetragonal Mg(OH)₂ together with other dense hydrous phases could act as an efficient carrier of water in cold subduction slabs. The emergence of this new, more stable compound at the edge of the MgO-H₂O-SiO₂ phase diagram has implications for the relative stability of more complex MSH phases at similar conditions.

We find that the tetragonal Mg(OH)₂ phase follows conventional high-pressure paradigms in that a layered structure is replaced by a more compact three-dimensional structure upon compression – the unexpected result is that this transition occurs (consistently in our calculations) before the decomposition reaction becomes favorable. Besides being more compact, the new phase is significantly stiffer than known brucite, which could lead to characteristic seismic signatures. A transition from the trigonal to the tetragonal phase is likely to be marked by an enhancement in both P and S-wave velocity. Under further compression, as tetragonal Mg(OH)₂ decomposes to a mixture of MgO and H₂O (ice) around 30 GPa, the P-wave velocity is likely to increase whereas the S-wave velocity is likely to decrease, owing to significantly lower S-wave velocity for ice-VII at high pressure. In combination (see Figure 3), both effects provide for a distinct test of the presence for the denser tetragonal phase of Mg(OH)₂ in cold subduction zones. However, it is very likely that the magnitude of the velocity discontinuity owing to the dissociation of tetragonal Mg(OH)₂ might be underlined by the presence of additional chemical components, which in turn is likely to stabilize other hydrous phases.

Tetragonal Mg(OH)₂ also features significantly stronger hydrogen bonds and weaker covalently bound hydroxyl groups compared to the trigonal phase, which we predict to lead to a very different spectroscopic signature, and could also result in qualitatively different proton diffusion behavior at elevated temperatures. The weaker covalent O-H bonds are likely to reduce the temperature where proton diffusivity sets in, and further stabilize the tetragonal phase over the trigonal phase at high temperature. On the other hand, due to the anatase-like structure of tetragonal Mg(OH)₂, protons can diffuse along one-dimensional channels of the MgO₂ polyhedral network, whereas in the low-pressure trigonal phase they can diffuse in two-dimensional wells between MgO₂ sheets. This is likely to significantly influence proton-induced electrical conductivity of the high-pressure phase of Mg(OH)₂. At the base of the mantle transition zone, several thermodynamic processes occur that might induce partial melting, as documented in seismological observations. First, the dissociation of high-pressure Mg(OH)₂ and other dense hydrous magnesium silicates such as phase-H(23) and phase-D(52) release water, which is likely to reduce the solidus of the lower mantle and lead to partial melting. In addition, it is known that there is a drastic reduction in the water storage capacity between the mantle transition zone minerals and lower mantle minerals, which also helps in reduction of the lower mantle solidus and thus helps in initiating partial melting in the lower mantle. Both processes may occur simultaneously and need to be understood to gain detailed insight into the deep Earth water budget.

Methods

We performed density functional theory calculations in conjunction with the projector augmented wave (PAW) method and plane wave basis sets as implemented in the Vienna Ab initio Simulation Package. Plane wave cutoffs of $E_k = 800$ eV and k-point sampling densities of 200$^{-1}$ were found to give sufficiently converged energies and forces. Electronic exchange-correlation energies are approximated with the PBE generalized gradient functional, and geometries were optimized until remaining forces on the atoms were smaller than 1 meV/Å. Crystal structure predictions were then run at 20, 50 and 100 GPa, with two and four formula units per unit cell, and utilizing approaches based on evolutionary algorithms and the particle swarm optimization method as implemented in the XtalOpt and CALYPSO packages. Around 600 structures were optimized in each search run. Phonon dispersions and densities of state were obtained with the finite displacement method using the PHON program and appropriate supercells of the relevant structures, with central difference dispersions of ±0.02 Å and up to 640 atoms. We applied ±1% strains to accurately determine the stresses in the limit of small strain. The elastic constants $C_{ij}$ were obtained from the stress-strain relation, $\sigma_{ij} = C_{ij} \varepsilon_{ij}$ (Voigt notation). The pressure de-
persistence of the full elastic stiffness tensor was fitted with the finite strain formulation. (60) The P-wave and S-wave anisotropy are defined as 
\[ A_{sP} = \frac{100 \times (V_{sP}^{\text{anisotropy}} - V_{sP}^{\text{reference}})}{V_{sP}^{\text{reference}}} \] 
and 
\[ A_{sS} = \frac{100 \times (V_{sS}^{\text{anisotropy}} - V_{sS}^{\text{reference}})}{V_{sS}^{\text{reference}}} \] respectively. We used petrophysical software to determine the elastic anisotropy. (62)

Acknowledgements

1. Pearson DG et al. (2014) Hydrous Mantle Transition Zone Indicated by Ringwoodite
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Footnote Author