Si-rich Mg-sursassite $Mg_4Al_5Si_7O_{23}(OH)_5$ with octahedrally coordinated Si: A new ultrahigh-pressure hydrous phase

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ABSTRACT

The crystal structure of a new high-pressure hydrous phase, Si-rich Mg-sursassite, of ideal composition $Mg_4Al_5Si_7O_{23}(OH)_5$, that was produced by sub-solidus reaction at 24 GPa and 1400 °C in an experiment using a model sedimentary bulk composition, has been determined by single-crystal X-ray diffraction. The phase was found to be topologically identical to Mg-sursassite, $Mg_5Al_5Si_6O_{21}(OH)_7$, and has space group $P2_1/m$ and lattice parameters $a = 8.4222(7)$, $b = 5.5812(3)$, $c = 9.4055(9)$ Å, $\beta = 106.793(8)°$, $V = 423.26(6)$ Å^3, and $Z = 1$. The empirical formula determined by electron microprobe analysis of the same crystal as was used in the X-ray experiment is $[Mg_{3.93(3)}Fe_{0.03(1)}]_{\Sigma3.96}[Al_{4.98(3)}Cr_{0.04(1)}]_{\Sigma5.02}Si_{7.02(4)}O_{23}(OH)_5$, with hydroxyl content implied by the crystal-structure analysis. The most significant aspect of the structure of Si-rich Mg-sursassite is the presence of octahedrally coordinated Si. Its structural formula is $^{M1,VII}Mg_2{}^{M2,VI}Mg_2^{2+}{}^{M3,VI}(Al_{0.5}Si_{0.5})_2{}^{M4,VI}Al_2{}^{M5,VI}Al_2{}^{T1,IV}Si_2{}^{T2,IV}Si_2{}^{T3,IV}Si_2O_{23}(OH)_5$. Si-rich Mg-sursassite joins the group of hydrous ultrahigh-pressure phases with octahedrally coordinated Si that have been discovered by experiment, and that may play a significant role in the distribution and hosting of water in the deep mantle at subduction zones. The reactions defining the stability of Si-rich Mg-sursassite are unknown, but are likely to be fundamentally different from those of Mg-sursassite, and involve other ultrahigh-pressure dense structures such as phase D, rather than phase A.

Keywords: Mg-sursassite, hydrous dense magnesium silicate, synthesis, microprobe analysis, X-ray diffraction, crystal structure

INTRODUCTION

Sursassite, ideally $Mn_4Al_6Si_6O_{22}(OH)_6$, occurs in Mn ore deposits (Nagashima et al. 2009) and is characteristically a low-pressure mineral. It is a sorosilicate with Si_2O_7 and SiO_4 groups that is related structurally to pumpellyite and ardennite. However, a fully Mg-substituted analog of composition $Mg_5Al_5Si_6O_{21}(OH)_7$ was first reported by Schreyer (1988) in experiments in the MgO-Al_2O_3-SiO_2-H_2O (MASH) system up to 5 GPa, 900 °C; he referred to this phase as "MgMgAl-pumpellyite." Fockenberg (1998) determined the maximum stability of this phase to 10 GPa and found that it had a thermal limit of 800 °C defined by the reactions Mg-sursassite = pyrope + topaz-OH + coesite/stishovite + H_2O. Using a model with ultrabasic bulk composition, Bromiley and Pawley (2002) determined the phase relations of Mg-sursassite to 10 GPa and showed that Mg-sursassite replaces chlorite as a major host of H_2O above 6 GPa via the reaction chlorite + enstatite = Mg-sursassite + forsterite + H_2O. The high-temperature limit of Mg-sursassite at 7–10 GPa (700–750 °C) for ultrabasic bulk compositions is defined by the reaction Mg-sursassite + phase A + enstatite = pyrope + H_2O. The general structural formula of sursassite-group minerals is $^{M1,VII}M_2^{2+}{}^{M2,VI}M_2^{M3,VI}(M^{2+},Al,Si)_2$ $^{M4,VI}Al_2{}^{M5,VI}Al_2{}^{T1,IV}Si_2{}^{T2,IV}Si_2{}^{T3,IV}Si_2O_{21-23}(OH)_{5-7}$. ^{T2}Si and ^{T3}Si

form a sorosilicate Si_2O_7 unit. Occupancies of H sites vary from 0.5 to 1. Compositional variation in sursassite-type phases involves (1) homovalent substitution at $M(1,2)$ sites, e.g., Mg, Mn^{2+}, Fe^{2+}; (2) heterovalent substitution at the $M3$ site, e.g., Mg for Al; and (3) charge balancing by $O^{2-} \rightarrow OH^-$. Two distinct stoichiometries have been reported: $M_4^{2+}Al_6Si_6O_{22}(OH)_6$ and $M_5^{2+}Al_5Si_6O_{21}(OH)_7$, being related by the substitution $Al + O^{2-} \leftrightarrow M^{2+} + OH^-$. In this paper we add a new stoichiometry, $M_4^{2+}Al_5Si_7O_{23}(OH)_5$, which we refer to as Si-rich Mg-sursassite.

In sursassite *sensu stricto*, the $M3$ site is fully occupied by Al, and there are five non-equivalent H sites bonded to three non-equivalent oxygen atoms; four of the H sites are half-occupied (Nagashima et al. 2009). The $M3$ site in Mg-sursassite has an average composition $Mg_{0.5}Al_{0.5}$ and there are four non-equivalent H sites, one of which is half-occupied. The structural formula of end-member Mg-sursassite is $^{M1,VII}Mg_2{}^{M2,VI}Mg_2^{2+}{}^{M3,VI}(Mg_{0.5}Al_{0.5})_2{}^{M4,VI}Al_2$ $^{M5,VI}Al_2{}^{T1,IV}Si_2{}^{T2,IV}Si_2{}^{T3,IV}Si_2O_{22}(OH)_7$. As described below, the new phase Si-rich Mg-sursassite has the structural formula $^{M1,VII}Mg_2{}^{M2,VI}Mg_2^{2+}{}^{M3,VI}(Al_{0.5}Si_{0.5})_2{}^{M4,VI}Al_2{}^{M5,VI}Al_2{}^{T1,IV}Si_2{}^{T2,IV}Si_2{}^{T3,IV}Si_2O_{23}(OH)_5$. The possible significance of this new type of sursassite is considered.

EXPERIMENTAL METHODS

A high-pressure experiment was performed at 24 GPa and 1400 °C using a 2000-ton Kawai-type multi-anvil apparatus at the Geodynamics Research Center, Ehime University, Matsuyama, Japan. A sintered mixture of 83% MgO + 17% CoO

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was used as the pressure medium. This mixture was formed into an octahedron of 8 mm edges and was compressed by eight cubic tungsten carbide anvils with 3 mm truncation edges. Pyrophyllite gaskets were placed between the anvils to support the anvil flanks. A cylindrical LaCrO$_3$ heater, 3.2/2.0 mm in outer/inner diameter and 4 mm long, was used. The samples were loaded into rhenium capsules isolated from heater by a MgO insulator.

The starting material, chosen to model "global subducted sediment" (GLOSS) of Plank and Langmuir (1998), was a mixture of high-purity reagents (in wt%): 58.66 SiO$_2$, 0.62 TiO$_2$, 11.93 Al$_2$O$_3$, 5.96 CaO, 5.22 FeO, 2.49 MgO, 0.32 MnO, 2.44 Na$_2$O, 2.04 K$_2$O, 3.02 CO$_2$, and 7.30 H$_2$O. Temperature was controlled by a W$_{97}$Re$_3$-W$_{75}$Re$_{25}$ thermocouple (0.1 mm diameter). Pressure was calibrated at room temperature using the semiconductor-to-metal transitions of Bi, ZnS, and GaAs (Irifune et al. 2004). The sample was initially pressurized to 24 GPa in 1 h and then heated to 1400 °C at a rate of 50 °C/min. The effect of temperature on pressure was further corrected using the α-β and β-γ transitions in Mg$_2$SiO$_4$ (Katsura and Ito 1989). The experiment lasted 4 h and was quenched by turning off power to the heater. The capsule was recovered, mounted in epoxy, sectioned, and polished.

CHEMICAL AND STRUCTURAL CHARACTERIZATION

The chemical composition of Mg-sursassite was first analyzed qualitatively with energy-dispersive X-ray spectroscopy (EDS) using a CamScan electron microscope MV2300. No elements with $Z > 9$ other than Al, Mg, Si, and minor Cr and Fe were detected. A small fragment of the of crystal analyzed by EDS ($15 \times 18 \times 24\ \mu m^3$) was extracted from the polished block for crystal structure determination by single-crystal X-ray diffraction (see below). After the X-ray experiment, this crystal fragment was analyzed by quantitative wavelength-dispersive X-ray (WDS) using a JEOL-JXA 8200 microprobe operated at 15 kV, 10 nA, and 1 μm beam size, with counting times of 20 s on-peak and 10 s for each background position. $K\alpha$ lines for all analyzed elements were referenced to synthetic mineral standards [olivine (Mg, Fe, Si), albite (Al), and knorringite (Cr)].

The crystal fragment was mounted on a 5 μm diameter carbon fiber, itself attached to a glass rod. Single-crystal X-ray diffraction intensity data were collected with a Bruker D8 Venture Photon 100 CMOS equipped with graphite-monochromatized Mo$K\alpha$ radiation. The detector-to-crystal distance was 50 mm. Data were collected using ω and φ scan modes, with a 0.5 ° frame-width and an exposure time of 50 s per frame. The data were corrected for Lorentz and polarization factors and absorption using the software package APEX3 (Bruker AXS Inc. 2016).

RESULTS AND DISCUSSION

Phases in the run product were identified using EMPA and single-crystal XRD. The product assemblage consisted of (vol%) Si-rich Mg-sursassite (1%) + phase D (20%) + hollandite (13%) + Al-phase D (13%) + Ca-perovskite (15%) + stishovite (38%) (Fig. 1). The compositions of run products are shown in Table 1.

As for the studied Si-rich sursassite, three very similar analyses were obtained by WDS microprobe analysis. The average has in wt% oxides (ranges in parentheses): MgO = 17.87 (17.69–17.93), Al$_2$O$_3$ = 28.66 (28.32–29.01), FeO = 0.29 (0.19–0.40), Cr$_2$O$_3$ = 0.37 (0.29–0.49), SiO$_2$ = 47.64 (47.40–48.11), total = 94.83 (94.22–95.05). The H$_2$O content, calculated from the crystal-structure analysis (see below), is 5.09 wt%, which gives an analysis total of 99.92 wt%. The empirical formula (16 cations pfu), assuming all Fe is divalent, all Cr is trivalent, and a H$_2$O content calculated from the ideal formula Mg$_4$Al$_5$Si$_7$O$_{23}$(OH)$_5$, is [Mg$_{3.93(3)}$Fe$_{0.03(1)}$]$_{\Sigma3.96}$[Al$_{4.98(3)}$Cr$_{0.04(1)}$]$_{\Sigma5.02}$Si$_{7.02(4)}$O$_{23}$(OH)$_5$. The minor Cr content (not present in the starting material) is likely due to a
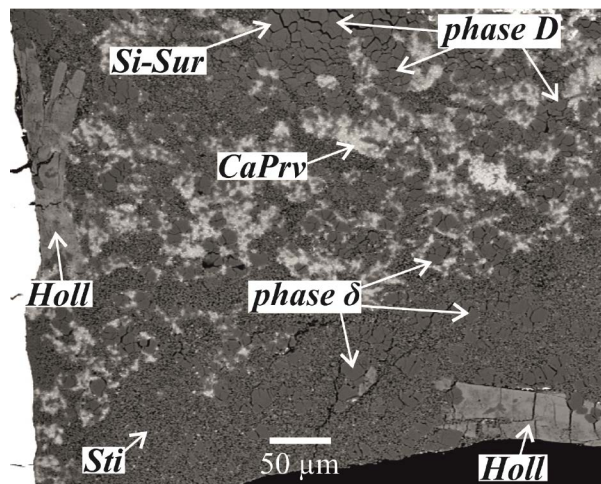

FIGURE 1. SEM-BSE image of the experimental run synthesized at $P = 24$ GPa and $T = 1400$ °C. Si-rich Mg-sursassite (Si-Sur) is associated with phase δ, hollandite (holl), stishovite (Sti), phase D, and Ca-perovskite (CaPrv). CamScan electron microscope MV2300.

TABLE 1. Microprobe data (wt% of oxides) of the different phases in the run product together with the atomic ratios calculated on the basis of atoms (phase δ and phase D) or oxygen content (Holl and Ca-Prv)

Phase	δ	D	Holl	Ca-Prv
SiO$_2$	13.99	38.39	65.97	57.58
TiO$_2$	0.86	0.21	–	0.16
Al$_2$O$_3$	63.48	23.40	19.70	–
FeO	2.47	6.61	0.31	0.57
MnO	–	0.15	–	–
MgO	5.85	17.25	0.36	0.54
CaO	–	0.05	0.60	40.26
Na$_2$O	–	–	0.53	0.23
K$_2$O	0.09	–	12.80	–
H$_2$O*	14.77	13.88	–	–
Total	101.51	99.94	100.27	99.34
O	–	–	8	3
Si	0.139	1.181	2.984	1.079
Ti	0.006	0.005	–	0.002
Al	0.746	0.848	1.050	–
Fe	0.021	0.170	0.012	0.009
Mn	–	0.004	–	–
Mg	0.087	0.790	0.024	0.015
Ca	–	0.002	0.029	0.808
Na	–	–	0.046	0.008
K	0.001	–	0.738	–
Total	1.000	3.000	4.883	1.921

Note: H$_2$O calculated from ideal formulas [Al-phase D: Mg(Si$_{1-x}$Al$_x$)$_2$O$_6$H$_{2+2x}$, phase δ: (AlMgSi)OOH].

contamination from the LaCrO$_3$ heater.

The diffraction data indicate that the structure is monoclinic. Systematic absences are consistent with space groups $P2_1$ and $P2_1/m$. Unit-cell parameters obtained from least-squares refinement of 198 reflections with $I/\sigma(I) > 10$ are $a = 8.4222(7)$, $b = 5.5812(3)$, $c = 9.4055(9)$ Å, $\beta = 106.793(8)°$, $V = 423.26(6)$ Å^3. The unit-cell parameters and $P2_1/m$ symmetry indicated a close correspondence with those of synthetic Mg-sursassite reported by Gottschalk et al. (2000), for which $a = 8.5424(8)$, $b = 5.5717(3)$, $c = 9.6484(6)$ Å, $\beta = 108.298(4)°$, $V = 447.0(1)$ Å^3. Consequently, the atom coordinates of the structure of Mg-sursassite reported by Gottschalk et al. (2000) were used as the starting model for

structure refinement by full-matrix least-squares methods using SHELXL-97 (Sheldrick 2008).

Scattering curves for neutral atoms were taken from the *International Tables for Crystallography* (Wilson 1992). In refining site-scattering at sites, vacancies were allowed on all M sites. Initially, site-scattering values were obtained by allowing unconstrained occupancies of sites using Mg ($M1$, $M2$), Al ($M4$, $M5$), and Si ($M3$, $T1$, $T2$, $T3$). Refined occupancy levels indicated that $M1$ and $M2$ are filled by Mg, whereas $M4$ and $M5$ are filled by Al. However, the refined occupancy of $M3$ using a neutral scattering factor for Si is 0.967(2) and corresponds to 13.47(2) electrons. Hence, the most reasonable interpretation of the site-scattering at $M3$ is that this site has an occupancy of $Al_{0.5}Si_{0.5}$. The high Si occupancy of this site is consistent with the small volume of the $M3$ octahedron (7.53 $Å^3$), which is much smaller than 9.40 $Å^3$ for $^{M3}AlO_6$ in sursassite (Nagashima et al. 2009) and 10.30 $Å^3$ for $^{M3}(Mg_{0.5}Al_{0.5})O_6$ in Mg-sursassite (Gottschalk et al. 2000). The SiO_6 octahedron in stishovite has a volume of 6.61 $Å^3$ (Hill et al. 1983). Thus, there is compelling evidence from chemistry and structure that the crystal of this study has stoichiometric amounts of excess Si relative to Mg-sursassite and that this excess Si is octahedrally coordinated Si.

On the basis of refined site-scattering values, the occupancies of sites were fixed at $M(1,2)$ = Mg, $M3$ = ($Al_{0.5}Si_{0.5}$), $M(4,5)$ = Al, $T(1,2,3)$ = Si for subsequent anisotropic refinement. With full anisotropic refinement to convergence gave agreement indices of R_1 = 0.040, wR_2 = 0.074, GoF = 0.935. Unsurprisingly for such a small crystal, no hydrogen atoms were located in difference-Fourier maps.

A list of observed and calculated structure factors and the CIF are deposited[1]. Details relating to the data collection and structure refinement are given in Table 2. Table 3 gives bond-valence sums (BVS), computed on the basis of bond-valence parameters of Brese and O'Keeffe (1991) for cations and oxygen atoms. The key features of the structure of Si-rich Mg-sursassite are summarized in Figure 2.

The interpretation of oxygen donors and acceptors in sursassite-group structures requires some care, as there are half-occupied and fully occupied H sites and mixed occupancies of cation sites. In the case of sursassite *sensu stricto*, these issues have been addressed in detail by Nagashima et al. (2009), and we have used their analysis to aid interpretation of the bond-valences of some of the more problematic oxygen atoms in Si-rich Mg-sursassite, namely O(5), O(7), and O(10).

In Si-rich Mg-sursassite, atoms O(6) (BVS = 1.21 v.u.) and O(11) (BVS = 1.16 v.u.) are obvious oxygen donors for OH groups and are very likely to be associated with fully occupied H atom sites. The BVS values for O(7) and O(10) are very similar to those of sursassite. As pointed out by Nagashima et al. (2009), O(10) is anomalous in that it is twofold-coordinated, being bonded only to ^{T1}Si and ^{M2}Mn (^{M2}Mg in Mg-sursassite and Si-rich Mg-sursassite). There is no evidence for protonation of this oxygen atom, as occurs in the related mineral macfallite (Nagashima et al. 2008), e.g., location of nearby H or lengthening of the Si1-O(10) bond. There is, however, the likelihood of O(10) receiving a strong hydrogen-bond from O(6)H, thereby raising its BVS value to ~1.7 v.u. (Nagashima et al. 2009): d[O(6)···O(10)] = 2.80 Å.

The O(7) atom is bonded to two $M3$ and one Mg1 sites. There are two possibilities for assigning its bond-valence deficiency: (1) O(7) receives a strong hydrogen-bond from O(6), or

TABLE 2. Data and experimental details for the selected Si-rich Mg-sursassite crystal

Crystal data	
Formula	$Mg_4Al_5Si_7O_{23}(OH)_5$
Crystal size (mm)	0.015 × 0.018 × 0.024
Form	block
Color	white
Crystal system	monoclinic
Space group	$P2_1/m$ (no. 11)
a (Å)	8.4222(7)
b (Å)	5.5812(3)
c (Å)	9.4055(9)
B (°)	106.793(8)
V ($Å^3$)	423.26(6)
Z	1
Data collection	
Instrument	Bruker D8 Venture
Radiation type	$MoK\alpha$ (λ = 0.71073)
Temperature (K)	295(3)
Detector to sample distance (cm)	5
Number of frames	1102
Measuring time (s)	50
Maximum covered 2θ (°)	66.08
Absorption correction	multi-scan
Collected reflections	3488
Unique reflections	1734
Reflections with $F_o > 4\sigma(F_o)$	850
R_{int}	0.0228
R_σ	0.0834
Range of h, k, l	$-12 \le h \le 11, -8 \le k \le 8, 0 \le l \le 13$
Refinement	
Refinement	Full-matrix least squares on F^2
Final R_1 [$F_o > 4\sigma(F_o)$]	0.0343
Final R_1 (all data)	0.0401
Number refined parameters	124
GoF	0.935
$\Delta\rho_{max}$ (e $Å^{-3}$)	0.50
$\Delta\rho_{min}$ (e $Å^{-3}$)	−0.39

TABLE 3. Bond valence sums (v.u.) in the structure of Si-rich Mg-sursassite

	M1	M2	M3	M4	M5	T1	T2	T3	ΣO
	(Mg)	(Mg)	($Al_{0.50}Si_{0.50}$)	(Al)	(Al)	(Si)	(Si)	(Si)	
O1	0.247×2↓	0.267×2↓	0.530×2↓					0.912×2↓	1.956
O2	0.375×2↓				0.452×2↓	1.079×2↓			1.906
O3		0.420×2↓		0.489×2↓			1.067×2↓		1.976
O4				0.544×2↓→		0.920			2.008
O5		0.124	0.660×2↓→			0.937			2.381
O6					0.605×2↓				1.210
O7	0.244		0.714×2↓→						1.672
O8	0.099				0.495×2↓→		1.093		2.182
O9	0.177						0.932	0.950	2.059
O10		0.425						1.036	1.461
O11				0.581×2↓→					1.162
	1.764	1.923	3.808	3.228	3.104	4.015	4.159	3.810	

(2) O(7) = 50% O/50% OH. How might we choose between these two options? The composition of Si-rich Mg-sursassite is very well-defined by EMPA (see above). The cation composition 4Mg:5Al:7Si requires 51 negative charges to charge-balance. There are 28 O atoms p.f.u and so five of these must be OH. O(6) and O(11) are fully occupied OH groups. Hence, an additional half-occupied OH group must be present that would have an oxygen atom BVS of ~1.5 v.u.: atoms O(7) and O(10) are the only candidates. However, we have seen above that O(10) is very unlikely to be an OH group, half or fully occupied. This leaves O(7) as the only other possibility. This atom also correlates with a hydroxyl group in sursassite ($M3$ = Al) and Mg-sursassite ($M3$ = $Mg_{0.5}Al_{0.5}$). Hence, it would seem reasonable to propose that it is a 50/50 O/OH site in Si-rich Mg-sursassite; O(6) with which
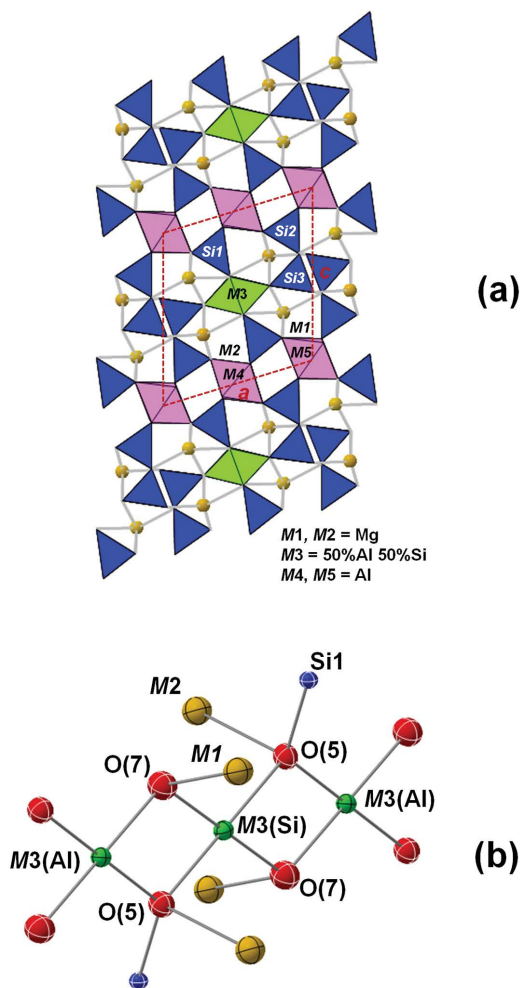
FIGURE 2. (**a**) View of the structure of Si-rich Mg-sursassite determined in this study projected onto the (010) plane. Blue = isolated SiO_4 and Si_2O_7 sorosilicate groups, pink = $M4$ and $M5$ octahedra (Al), green = $M3$ octahedron (50%Al, 50%Si), orange spheres = $M1$ (Mg) and $M2$ (Mg). Rows of $M(2,3,4,5)$ octahedra and $^{VII}M1$ polyhedra extend into the page parallel to [010]. (**b**) A fragment of a row of $M3$ octahedra in Si-rich Mg-sursassite showing the coordination of O(5) and O(7) oxygen atoms. The two O(1) atoms of the $M3O_6$ octahedron have been omitted for clarity. The proposed local ordering of Al and Si in the $M3$ sites is indicated. All atoms are shown as displacement ellipsoids at the 68% probability level. (Color online.)

it likely forms a strong hydrogen bond has two half-occupied H sites and so has full OH occupancy overall (as its BVS value of 1.21 v.u. indicates). The corresponding configuration occurs in sursassite (Nagashima et al. 2009).

IMPLICATIONS

The experiment reported in this paper was a synthesis, and as such it is not proof *sensu stricto* of the thermodynamic stability under these *P-T* conditions of any of the product phases. However, as noted above, Si-rich Mg-sursassite grew at 24 GPa during heating to 1400 °C and persisted to the end of the experi-

ment. This temperature is much higher than the 800 °C limit at 10 GPa of Mg-sursassite (Fockenberg 1998).

The presence of octahedrally coordinated Si in Si-rich Mg-sursassite suggests that the reactions defining its *P-T* stability in ultrabasic and basic bulk compositions are likely to be fundamentally different from those of Mg-sursassite (which, in turn, has a much greater *P-T* stability than sursassite) and involve ultrahigh-pressure structures such as phase D, rather than phase A. Future experiments at 10–25 GPa and 800–1400 °C on ultrabasic, basic, and felsic model bulk compositions, and on Si-rich Mg-sursassite itself, should provide insights into the significance of this phase for the hydrous mineralogy of deep subduction.

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Endnote:

[1]Deposit item AM-20-97533, CIF. Deposit items are free to all readers and found on the MSA website, via the specific issue's Table of Contents (go to http://www.minsocam.org/MSA/AmMin/TOC/2020/Sep2020_data/Sep2020_data.html).