minerals

Supplementary materials

Thermoelastic Properties of $K_{0.7}Na_{0.3}AlSi_3O_8$ Hollandite and $NaAlSi_2O_6$ Jadeite: Implication for the Fate of the Subducted Continental Crust in the Deep Mantle

Steeve Gréaux [1,2,*], Youmo Zhou [1], Yoshio Kono [1], Akihiro Yamada [1,§], Yuji Higo [3] and Tetsuo Irifune [1,2]

1 Geodynamics Research Center, Ehime University, Matsuyama, Ehime 790-8577, Japan; youmo@sci.ehime-u.ac.jp (Y.Z.); kono@sci.ehime-u.ac.jp (Y.K.); yamada.ak@mat.usp.ac.jp (A.Y.); irifune@dpc.ehime-u.ac.jp (T.I.)
2 Earth-Life Science Institute, Tokyo Institute of Technology, Tokyo 152-8550, Japan
3 Japan Synchrotron Radiation Institute, SPring-8, Hyogo 679-5198, Japan; higo@spring8.or.jp
* Correspondence: greaux@sci.ehime-u.ac.jp
§ Current address: Center for the Glass Science and Technology, The University of Shiga Prefecture, Hikone 522-8533, Japan

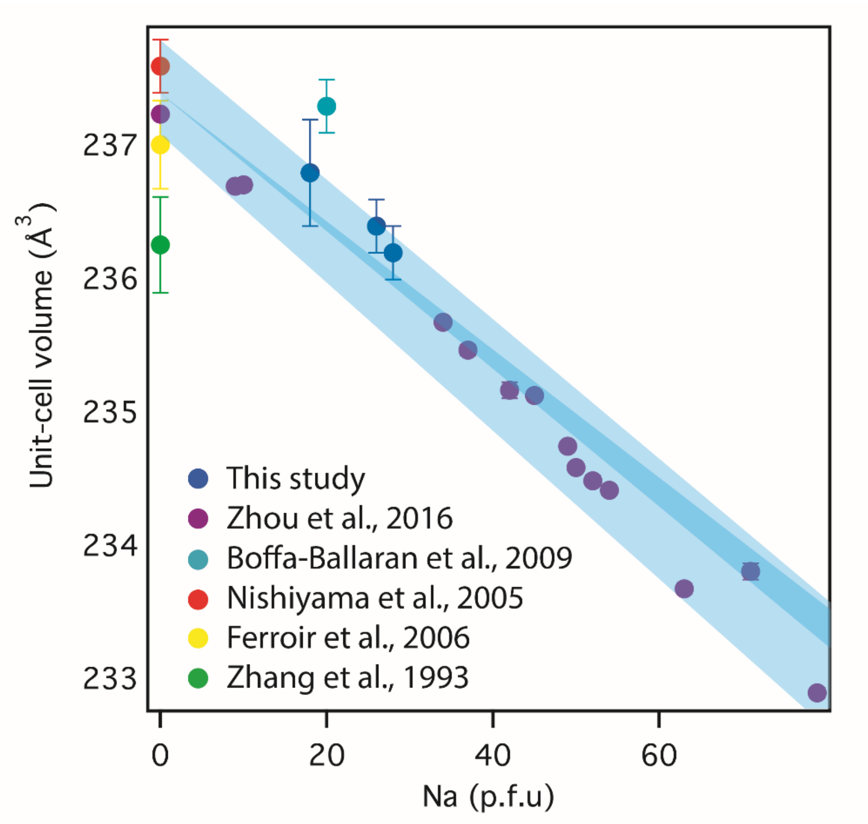

Figure S1. Unit-cell volume of liebermannite as a function of Na-content. The shaded area represents the uncertainties on the determination of the unit-cell volume of the $KAlSi_3O_8$ endmember on the basis of the data of Nishiyama et al. [18] and Ferroir et al. [19], which is translated to the other compositions.

Table S1. Raw data for: Pressure (NaCl scale), Pressure (Au scale), Temperature (Kelvin), Unit-cell volume of Na-liebermannite (Angstrom cube), Unit-cell volume of Jadeite (Angstrom cube).

P_NaCl (Gpa)	P_Au (Gpa)	T (K)	V_Lieb (Å^3)	err_V_Lieb	V_Jd (Å^3)	err_V_Jd
7.026	7.646	300	228.105608	0.034	381.300604	0.059
11.627	11.628	300	225.033551	0.028	373.256031	0.055
13.802	13.893	300	223.031548	0.032	368.154679	0.053
14.614	14.922	300	222.136033	0.029	365.320207	0.051
16.107	16.107	300	220.387379	0.026	362.611472	0.044
17.164	17.764	300	218.494467	0.02	360.391433	0.044
11.896	12.006	500	225.437117	0.028	374.092062	0.053
14.091	14.238	500	223.087682	0.033	368.247367	0.05
14.917	15.207	500	222.636561	0.028	365.233569	0.058
16.553	16.553	500	220.798399	0.023	362.290041	0.046
17.668	17.968	500	218.67797	0.017	361.326151	0.057
12.235	12.269	700	225.91973	0.029	374.621195	0.056
14.483	14.835	700	223.116743	0.032	367.85144	0.054
15.296	15.355	700	223.023533	0.028	365.702597	0.048
16.88	16.743	700	221.172484	0.022	363.113605	0.044
17.946	18.363	700	219.184782	0.018	362.056882	0.05
12.625	12.407	900	226.90488	0.034	374.929213	0.048
15.095	15.17	900	223.595875	0.031	368.804352	0.054
15.662	15.709	900	223.615671	0.028	366.374774	0.046
17.277	17.327	900	221.681429	0.024	364.128547	0.045
18.268	18.684	900	219.65628	0.018	362.632346	0.05
13.072	13.168	1100	227.220517	0.034	375.61337	0.048
15.397	15.493	1100	224.083194	0.033	369.484882	0.053
16.016	16.384	1100	223.961007	0.03	367.085907	0.051
17.671	17.518	1100	222.138232	0.024	365.043653	0.046
18.83	18.83	1100	220.188129	0.019	362.943756	0.055
16.607	16.992	1300	224.326985	0.03	367.466495	0.051
17.975	18.338	1300	222.792246	0.027	366.198889	0.051
19.143	19.143	1300	220.706067	0.019	363.762981	0.053
18.66	18.744	1500	223.167134	0.025	366.494264	0.05
19.637	19.826	1500	221.248695	0.019	363.844074	0.049
20.202	20.38	1700	221.909056	0.022	363.811834	0.042

Abbreviations stand for: P, pressure; T, temperature; V_Lieb, unit-cell volume of Na-liebermannite; V_Jd, unit-cell volume of jadeite.

Table S2. Thermoelastic parameters of major mantle minerals.

Mineral	V_0 (Å)	K_0 (GPa)	K′	∂K/∂T ($GPa \cdot K^{-1}$)	a_0 (10^{-5} K^{-1})	b_0 (10^{-8} K^{-2})	Ref.
				Pyrolite			
Olivine	292.1	129	4.6	−0.038	2.27	2.22	a
Wadsleyite	538.5	169	4.1	−0.021	2.31	1.18	b
Ringwoodite	527.8	187	4.4	−0.028	1.90	1.20	c
Pyroxene	423.46	126	4.0	−0.015	2.20	-	d
Garnet	1500.4	167	4.6	−0.021	2.58	1.02	e
Majorite	1509.1	156	4.4	−0.019	2.88	2.93	f
CaPv	45.6	244	4.0	−0.035	3.06	0.87	g
				Harzburgite			
Olivine	292.1	129	4.6	−0.038	2.27	2.22	a
Wadsleyite	538.5	169	4.1	−0.021	2.31	1.18	b
Ringwoodite	527.8	187	4.4	−0.028	1.90	1.20	c
Pyroxene	423.46	126	4.0	−0.015	2.20	-	d
Garnet	1500.4	167	4.6	−0.021	2.58	1.02	e
Akimotoite	263.9	210	5.6	−0.040	2.41	-	h
				Oceanic crust			
Coesite	546.5	97.4	4.3	−0.020	1.03	-	i
Stishovite	46.64	294	5.3	−0.041	1.40	1.09	j
Pyroxene	423.46	126	4.0	−0.015	2.20	-	d
Garnet	1500.4	167	4.6	−0.021	2.58	1.02	e
Majorite	1574.1	170	4.0	−0.015	2.20	0.70	k
CaPv	45.58	209	4.8	−0.021	2.86	-	g
				Continental crust and sediments			
Coesite	546.5	97.4	4.3	−0.020	1.03	-	i
Stishovite	46.76	292	4.95	−0.042	1.90	1.03	J
Garnet	1500.4	167	4.6	−0.021	2.58	1.02	e
Pyroxene	402.4	127	4.0	−0.012	2.60	-	*
Kyanite	294.05	196	4.0	−0.021	2.53	-	l
CAS phase	324.2	171	5.1	−0.023	2.94	0.51	m
Orthoclase	723.66	67	4.0	−0.015	4.10	-	n
Hollandite-I	236.24	211	4.0	−0.043	2.90	-	**
Hollandite-II	237.01	184	4.0	−0.031	3.30	-	**
CaPv	45.58	209	4.0	−0.011	2.21	-	g

This study: * $NaAlSi_2O_6$ Jadeite and ** $K_{0.7}Na_{0.3}AlSi_3O_8$ hollandite; a: Liu and Li [1]; b: Katsura et al. [2]; c: Nishihara et al. [3]; d: Nishihara et al. [4]; e: Zou et al. [5]; f: Morishima et al. [6]; g: Ricolleau et al. [7]; h: Wang et al. [8]; i: Angel et al. [9]; j: Nishihara et al. [10]; k: Nishihara et al. [11]; l: He et al. [12]; m: Gréaux et al. [13]; n: Angel et al. [14].

References list for Table S2:

1. Liu, W.; Li, B. Thermal equation of state of $(Mg_{0.9}Fe_{0.1})_2SiO_4$ olivine. *Phys. Earth Planet. Inter.* **2006**, *157*, 188–195.
2. Katsura, T.; Shatskiy, A.; Manthilake, M.G.M.; Zhai, S.; Yamazaki, D.; Matsuzaki, T.; Yoshino, T.; Yoneda, A.; Ito, E.; Sugita, M.; et al. P-V-T relations of wadsleyite determined by in situ X-ray diffraction in a large-volume high-pressure apparatus. *Geophys. Res. Lett.* **2009**, *36*, L11307–5.
3. Nishihara, Y.; Takahashi, E.; Matsukage, K. N.; Iguchi, T.; Nakayama, K.; Funakoshi, K.-I. Thermal equation of state of $(Mg_{0.91}Fe_{0.09})_2SiO_4$ ringwoodite. *Phys. Earth Planet. Inter.* **2004**, *143–144*, 33–46.
4. Nishihara, Y.; Takahashi, E.; Matsukage, K.; Kikegawa, T. Thermal equation of state of omphacite. *Am. Mineral.* **2003**, *88*, 80–86.
5. Zou, Y.; Gréaux, S.; Irifune, T.; Whitaker, M.L.; Shinmei, T.; Higo, Y. Thermal equation of state of $Mg_3Al_2Si_3O_{12}$ pyrope garnet up to 19 GPa and 1,700 K. *Phys. Chem. Miner.* **2012**, *39*, 589–598.
6. Morishima, H.; Ohtani, E.; Kato, T.; Kubo, T.; Suzuki, A.; Kikegawa, T.; Shimomura, O. The high-pressure and temperature equation of state of a majorite solid solution in the system of $Mg_4Si_4O_{12}$-$Mg_3Al_2Si_3O_{12}$. *Phys. Chem. Miner.* **1999**, *27*, 3–10.

7. Ricolleau, A.; Fei, Y.; Cottrell, E.; Watson, H.; Deng, L.; Zhang, L.; Fiquet, G.; Auzende, A.-L.; Roskosz, M.; Morard, G.; et al. Density profile of pyrolite under the lower mantle conditions. *Geophys. Res. Lett.* **2009**, *36*, L06302.
8. Wang, Y.; Uchida, T.; Zhang, J.; Rivers, M.L.; Sutton, S. R. Thermal equation of state of akimotoite $MgSiO_3$ and effects of the akimotoite–garnet transformation on seismic structure near the 660 km discontinuity. *Phys. Earth Planet. Inter*. **2004**, *143–144*, 57–80.
9. Angel, R.J.; Mosenfelder, J.L.; Shaw, C. Anomalous compression and equation of state of coesite. *Phys. Earth Planet. Inter.* **2001**, *124*, 71–79.
10. Nishihara, Y.; Nakayama, K.; Takahashi, E.; Iguchi, T.; Funakoshi, K.-I. P-V-T equation of state of stishovite to the mantle transition zone conditions. *Phys. Chem. Miner.* **2004**, *31*, 660–670.
11. Nishihara, Y.; Aoki, I.; Takahashi, E.; Matsukage, K.N.; Funakoshi, K.-I. Thermal equation of state of majorite with MORB composition. *Phys. Earth Planet. Inter*. **2005**, *148*, 73–84.
12. He, Q.; Liu, X.; Li, B.; Deng, L.; Liu, W.; Wang, L. Thermal equation of state of a natural kyanite up to 8.55 GPa and 1273 K. *Matter Radiat. Extrem.* **2016**, *1*, 269–276.
13. Gréaux, S.; Nishiyama, N.; Kono, Y.; Irifune, T.; Gautron, L. P-V-T equation of state of $CaAl_4Si_2O_{11}$ CAS phase. *Phys. Chem. Miner.* **2011**, *38*, 581–590.
14. Angel, R.J.; Hazen, R.M.; McCormick, T.C.; Prewitt, C.T.; Smyth, J.R. Comparative compressibility of end-member feldspars. *Phys. Chem. Miner.* **1988**, *15*, 313–318.