

Wide distribution and partial melting of eclogite indicated by the X-discontinuity in the upper mantle

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Contents of this file

Figures S1

Tables S1 to S4

Introduction

The following supplementary materials provide first-principle calculation results of EOS of high-pressure clinoenstatite (HPCEN, MgSiO_3) together with previous experimental results (Table S1-S2), elastic constants of HPCEN (Figure S1, Table S3), the pressure and temperature dependency of elastic properties of HPCEN (Table S4).

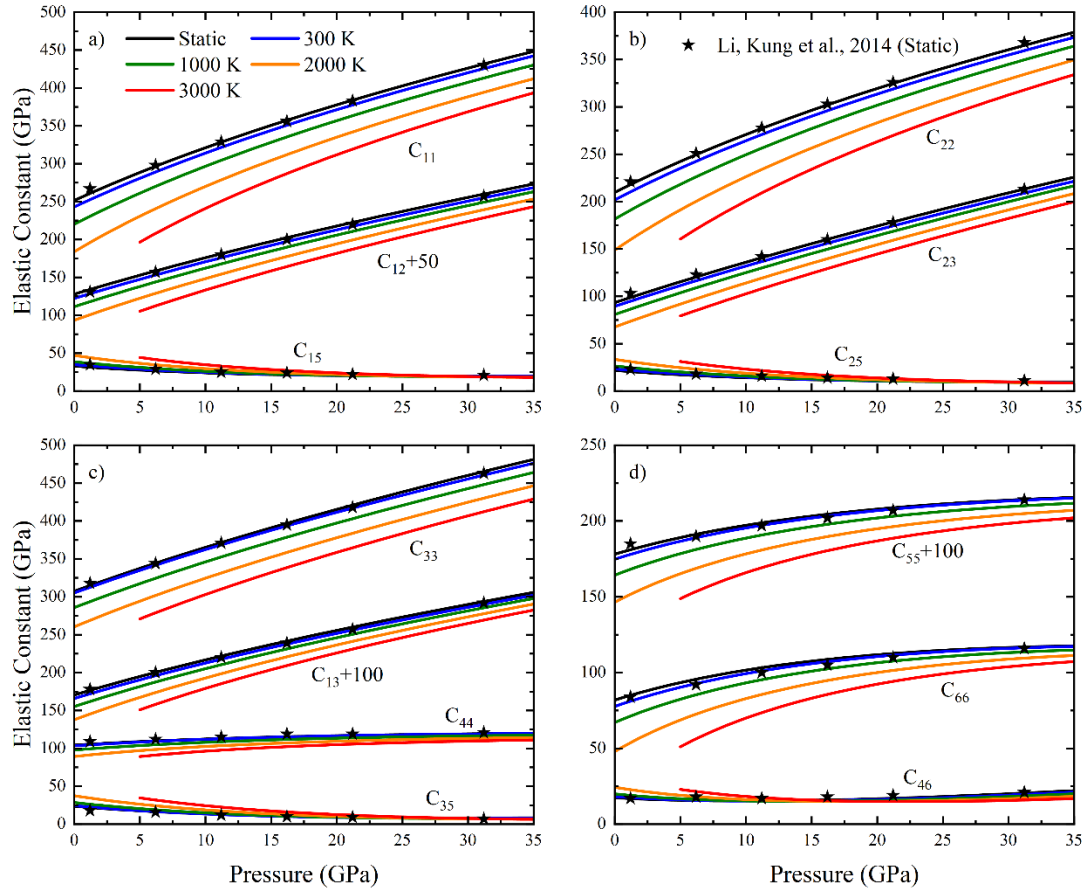


Figure S1. Elastic constants of HPCEN as a function of pressure at different temperature, in contrast to static GGA results of *Li et al.* (2014).

P (GPa)	T (K)	V (Å ³)	
		<i>Shinmei et al.</i> (1999)	This study
6.61	1173	392.4	393.3
7.32	300	381.9	383.7
8.69	300	378.5	380.3
9.20	300	377.0	379.2
10.68	300	373.8	375.9
11.22	573	374.2	376.8
11.27	873	376.3	379.3
9.23	300	376.9	379.2
9.04	300	377.6	379.4
10.19	573	376.4	378.9
11.35	873	376.1	379.2
11.75	1073	376.2	379.9
11.92	1273	378.2	381.7
11.14	1473	382.8	384.8
7.11	300	382.2	383.7
7.01	300	382.9	383.7
6.80	300	383.9	384.9
6.04	300	385.5	386.1
5.26	300	387.4	388.6
4.02	300	391.2	391.2
5.03	300	388.6	388.6
6.52	573	386.3	387.1
8.12	873	384.5	386.2
8.73	1173	385.5	388.0

Table S1. The volume of HPCEN at high pressure and high temperature.

	V_0 (\AA^3)	K_{T0} (GPa)	K'_{T0}	
This study	402.4	127.4	5.25	
<i>Lazarz et al.</i> (2019)	401.2	129	4 (fixed)	
<i>Lazarz et al.</i> (2019) ^a	403.9	121	4 (fixed)	0 GPa, 300 K
<i>Jacobsen et al.</i> (2010)	404	119	6.1	
<i>Shinmei et al.</i> (1999)	405	106	5	
This study	384.5	160.6	5	6.5 GPa, 300 K
<i>Kung et al.</i> (2005)	385	155	5.5	

^a. *Lazarz et al.* (2019) combined their results with those of *Angel and Hugh-Jones* (1994) together to fit the Birch-Murnaghan Equation with fixed K'_{T0} .

Table S2. Volume, isothermal bulk modulus and its derivative to pressure of HPCEN at 300 K.

	<i>Li et al. (2014) / This study</i>												
P (GPa)	C ₁₁	C ₂₂	C ₃₃	C ₁₂	C ₁₃	C ₂₃	C ₄₄	C ₅₅	C ₆₆	C ₁₅	C ₂₅	C ₃₅	C ₄₆
1.2	267/261	221/218	318/315	109/106	85/81	84/85	81/84	78/77	103/99	35/32	23/21	18/22	17/17
6.2	298/297	251/250	344/344	112/110	90/91	96/92	107/109	100/100	123/120	29/27	18/16	16/16	18/16
11.2	329/328	278/277	372/371	115/113	97/99	103/100	131/130	120/122	142/141	25/23	16/14	12/13	17/15
16.2	356/357	303/302	395/397	119/115	102/104	105/109	150/152	139/142	160/160	24/21	12/14	10/10	18/16
21.2	383/384	326/325	418/421	119/117	107/109	110/113	170/173	157/160	178/179	22/20	13/10	9/9	19/17
31.2	430/432	365/368	463/465	121/119	114/114	117/116	207/210	192/194	213/213	21/20	11/10	8/7	21/21

Table S3. Elastic Constants (GPa) of HPCEN at static conditions. Both GGA results of *Li et al. (2014)* after pressure correction and LDA results of this study are listed.

Parameters	K_S	G	Parameters	V_P	V_S
M_0 (GPa)	126.7	82.73	M_0 (km s ⁻¹)	8.452	4.995
$\frac{\partial M}{\partial P}$	6.425	2.042	$\frac{\partial M}{\partial P}$ (km s ⁻¹ GPa ⁻¹)	0.128	0.0424
$\frac{\partial M}{\partial T}$ (MPa/K)	-21.38	-11.17	$\frac{\partial M}{\partial T}$ ($\times 10^{-3}$ km s ⁻¹ K ⁻¹)	-0.525	-0.266
$\frac{\partial^2 M}{\partial P^2}$ ($\times 10^{-3}$ GPa ⁻¹)	-68.89	-44.04	$\frac{\partial^2 M}{\partial P^2}$ ($\times 10^{-3}$ km s ⁻¹ GPa ⁻²)	-2.659	-1.273
$\frac{\partial^2 M}{\partial P \partial T}$ ($\times 10^{-3}$ K ⁻¹)	0.5886	0.3755	$\frac{\partial^2 M}{\partial P \partial T}$ ($\times 10^{-6}$ km s ⁻¹ GPa ⁻¹ K ⁻¹)	23.56	12.08
$\frac{\partial^2 M}{\partial T^2}$ ($\times 10^{-6}$ GPa K ⁻¹)	-1.932	-0.088	$\frac{\partial^2 M}{\partial T^2}$ ($\times 10^{-6}$ km s ⁻¹ K ⁻²)	-0.070	-0.032

Table S4. Elastic moduli and velocities of HPCEN and their first and second derivatives with respect to pressure and temperature. The polynomial fitting equation is $M = M_0 + \left(\frac{\partial M}{\partial P}\right) \cdot P + \left(\frac{\partial M}{\partial T}\right) \cdot (T - 300) + \left(\frac{\partial^2 M}{\partial P^2}\right) \cdot P^2 + \left(\frac{\partial^2 M}{\partial T^2}\right) \cdot (T - 300)^2 + \left(\frac{\partial^2 M}{\partial P \partial T}\right) \cdot P \cdot (T - 300)$, $M = K_S, G, V_P$, and V_S . The fitting range is 0-25 GPa and 300-2000 K for pressure and temperature, respectively.