Table S1. Chemical composition of diopside used in this study and previous studies

Element	Fe-bearing diopside [a]	Diopside [b]	Diopside [b]
SiO_2	53.3(4) [c]	55.4(3)	53.6(3)
CaO	25.2(3)	26.1(1)	25.4(1)
Na_2O	0.04(2)	0.03(2)	/
K_2O	0.02(1)	/	/
MgO	14.6(2)	18.6(1)	17.8(1)
Fe_2O_3	6.7(4)	0.14(1)	0.79(4)
Cr_2O_3	/	0.05(1)	/
Al_2O_3	0.04(2)	0.03(1)	0.56(2)
TiO_2	0.03(1)	0.02(2)	/
MnO	0.04(2)	0.02(2)	0.06(1)
Total	99.97	100.37	98.11

a) This study; b) Sang et al. (2011);

c) Numbers in parentheses are the standard deviation of measurements.

Table S2. Single-crystal elastic moduli of diopside and hedenbergite at ambient conditions

Elastic constants	Diopside [a]	Diopside [b]	Diopside [c]	Diopside [d]	Hedenbergite [e]
Methods	BLS	BLS	BLS	BLS	BLS
C_{11}	225.8(6)	229.0(4)	226.1(9)	223(2)	222(6)
C_{22}	178.3(8)	179.0(4)	179.5(8)	171(2)	176(5)
C_{33}	246.7(7)	242.5(4)	239.2(9)	235(2)	249(5)
C_{44}	72.5(7)	78.9(3)	78.1(6)	74(1)	55(3)
C_{55}	65.6(8)	68.1(2)	69.2(4)	67(1)	63(2)
C_{66}	73.8(6)	78.2(3)	76.4(8)	66(2)	60(4)
C_{12}	77.5(8)	78.0(7)	77(1)	77(3)	69(14)
C_{13}	71.7(6)	69.8(6)	70(1)	81(2)	79(9)
C_{23}	65.6(7)	58.0(7)	57(2)	57(2)	86(10)
C_{15}	10.8(5)	9.9(3)	9.9(7)	17(1)	12(3)
C_{25}	8.5(4)	6.1(5)	6(1)	7(2)	13(7)
C_{35}	38.6(8)	40.9(3)	41.0(7)	43(1)	26(3)
C_{46}	5.3(3)	6.6(2)	6.8(4)	7.3(9)	-10(3)
K_S (GPa)	117(2)	114.6(7)	113.7(8)	113(4)	120.4[f]
G (GPa)	70(1)	72.7(4)	72.2(5)	67(2)	61.8[f]
V_P (km/s)	7.92(1)	8.06[f]	8.01[f]	7.838[f]	7.45[f]
V_S (km/s)	4.57(1)	4.72[f]	4.70[f]	4.513[f]	4.11[f]
ρ (g/cm^3)	3.345(1)	3.264(6)	3.270(1)	3.286[f]	3.657[f]

a) $Di_{80}Hd_{20}$, This study; b) Di_{100}, Sang et al. (2011); c) $Di_{97}Hd_2Jd_1$, Sang et al. (2011);

d) $Di_{98}Hd_1Jd_1$, Levien et al. (1979); e) Hd_{100}, Kandelin and Weidner (1988a);

f) The uncertainties are not available in the text.

Di: Diopside; Hd: Hedenbergite; Jd: Jadeite. BLS: Brillouin Light Scattering.

Table S3. Single-crystal elastic moduli of $Di_{80}Hd_{20}$ at high pressure in this study

Elastic constants	2.0(1) GPa	5.0(2) GPa	7.7(2) GPa	10.5(2) GPa	12.7(3) GPa	15.3(3) GPa	18.5(3) GPa
C_{11}	241.9(8)	256(1)	274(1)	285(1)	299(1)	314(2)	325(1)
C_{22}	190.2(7)	213(2)	230(1)	244(2)	251(1)	266(2)	276(3)
C_{33}	260.8(9)	280(1)	293(1)	312(1)	323(1)	341(2)	356(2)
C_{44}	78.3(8)	80(1)	83(1)	89(2)	91(1)	94(1)	95(2)
C_{55}	67.3(7)	72(1)	74(1)	78(1)	81(2)	84(1)	85(2)
C_{66}	75.7(8)	82(1)	84(1)	92(1)	96(2)	97(2)	103(1)
C_{12}	84.2(8)	91(2)	103(2)	112(3)	118(3)	121(2)	129(3)
C_{13}	80.1(7)	91(1)	106(2)	110(2)	121(3)	127(3)	129(3)
C_{23}	72.1(9)	75(2)	88(1)	96(2)	103(2)	116(2)	122(3)
C_{15}	9.2(6)	7(1)	5(2)	5(3)	6(2)	4(2)	2(2)
C_{25}	6.3(7)	7(2)	5(2)	4(3)	2(3)	-4(3)	-6(2)
C_{35}	33.3(6)	33(1)	31(1)	27(2)	26(2)	26(2)	19(2)
C_{46}	6.2(8)	4(2)	-3(2)	3(3)	-1(3)	3(2)	-4(2)
K_S (GPa)	127(2)	138(2)	153(2)	163(2)	171(2)	181(3)	190(2)
G (GPa)	73(1)	78(1)	81(1)	86(1)	88(1)	91(1)	94(1)
V_P (km/s)	8.12(2)	8.35(2)	8.57(2)	8.76(2)	8.90(2)	9.06(3)	9.17(3)
V_S (km/s)	4.64(1)	4.75(1)	4.77(1)	4.88(1)	4.92(1)	4.97(2)	5.01(2)
ρ (g/cm^3)	3.400(1)	3.476(1)	3.539(1)	3.603(1)	3.645(1)	3.695(1)	3.748(2)

Table S4. The first and second pressure derivatives of single-crystal elastic moduli for diopside at ambient conditions

	$Di_{80}Hd_{20}$ (This study)	Di_{100} [a] (Sang and Bass 2014)
$(\partial C_{11}/\partial P)_T$	6.7(4)	6.6(2)
$(\partial^2 C_{11}/\partial P^2)_T$	-0.16(6)	-0.16(4)
$(\partial C_{22}/\partial P)_T$	7.6(3)	6.7(3)
$(\partial^2 C_{22}/\partial P^2)_T$	-0.30(5)	-0.23(6)
$(\partial C_{33}/\partial P)_T$	6.88(6)	6.8(2)
$(\partial C_{44}/\partial P)_T$	1.9(2)	1.8(2)
$(\partial^2 C_{44}/\partial P^2)_T$	-0.08(3)	-0.08(7)
$(\partial C_{55}/\partial P)_T$	1.3(1)	2.2(2)
$(\partial^2 C_{55}/\partial P^2)_T$	-0.02(2)	-0.15(4)
$(\partial C_{66}/\partial P)_T$	1.90(5)	2.4(2)
$(\partial C_{12}/\partial P)_T$	3.6(3)	4.9(6)
$(\partial^2 C_{12}/\partial P^2)_T$	-0.10(5)	-0.3(1)
$(\partial C_{13}/\partial P)_T$	5.0(4)	4.5(2)
$(\partial^2 C_{13}/\partial P^2)_T$	-0.24(7)	-0.18(4)
$(\partial C_{23}/\partial P)_T$	3.3(1)	3.5(5)
$(\partial C_{15}/\partial P)_T$	-0.44(4)	-0.2(1)
$(\partial C_{25}/\partial P)_T$	-0.63(7)	-0.9(4)
$(\partial C_{35}/\partial P)_T$	-0.88(6)	-0.71(8)
$(\partial C_{46}/\partial P)_T$	-0.37(9)	-0.02(24)

[a)] Refitting using the third- or fourth-order Eulerian finite-strain equation

Table S5. Thermoelastic parameters of upper mantle minerals used in our thermoelastic modeling

Parameters	Olivine [a] (X_{Mg}=0.80)	Opx [b] (X_{Mg}=0.80)	Cpx [c] (X_{Mg}=0.80)	Cpx [d] (X_{Mg}=1.00)
Density	3.443	3.369	3.344	3.264
K_{S0} (GPa)	130.8	110	118	114.6
$(\partial K_S/\partial P)_T$	4.7	10.8	5.0	5.4
$(\partial^2 K_S/\partial P^2)_T$ (GPa^{-1})	— [f]	-1.6	-0.12	-0.2
$(\partial K_S/\partial T)_P$ (GPa/K)	-0.020	-0.0263	-0.0123	-0.012
G_0 (GPa)	74.0	75.5	70.5	72.7
$(\partial G/\partial P)_T$	1.90	2.06	1.72	1.9
$(\partial^2 G/\partial P^2)_T$ (GPa^{-1})	-0.10	-0.12	-0.05	-0.07
$(\partial G/\partial T)_P$ (GPa/K)	-0.010	-0.0136	-0.00998	-0.011
α (K^{-1})	3.5×10^{-5}	3.45×10^{-5}	3.1×10^{-5}	3.1×10^{-5}

[a] Mao et al. (2015); Zha et al. (1996); Zhang and Bass (2016a)
[b] Jackson et al. (2003, 2007); Webb and Jackson (1993); Zhang and Bass (2016b)
[c] Finger and Ohashi (1976); Isaak et al. (2006); Hao et al. (2019a); This study
[d] Finger and Ohashi (1976); Li and Neuville (2010); Sang and Bass (2014)
[f] The values are not available in the literature.