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Seismic visibility of eclogite in the Earth's upper mantle – implications from high pressure-temperature single-crystal elastic properties of omphacite

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Elements	Wt%
Na_2O	4.13
MgO	11.77
Al_2O_3	7.59
SiO_2	54.73
CaO	17.59
Total	99.42

Table 1. Chemical composition of the omphacite sample. The EPMA is performed using the JEOL 8200 Electron Microprobe facility with 20 nA beam current and 15 kV accelerating voltage at the Institute of Meteroritics at UNM. Experimental conditions can be found from the main text section 2. The element standards were albite for Na, forsterite for Mg, almandine for Al and Fe, diopside for Si and Ca. Oxygen was calculated by stoichiometry from the cations.

	1 atm 300 K	3.0(1) GPa 300 K	6.0(1) GPa 300 K	8.9(1) GPa 300 K	12.0(1) GPa 300 K	15.0(1) GPa 300 K	18.0(1) GPa 300 K
ρ (g/cm^3)	3.34(1)	3.419	3.492	3.558	3.625	3.686	3.744
C_{11} (GPa)	231.5(8)	259(1)	277.2(8)	294.3(7)	315.3(8)	333.2(7)	348.6(6)
C_{22} (GPa)	201(1)	213(2)	229(1)	247(1)	262(1)	277(1)	289(1)
C_{33} (GPa)	253.8(8)	275(1)	297.6(8)	314.2(7)	326.3(8)	346.8(8)	356.7(6)
C_{44} (GPa)	79.1(5)	82.3(6)	86.0(6)	87.6(5)	91.0(6)	92.5(6)	97.7(6)
C_{55} (GPa)	68.9(4)	70.7(5)	74.0(5)	78.4(4)	81.9(4)	84.5(4)	88.1(3)
C_{66} (GPa)	74.0(4)	80.3(7)	89.7(5)	95.7(6)	101.4(5)	109.6(5)	119.1(5)
C_{12} (GPa)	84.4(9)	96(1)	107.6(8)	120.7(8)	131.6(9)	144.5(9)	146.7(9)
C_{13} (GPa)	76(1)	85(1)	93(1)	104.2(9)	118(1)	122(1)	132.6(8)
C_{23} (GPa)	60(2)	71(2)	77(2)	89(2)	89(2)	99(2)	120(2)
C_{15} (GPa)	7.6(5)	5.6(6)	5.6(5)	4.4(4)	4.6(5)	6.3(5)	6.5(4)
C_{25} (GPa)	5.4(10)	4(1)	5.9(9)	6(1)	10(1)	11(1)	22(1)
C_{35} (GPa)	39.8(5)	33.2(6)	28.5(5)	26.4(4)	23.8(5)	21.5(5)	23.2(4)
C_{46} (GPa)	5.9(4)	6.4(6)	7.0(5)	7.2(6)	6.5(6)	2.2(6)	-1.8(5)
K_S^R (GPa)	119.9(5)	134.7(6)	146.7(6)	161.3(5)	171.3(6)	183.4(6)	193.6(5)
G^R (GPa)	71.9(2)	76.7(3)	82.2(3)	85.8(3)	90.0(3)	94.0(3)	97.8(2)
K_S^V (GPa)	125.3(5)	138.8(6)	150.8(6)	164.8(5)	175.8(6)	187.6(6)	199.2(5)
G^V (GPa)	75.4(2)	79.7(3)	85.0(3)	88.4(3)	92.5(3)	96.7(3)	100.7(2)
K_S^{VRH} (GPa)	123(3)	137(3)	149(2)	163(2)	174(3)	186(3)	196(3)
G^{VRH} (GPa)	74(2)	78(2)	84(2)	87(2)	91(2)	95(2)	99(2)
Vp (km/s)	8.13(4)	8.40(3)	8.63(3)	8.86(2)	9.02(3)	9.21(3)	9.37(3)
Vs (Km/s)	4.70(3)	4.78(3)	4.89(3)	4.95(2)	5.02(2)	5.09(2)	5.15(2)

	1.4(1) GPa 400 K	3.8(1) GPa 400 K	10.0(1) GPa 400 K	14.8(1) GPa 400 K	17.0(1) GPa 400 K	4.3(2) GPa 500 K	10.9(1) GPa 500 K
ρ (g/cm^3)	3.369	3.432	3.579	3.679	3.722	3.436	3.591
C_{11} (GPa)	237.9(6)	255(1)	296.1(7)	329.2(9)	341(1)	253(1)	297.8(7)
C_{22} (GPa)	201.1(9)	208(2)	241.7(9)	263(1)	275(2)	208(1)	241(1)
C_{33} (GPa)	258.2(6)	277(1)	312.4(9)	340.8(7)	352(1)	277.1(9)	313(1)
C_{44} (GPa)	78.8(4)	83.2(6)	87.6(6)	91.5(7)	93(1)	82.9(6)	87.9(7)
C_{55} (GPa)	68.9(4)	70.8(6)	79.1(4)	83.0(4)	84.8(6)	71.1(6)	78.5(4)
C_{66} (GPa)	75.4(3)	81.3(7)	96.1(4)	107.4(7)	112.2(8)	80.2(6)	95.3(5)
C_{12} (GPa)	85.3(7)	94(1)	118.6(8)	139(1)	145(1)	94(1)	120(1)
C_{13} (GPa)	75.6(7)	82(1)	103.2(9)	122(1)	132(1)	81(1)	104(1)
C_{23} (GPa)	62(2)	76(2)	93(3)	107(2)	111(3)	68(2)	92(3)
C_{15} (GPa)	8.4(4)	7.7(6)	6.8(4)	3.4(5)	4.7(8)	7.7(6)	5.3(4)
C_{25} (GPa)	8.0(9)	7(1)	5.4(8)	8(1)	9(2)	4(1)	6.2(9)
C_{35} (GPa)	34.6(4)	34.5(6)	25.5(5)	23.1(5)	21.6(7)	32.4(6)	27.8(5)
C_{46} (GPa)	7.1(3)	5.1(6)	4.8(4)	6.8(7)	1.3(9)	6.0(6)	7.0(5)
K_S^R (GPa)	121.8(4)	133.1(7)	160.9(7)	181.2(6)	189.2(8)	131.6(6)	160.9(8)
G^R (GPa)	73.3(2)	76.6(3)	85.9(3)	91.2(3)	94.0(4)	76.8(3)	85.3(3)
K_S^V (GPa)	127.0(4)	138.1(7)	164.5(7)	185.3(6)	193.5(8)	135.9(6)	164.9(8)
G^V (GPa)	76.2(2)	79.6(3)	88.2(3)	94.1(3)	96.6(4)	79.8(3)	88.1(3)
K_S^{VRH} (GPa)	124(3)	136(3)	163(2)	183(2)	191(3)	134(3)	163(3)
G^{VRH} (GPa)	75(2)	78(2)	87(1)	93(2)	95(2)	78(2)	87(2)
Vp (km/s)	8.16(4)	8.36(4)	8.83(3)	9.13(3)	9.25(3)	8.33(3)	8.81(3)
Vs (Km/s)	4.71(3)	4.77(3)	4.93(2)	5.02(2)	5.06(2)	4.77(3)	4.91(2)

	14.9(1) GPa 500 K	16.9(1) GPa 500 K	2.7(3) GPa 700 K	11.5(2) GPa 700 K	14.9(2) GPa 700 K	18.4(1) GPa 700 K
ρ (g/cm^3)	3.673	3.713	3.346	3.587	3.658	3.727
C_{11} (GPa)	327(1)	337(1)	233(1)	293(1)	319(1)	341.1(8)
C_{22} (GPa)	258(1)	270(1)	196(2)	237(2)	255(2)	272(1)
C_{33} (GPa)	337.5(9)	345(1)	251(1)	304(1)	335(1)	348.7(7)
C_{44} (GPa)	89.8(7)	92.8(9)	75.4(7)	86.2(9)	88(1)	92.6(8)
C_{55} (GPa)	81.8(5)	84.4(5)	68(1)	77.1(6)	79.5(5)	84.8(4)
C_{66} (GPa)	105.5(7)	110.6(7)	71.5(6)	93.4(7)	103.3(8)	109.5(5)
C_{12} (GPa)	137(1)	142(1)	81(1)	114(1)	132(1)	143.9(8)
C_{13} (GPa)	118(1)	128(1)	71(1)	100(1)	117(1)	128.5(9)
C_{23} (GPa)	110(3)	115(3)	61(3)	94(4)	99(3)	117(2)
C_{15} (GPa)	3.0(7)	5.3(7)	9.2(7)	5.7(7)	4.0(7)	6.0(5)
C_{25} (GPa)	10(1)	13(1)	7(1)	10(1)	13(1)	14.1(9)
C_{35} (GPa)	21.7(6)	21.6(7)	33.0(8)	30.0(8)	18.8(7)	19.8(4)
C_{46} (GPa)	3.4(7)	0.5(6)	7.4(7)	6.2(7)	1.0(8)	2.5(6)
K_S^R (GPa)	179.8(7)	186.8(7)	118.1(8)	157(1)	173.5(8)	188.7(5)
G^R (GPa)	89.8(3)	92.7(4)	71.5(4)	83.9(4)	88.9(4)	93.1(3)
K_S^V (GPa)	183.9(7)	191.4(7)	122.9(8)	161(1)	178.2(8)	193.4(5)
G^V (GPa)	92.6(3)	95.4(4)	74.2(4)	86.4(4)	91.5(4)	95.5(3)
K_S^{VRH} (GPa)	182(3)	189(3)	121(3)	159(3)	176(3)	191(3)
G^{VRH} (GPa)	91(2)	94(2)	73(2)	85(2)	90(2)	94(2)
Vp (km/s)	9.09(3)	9.21(3)	8.06(4)	8.72(3)	9.00(3)	9.22(3)
Vs (Km/s)	4.98(2)	5.04(2)	4.67(3)	4.87(2)	4.97(2)	5.03(2)

Table 2. Single-crystal elastic properties of omphacite at each P-T condition determined in this study. The superscripts R and V denote the Reuss and Voigt bounds of the homogeneous isotropic aggregate under the VRH averaging scheme.

Mineral	Density (g/cm^3)	K_{S0} (GPa)	$\partial K_S/\partial P$	$\partial K_S/\partial T$ (GPa/K)	G_0 (GPa)	$\partial G/\partial P$	$\partial G/\partial T$ (GPa/K)	a_0 (10^{-4} K^{-1})	a_1 (10^{-8} K^{-2})	a_2 (K)
Jadeite[1]	3.302(5)	138(3)	3.9(1)	-0.029(5)	84(2)	1.09(4)	-0.013(5)	0.34(5)	0	0
Diopside[2]	3.272(6)	116.4(7)	4.9(1)	-0.029(5)	73.0(4)	1.6(1)	-0.013(5)	0.19	2.08	0
Pyrope[3,4,5,6,8]	3.56(2)	171.0(5)	4.4(1)	-0.014(3)	94.9(2)	1.15(6)	-0.011(2)	0.288	0.2787	-0.5521
Mg-majorite[3,4,5,6,9]	3.56(2)	162.0(5)	4.4(1)	-0.014(3)	86.2(2)	1.15(6)	-0.011(2)	0.288	0.2787	-0.5521
Jd-majorite[7,8]	3.644(7)	178(4)	4.47(2)	-0.0138(3)	125(2)	1.29(5)	-0.0128(2)	0.1951	0.8089	-0.4972
Grossular[8,9]	3.605(2)	171.2(8)	4.47(2)	-0.0138(3)	107.4(2)	1.29(5)	-0.0128(2)	0.1951	0.8089	-0.4972
Almandine[10]	4.3188(2)	174.2(12)	4.61(14)	-0.0267(7)	94.9(7)	1.06(6)	-0.0131(8)	0.26(5)	2.3(14)	0
Coesite[11,12]	2.91(2)	106.5(6)	2.7(15)	-0.0016(16)	60.7(3)	0.33(5)	-0.0044(5)	0.106(14)	-0.028(166)	-0.48(12)
Stishovite[13,14]	4.381(2)	296(5)	4.2(4)	-0.046(5)				0.126(11)	1.29(17)	0
Hedenbergite[9,15]	3.657(1)	120(4)	4	-0.029(5)	62(2)	1.6(1)	-0.013(5)	0.298	0	0

1. Hao et al. (2020) 2. Li and Neuville (2010) 3. Irifune et al. (2008) 4. Liu et al. (2000) 5. Sinogeikin and Bass (2002) 6. Suzuki and Anderson (1983) 7. Reichmann et al. (2002) 8. Gwanmesia et al. (2014) 9. Fei (1995) 10. Arimoto et al. (2015) 11. Chen et al. (2017) 12. Kulik et al. (2018) 13. Yang and Wu (2014) 14. Nishihara et al. (2005) 15. Kandelin and Weidner (1988)

Table 3. Thermoelastic parameters of all the relevant mineral phases for calculating the density and velocity. The a_0, a_1 and a_2 are the thermal expansion parameters, defined in Fei (1995): $a(T)=a_0+a_1T+a_2T^{-2}$. The thermal expansion parameters for jadeite using the equations in Hao et al. (2020). The elasticity data of stishovite are directly obtained from the first-principles calculation study by Yang and Wu (2014). The parameters for stishovite listed in the table are for density calculation. The parameters (except the thermal expansion parameters) for pyrope and coesite are recalculated based on the experimental values presented in Irifune et al. (2008) and Chen et al. (2017). Some parameters are listed without uncertainties because the uncertainties were not reported in the references.