Supporting Information for

**Effect of thermoelastic properties of the pyrope-almandine solid solutions on the entrapment pressure of garnet-related elastic geobarometer**

Bo Li 1,2,3, Junjie Jiang 4, Jingui Xu 5, Sergey N. Tkachev 6, Zhilin Ye 2,3, Shijie Huang 2,3, Weihua Guo 1, Yongjun Zeng 1, Vitali B. Prakapenka 6, Dawei Fan 2\*, Wenge Zhou 2

1 Research Institute of Petroleum Exploration & Development-Northwest (NWGI), PetroChina Lanzhou 730020, China

2 Key Laboratory of High-Temperature and High-Pressure Study of the Earth’s Interior, Institute of Geochemistry, Chinese Academy of Sciences, Guiyang 550081, China

3 University of Chinese Academy of Sciences, Beijing 100049, China

4 Basic Geological Survey Institute of Jiangxi Geological Survey Institute, Nanchang, 330030, China

5 Hawaii Institute of Geophysics and Planetology, School of Ocean and Earth Science and Technology, University of Hawaii at Manoa, Honolulu, Hawaii 96822, USA

6 Center for Advanced Radiation Sources, University of Chicago, Chicago, Illinois 60437, USA

\* Corresponding Authors:

Dawei Fan (fandawei@vip.gyig.ac.cn)

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TABLE S1. Unit-cell parameters of Prp-Alm garnets at high pressure and room temperature

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| *P*(GPa) | *V0* (Å3) | | | *P*(GPa) | *V0* (Å3) | *P*(GPa) | *V0* (Å3) | | | |
| Prp9Alm91 | Prp31Alm68 | Prp48Alm52 | Prp23Alm76 | Prp57Alm43 | Prp67Alm32 | Prp78Alm22 | Prp87Alm12 |
| 0.0001 | 1536.2(3) | 1525.06(2) | 1524.8(5) | 0.0001 | 1529.4(5) | 0.0001 | 1519.3(2) | 1516.2(3) | 1513.04(3) | 1507.1(2) |
| 0.37(1) | 1535.1(2) | 1522.2(2) | 1521.4(2) | 0.51(1) | 1524.26(8) | 0.44(1) | 1515.3(2) | 1512.3(3) | 1509.6(2) | 1503.7(3) |
| 0.68(1) | 1531.8(2) | 1519.4(2) | 1518.3(2) | 0.95(2) | 1521.39(6) | 0.66(1) | 1513.6(2) | 1510.4(2) | 1507.7(3) | 1501.2(3) |
| 1.25(2) | 1526.5(2) | 1514.4(2) | 1513.7(2) | 1.54(4) | 1516.07(6) | 1.02(3) | 1510.8(2) | 1507.3(2) | 1504.2(3) | 1498.8(3) |
| 1.99(3) | 1520.5(2) | 1508.1(2) | 1506.8(2) | 2.07(4) | 1512.72(6) | 1.58(4) | 1505.7(2) | 1502.5(3) | 1499.3(3) | 1493.9(3) |
| 2.64(4) | 1515.2(2) | 1502.7(2) | 1501.6(2) | 2.65(4) | 1507.33(6) | 2.05(7) | 1501.6(2) | 1498.3(3) | 1495.8(3) | 1490.1(3) |
| 3.15(4) | 1510.9(2) | 1498.9(2) | 1497.4(2) | 3.11(6) | 1503.77(5) | 2.44(5) | 1498.7(2) | 1495.3(3) | 1492.2(3) | 1486.6(3) |
| 3.71(5) | 1507.0(2) | 1494.5(2) | 1492.6(2) | 4.10(9) | 1496.14(6) | 3.09(6) | 1493.2(2) | 1489.6(3) | 1486.9(3) | 1481.3(3) |
| 4.43(5) | 1499.8(2) | 1489.2(2) | 1486.3(2) | 4.89(8) | 1489.60(6) | 3.57(8) | 1489.7(3) | 1485.4(3) | 1482.9(3) | 1477.6(3) |
| 5.03(1) | 1496.7(2) | 1484.9(2) | 1482.6(2) | 5.64(10) | 1483.82(4) | 4.17(4) | 1485.0(3) | 1482.0(3) | 1477.8(3) | 1473.4(3) |
| 6.01(6) | 1488.6(2) | 1477.3(3) | 1476.0(2) | 6.59(9) | 1477.12(4) | 4.55(4) | 1481.8(3) | 1478.8(3) | 1474.8(4) | 1470.2(3) |
| 6.79(7) | 1482.4(2) | 1471.6(2) | 1469.8(2) | 7.60(11) | 1470.24(4) | 5.23(8) | 1476.5(4) | 1473.5(4) | 1469.9(3) | 1465.1(3) |
| 7.64(6) | 1477.2(2) | 1465.5(2) | 1464.1(2) | 8.65(9) | 1462.70(4) | 5.96(5) | 1471.5(4) | 1467.5(4) | 1464.3(3) | 1459.7(3) |
| 8.48(7) | 1471.4(2) | 1459.7(2) | 1457.7(2) | 9.77(11) | 1454.96(4) | 7.09(3) | 1462.9(3) | 1459.6(4) | 1456.1(3) | 1451.3(3) |
| 9.23(9) | 1467.3(2) | 1454.9(2) | 1453.2(2) | 10.73(10) | 1448.56(5) | 7.75(5) | 1458.3(3) | 1454.9(4) | 1451.4(4) | 1446.7(3) |
| 9.93(7) | 1461.0(2) | 1449.6(2) | 1448.2(2) | 11.69(10) | 1442.16(6) | 8.20(6) | 1455.2(3) | 1451.9(3) | 1447.9(4) | 1443.1(3) |
| 10.84(9) | 1456.6(2) | 1444.4(2) | 1442.8(2) | 12.93(11) | 1434.80(5) | 8.66(5) | 1452.1(2) | 1448.7(3) | 1445.0(4) | 1439.4(3) |
| 11.37(7) | 1453.5(2) | 1440.5(2) | 1439.0(2) | 14.21(13) | 1426.61(5) | 9.01(3) | 1449.4(2) | 1446.6(4) | 1442.7(3) | 1437.0(3) |
| 12.00(8) | 1448.5(2) | 1436.8(2) | 1435.5(2) | 15.35(14) | 1420.10(4) | 9.37(5) | 1447.1(2) | 1444.2(3) | 1440.3(4) | 1435.1(3) |
| 12.62(9) | 1444.6(2) | 1433.1(3) | 1431.4(2) | 16.61(11) | 1412.72(5) | 9.73(5) | 1444.2(2) | 1441.0(3) | 1437.3(3) | 1432.6(3) |
| 13.29(10) | 1440.6(2) | 1428.8(2) | 1426.9(2) | 17.91(11) | 1404.84(6) | 10.19(6) | 1441.4(2) | 1438.8(3) | 1434.1(3) | 1429.8(3) |
| 14.03(10) | 1435.9(2) | 1424.0(2) | 1423.1(2) | 19.04(10) | 1398.50(6) | 10.57(6) | 1438.8(2) | 1435.5(3) | 1431.7(3) | 1426.8(3) |
| 15.01(12) | 1429.3(2) | 1417.6(3) | 1416.5(2) | 20.58(10) | 1389.83(6) | 11.25(9) | 1434.2(2) | 1430.6(3) | 1427.8(3) | 1422.4(3) |
| 16.06(12) | 1422.3(2) | 1411.1(2) | 1410.0(2) | - | - | 11.75(7) | 1430.8(2) | 1427.2(3) | 1424.6(3) | 1419.0(3) |
| Numbers in parenthesis represent 1σ in the last digit  -: none | | | | | | | | | | |

Table S2. A summary of previous experimentally determined bulk modulus and its pressure derivative of garnets along the Prp-Alm join

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Composition | *V0* (Å3) | *K0* (GPa) | *K' 0* | Method | References |
| Prp100 | 1502.9(3) | 171(2) | 4.4(2) | SCXRD | Zhang et al. (1998b) |
| Prp100 | 1500(1) | 167(6) | 4.6(3) | PXRD | Zou et al. (2012a) |
| Prp100 | 1506.15(16) | 163.7(17) | 6.4(4) | SCXRD | Milani et al. (2015) |
| Prp100 | 1502.6(7) | 170.4(35) | 4.3fixed | PXRD | Du et al. (2015) |
| Hydrous Prp100b | - | 168.6(4) | 4.6(1) | BLS | Fan et al. (2019b) |
| Prp100 | - | 171.2(20) | 4.1(3) | BLS | Sinogeikin and Bass (2000) |
| Prp100 | - | 175(2) | 3.9(3) | UI | Gwanmesia et al. (2006) |
| Prp100 | - | 170.0(2) | 4.51(2) | UI | Zou et al. (2012b) |
| Prp100 | - | 172.0(16) | 4.38(8) | UI | Chantel et al. (2016) |
| Prp30Alm70 | 1526(1) | 183(2) | 4.3a | PXRD | Huang and Chen (2014) |
| Prp54Alm46 | 1515(2) | 174(2) | 4.3a | PXRD | Huang and Chen (2014) |
| Prp83Alm17 | 1511(1) | 172(4) | 4.3a | PXRD | Huang and Chen (2014) |
| Prp60Alm40 | 1516.32(13) | 167.2(1.7) | 5.6(5) | SCXRD | Milani et al. (2015) |
| Alm100 | 1528.6 | 185(3) | 4.2(3) | SCXRD | Zhang et al. (1999) |
| Alm100 | 1531.05(7) | 179(3) | 4a | PXRD | Arimoto et al. (2015) |
| Alm100 | 1533.52(10) | 172.6(1.5) | 5.8(5) | SCXRD | Milani et al. (2015) |
| Alm100 | 1531.05(7) | 174.2(12) | 4.61(14) | UI | Arimoto et al. (2015) |
| a Values were fixed during data processing;  b ~900 ppmw H2O;  SCXRD: single-crystal X-ray diffraction; PXRD: powder X-ray diffraction;  BLS: Brillouin light spectroscopy; UI: Ultrasonic interferometry.  Numbers in parenthesis represent standard deviations  -: none | | | | | |

TABLE S3. Unit-cell parameters of Prp-Alm garnets at high pressure and high temperature

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| *P*(GPa) | *T*(K) | *V0* (Å3) | | | |
| Prp14Alm86 | Prp31Alm68 | Prp48Alm52 | Prp67Alm32 |
| 0.0001 | 300 | 1530.46(12) | 1525.06(2) | 1524.8(5) | 1516.2(3) |
| 1.39(1) | 300 | 1519.5(2) | 1513.5(2) | 1511.5(3) | 1504.1(3) |
| 2.48(1) | 300 | 1510.6(3) | 1503.7(2) | 1501.6(3) | 1495.0(4) |
| 3.27(6) | 300 | 1503.7(3) | 1497.4(3) | 1494.5(3) | 1488.5(6) |
| 5.24(1) | 300 | 1489.3(9) | 1482.1(2) | 1478.3(4) | 1473.2(2) |
| 6.26(1) | 300 | 1481.9(4) | 1474.8(3) | 1470.3(3) | 1465.5(2) |
| 8.40(1) | 300 | 1466.9(3) | 1460.4(2) | 1454.8(3) | 1450.1(2) |
| 8.99(1) | 300 | 1462.9(4) | 1455.9(2) | 1450.5(3) | 1446.2(2) |
| 11.15(3) | 300 | 1449.5(4) | 1442.3(7) | 1435.6(3) | 1431.7(4) |
| 11.71(4) | 300 | 1445.1(8) | 1438.3(7) | 1432.3(3) | 1427.8(7) |
| 12.04(2) | 300 | 1443.0(6) | 1436.4(4) | 1430.0(3) | 1425.9(7) |
| 12.75(1) | 300 | 1438.0(5) | 1431.8(3) | 1425.6(3) | 1421.1(3) |
| 13.96(2) | 300 | 1431.3(6) | 1424.8(3) | 1417.7(3) | 1413.7(4) |
| 14.70(1) | 300 | 1426.5(5) | 1420.2(2) | 1413.0(4) | 1409.1(2) |
| 4.74(6) | 400 | 1498.1(3) | 1491.2(3) | 1487.8(4) | 1481.9(4) |
| 6.58(1) | 400 | 1484.4(2) | 1477.4(3) | 1473.1(3) | 1467.8(3) |
| 7.35(3) | 400 | 1479.1(7) | 1471.9(2) | 1467.1(3) | 1462.1(2) |
| 9.13(1) | 400 | 1466.3(3) | 1459.7(2) | 1454.0(3) | 1449.3(2) |
| 9.77(1) | 400 | 1462.1(3) | 1455.9(2) | 1449.5(3) | 1444.8(2) |
| 10.45(1) | 400 | 1457.6(4) | 1450.9(2) | 1444.7(3) | 1440.2(2) |
| 11.87(2) | 400 | 1448.1(3) | 1441.8(3) | 1435.3(3) | 1430.8(4) |
| 13.23(5) | 400 | 1439.2(4) | 1433.5(3) | 1426.6(3) | 1422.1(4) |
| 13.64(6) | 400 | 1437.1(5) | 1431.0(3) | 1423.9(3) | 1419.4(3) |
| 15.04(2) | 400 | 1428.6(5) | 1422.7(2) | 1415.3(3) | 1410.7(4) |
| 15.47(1) | 400 | 1425.4(7) | 1420.2(2) | 1412.6(3) | 1408.1(2) |
| 6.31(5) | 500 | 1491.2(4) | 1484.5(2) | 1480.4(4) | 1474.5(4) |
| 7.30(1) | 500 | 1483.7(2) | 1477.2(4) | 1472.3(3) | 1467.1(2) |
| 8.73(3) | 500 | 1473.7(5) | 1467.2(2) | 1461.6(4) | 1456.6(2) |
| 9.85(3) | 500 | 1465.7(3) | 1459.7(2) | 1453.5(4) | 1448.7(2) |
| 11.68(2) | 500 | 1453.7(3) | 1447.6(2) | 1440.8(3) | 1436.2(2) |
| 12.09(49) | 500 | 1450.9(4) | 1444.8(5) | 1438.1(3) | 1433.3(2) |
| 12.63(1) | 500 | 1447.5(4) | 1441.4(4) | 1434.5(3) | 1429.9(3) |
| 14.43(2) | 500 | 1436.1(4) | 1430.7(5) | 1422.9(3) | 1418.3(4) |
| 14.66(3) | 500 | 1434.4(5) | 1429.3(3) | 1421.5(3) | 1416.9(3) |
| 16.20(2) | 500 | 1425.2(3) | 1420.2(2) | 1412.2(3) | 1407.4(3) |
| 16.38(1) | 500 | 1424.3(2) | 1419.3(2) | 1411.2(3) | 1406.3(2) |
| 8.36(23) | 600 | 1480.7(3) | 1474.4(3) | 1469.2(3) | 1463.7(3) |
| 8.83(9) | 600 | 1477.4(3) | 1471.1(2) | 1465.6(2) | 1460.1(3) |
| 10.84(4) | 600 | 1463.4(4) | 1457.4(2) | 1450.9(4) | 1446.0(2) |
| 10.88(4) | 600 | 1463.1(3) | 1457.1(2) | 1450.6(3) | 1445.7(2) |
| 13.54(3) | 600 | 1445.8(5) | 1440.1(2) | 1432.7(4) | 1427.9(2) |
| 13.81(5) | 600 | 1443.9(4) | 1438.5(5) | 1430.8(3) | 1426.2(3) |
| 16.09(1) | 600 | 1429.6(8) | 1424.9(3) | 1416.6(3) | 1411.9(4) |
| 16.15(1) | 600 | 1429.1(5) | 1424.5(2) | 1416.2(3) | 1411.4(4) |
| 17.80(3) | 600 | 1419.6(5) | 1415.2(2) | 1406.4(3) | 1401.5(3) |
| 17.75(1) | 600 | 1419.9(3) | 1415.4(2) | 1406.7(3) | 1401.8(2) |
| 11.95(6) | 700 | 1460.3(7) | 1454.4(2) | 1447.2(3) | 1442.7(3) |
| 12.72(4) | 700 | 1454.9(3) | 1449.6(2) | 1442.1(3) | 1437.3(2) |
| 15.81(10) | 700 | 1435.2(4) | 1430.6(2) | 1421.8(3) | 1417.3(3) |
| 18.04(9) | 700 | 1421.7(4) | 1417.6(2) | 1408.4(3) | 1403.7(4) |
| 19.67(3) | 700 | 1411.9(4) | 1408.0(3) | 1399.1(3) | 1394.3(2) |
| Numbers in parenthesis represent 1σ in the last digit  -: none | | | | | |

TABLE S4. Isomeke sensitivity calculations for the garnets-quartz host-inclusion system: entrapment pressure calculated for different values of garnet (Prp14Alm86) thermoelastic properties and inclusion pressure.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| T(K) | Control groupa | *K0* (GPa)b | | *α300* (10-5K-1) | |
| -σ | +σ | -σ | +σ |
| 500 | 1.183 | 1.184 | 1.182 | 1.190 | 1.177 |
| 600 | 1.210 | 1.211 | 1.209 | 1.220 | 1.200 |
| 700 | 1.246 | 1.247 | 1.245 | 1.259 | 1.233 |
| 800 | 1.298 | 1.299 | 1.298 | 1.315 | 1.282 |
| 900 | 1.373 | 1.374 | 1.372 | 1.393 | 1.354 |
| 1000 | 1.478 | 1.479 | 1.477 | 1.499 | 1.457 |
| 1100 | 1.620 | 1.621 | 1.619 | 1.642 | 1.598 |
| 1200 | 1.807 | 1.808 | 1.806 | 1.828 | 1.787 |
| 1300 | 2.048 | 2.049 | 2.048 | 2.066 | 2.032 |
| a: in this group, the thermoelastic coefficients used for calculation are shown in Table 6  b: in this group, the thermoelastic coefficient is changed according to its uncertainty, while the other thermoelastic coefficients are the same as the control group. | | | | | |

TABLE S5. Isomeke sensitivity calculations for the diamond-garnets host-inclusion system: entrapment pressure calculated for different values of garnet (Prp14Alm86) thermoelastic properties and inclusion pressure.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| T(K) | Control groupa | *K0* (GPa)b | | *α300* (10-5K-1) | |
| -σ | +σ | -σ | +σ |
| 800 | 4.667 | 4.651 | 4.683 | 4.575 | 4.759 |
| 900 | 5.469 | 5.450 | 5.489 | 5.357 | 5.581 |
| 1000 | 6.260 | 6.238 | 6.283 | 6.129 | 6.393 |
| 1100 | 7.043 | 7.018 | 7.068 | 6.891 | 7.195 |
| 1200 | 7.819 | 7.790 | 7.847 | 7.647 | 7.991 |
| 1300 | 8.589 | 8.558 | 8.620 | 8.396 | 8.781 |
| 1400 | 9.354 | 9.320 | 9.388 | 9.142 | 9.567 |
| 1500 | 10.116 | 10.079 | 10.153 | 9.883 | 10.349 |
| 1600 | 10.874 | 10.835 | 10.914 | 10.621 | 11.128 |
| a: in this group, the thermoelastic coefficients used for calculation are shown in Table 6  b: in this group, the thermoelastic coefficient is changed according to its uncertainty, while the other thermoelastic coefficients are the same as the control group. | | | | | |



FIGURE S1. Crystal structure of pyrope-almandine solid solution garnet at ambient conditions. The red ball indicates oxygen. In this structure, Si4+ is occupied at tetrahedral sites, Al3+ is occupied at octahedral sites, and Mg2+, Fe2+ are occupied at dodecahedral sites.