# Supporting Information for:

# Pressure destabilizes oxygen vacancies in bridgmanite

Hongzhan Fei1\*, Zhaodong Liu1,2, Rong Huang1,3, Seiji Kamada4,5, Naohisa Hirao6, Saori Kawaguchi6, Catherine McCammon1, Tomoo Katsura1,7

1. Bayerisches Geoinstitut, University of Bayreuth, Bayreuth, D95440, Germany.
2. State Key Laboratory of Superhard Materials, Jilin University, Changchun 130012, China.
3. Department of Earth Sciences, University College London, Gower Street, London WC1E 6BT, UK.
4. Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Miyagi, Sendai, 980-8578, Japan.
5. Department of Earth Science, Tohoku University, Miyagi, Sendai, 980-8578, Japan.
6. Japan Synchrotron Radiation Research Institute (JASRI), Sayo, Hyogo, 679-5198, Japan.
7. Center for High Pressure Science and Technology Advanced Research, Beijing 100097, China.

This Supporting Information file contains:

* **Table S1.** Lattice parameters and d-spacings of bridgmanite from runs I-574, I-873, and I-909 based on the X-ray diffraction spectra in Fig. 4.
* **Table S1** Lattice parameters and d-spacings of bridgmanite from runs I-574, I-873, and I-909 based on the X-ray diffraction spectra in Fig. 4.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | I-574-MgO  a=4.978(2), b=4.976(2), c=6.963(3) V=166.2(3) Å3 | | | I-574-MgO  a=4.961(3), b=4.967(3), c=6.955(4) V=164.4(3) Å3 | | | I-909-MgO  a=4.773(4), b=4.948(4), c=6.901(3) V=163.0(3) Å3 | | |
| (hkl) | 2θobs | 2θcal | d-spacing (Å) | 2θobs | 2θcal | d-spacing (Å) | 2θobs | 2θcal | d-spacing (Å) |
| 0 0 2 | 29.80 | 29.80 | 3.482 | 29.74 | 29.81 | 3.488 | 30.00 | 30.08 | 3.459 |
| 1 1 0 | 30.00 | 30.04 | 3.459 | 30.24 | 30.19 | 3.431 | 30.24 | 30.21 | 3.432 |
| 1 1 1 | 33.69 | 33.63 | 3.089 |  |  |  |  |  |  |
| 0 2 0 | 42.10 | 42.16 | 2.492 |  |  |  |  |  |  |
| 1 1 2 | 42.69 | 42.83 | 2.459 | 43.04 | 42.94 | 2.440 | 43.13 | 43.15 | 2.435 |
| 2 0 0 | 43.77 | 43.83 | 2.401 |  |  |  |  |  |  |
| 1 2 0 | 47.84 | 47.80 | 2.208 |  |  |  |  |  |  |
| 1 0 3 | 50.84 | 50.74 | 2.085 |  |  |  |  |  |  |
| 2 1 1 | 51.41 | 51.41 | 2.064 |  |  |  |  |  |  |
| 0 2 2 | 52.54 | 52.48 | 2.023 |  |  |  |  |  |  |
| 2 0 2 | 53.81 | 53.90 | 1.978 |  |  |  |  |  |  |
| 1 1 3 | 55.41 | 55.38 | 1.925 |  |  |  |  |  |  |
| 1 2 2 | 57.23 | 57.36 | 1.869 |  |  |  |  |  |  |
| 2 1 2 | 58.35 | 58.37 | 1.836 |  |  |  |  |  |  |
| 0 0 4 | 61.86 | 61.90 | 1.742 | 61.97 | 61.92 | 1.739 | 62.55 | 62.53 | 1.724 |
| 2 2 0 | 62.45 | 62.44 | 1.727 | 62.83 | 62.78 | 1.717 | 62.79 | 62.81 | 1.718 |
| 0 2 3 | 63.62 | 63.66 | 1.698 |  |  |  |  |  |  |
| 2 2 1 | 64.52 | 64.55 | 1.677 |  |  |  |  |  |  |
| 1 3 0 | 69.68 | 69.61 | 1.567 |  |  |  |  |  |  |
| 3 0 1 | 70.18 | 70.12 | 1.557 |  |  |  |  |  |  |
| 1 1 4 | 70.41 | 70.33 | 1.553 | 70.71 | 70.63 | 1.547 | 70.96 | 71.00 | 1.542 |
| 2 2 2 | 70.81 | 70.70 | 1.545 | 71.07 | 71.03 | 1.540 | 71.18 | 71.20 | 1.538 |
| 1 3 1 | 71.72 | 71.62 | 1.528 | 71.79 | 71.90 | 1.527 |  |  |  |
| 1 3 2 | 77.49 | 77.52 | 1.430 | 77.74 | 77.79 | 1.426 | 78.16 | 78.13 | 1.420 |
| 0 2 4 | 77.73 | 77.74 | 1.427 | 77.93 | 77.85 | 1.423 | 78.42 | 78.50 | 1.416 |
| 2 0 4 | 78.85 | 78.91 | 1.409 | 79.22 | 79.14 | 1.404 | 79.72 | 79.62 | 1.397 |
| 3 1 2 | 79.83 | 79.85 | 1.395 | 80.35 | 80.37 | 1.387 | 80.35 | 80.37 | 1.387 |