Supplementary materials for "**Single-Crystal X-ray Diffraction on the Structure of (Al,Fe)-bearing Bridgmanite in the Lower Mantle**"

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This document contains supplementary materials for the single-crystal x-ray diffraction results on bridgmanite at high pressure:

Figures S1-S5

Tables S1-S2

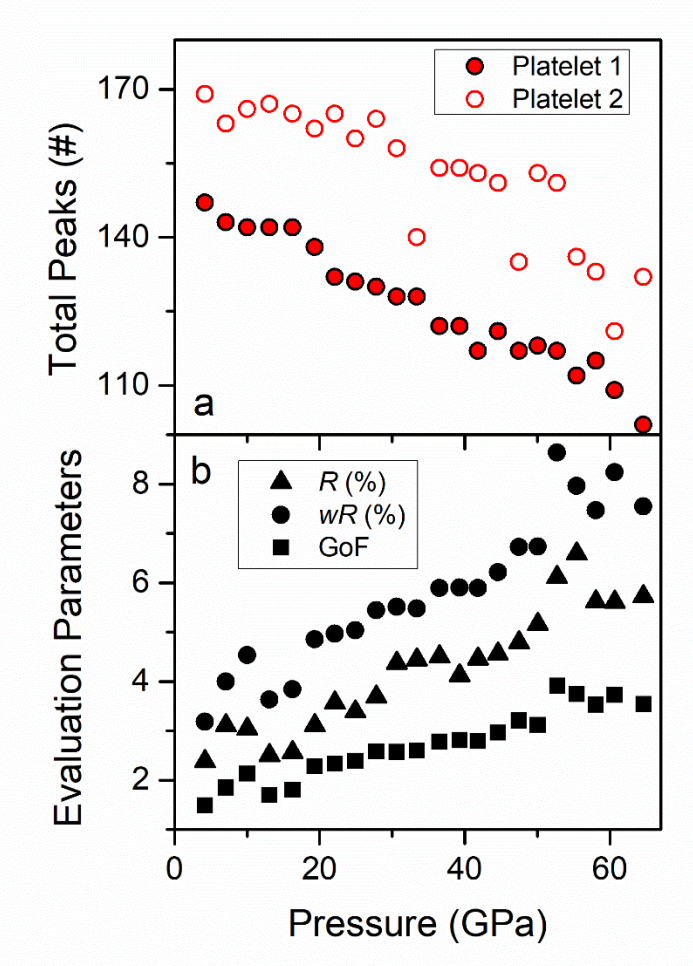

Figure S1. Data analyses on single-crystal X-ray diffraction patterns of Fe10-Al14-Bgm at high pressure. **a** The number of high-quality reflection peaks of each bridgmanite platelet used for structure refinements. These reflections were selected with intensities (I) of I>3σ(I). Solid and open red circles are for platelets 1 and 2, respectively. **b** Evaluation parameters during the structure refinements on Fe10-Al14-Bgm using JANA software (Petříček et al. 2014). Circles: weighted R-factor ($wR(F^2)$) in percentage; triangles: R-factor ($R(F^2>2\sigma(F^2))$) in percentage; squares: goodness of fit (GoF).

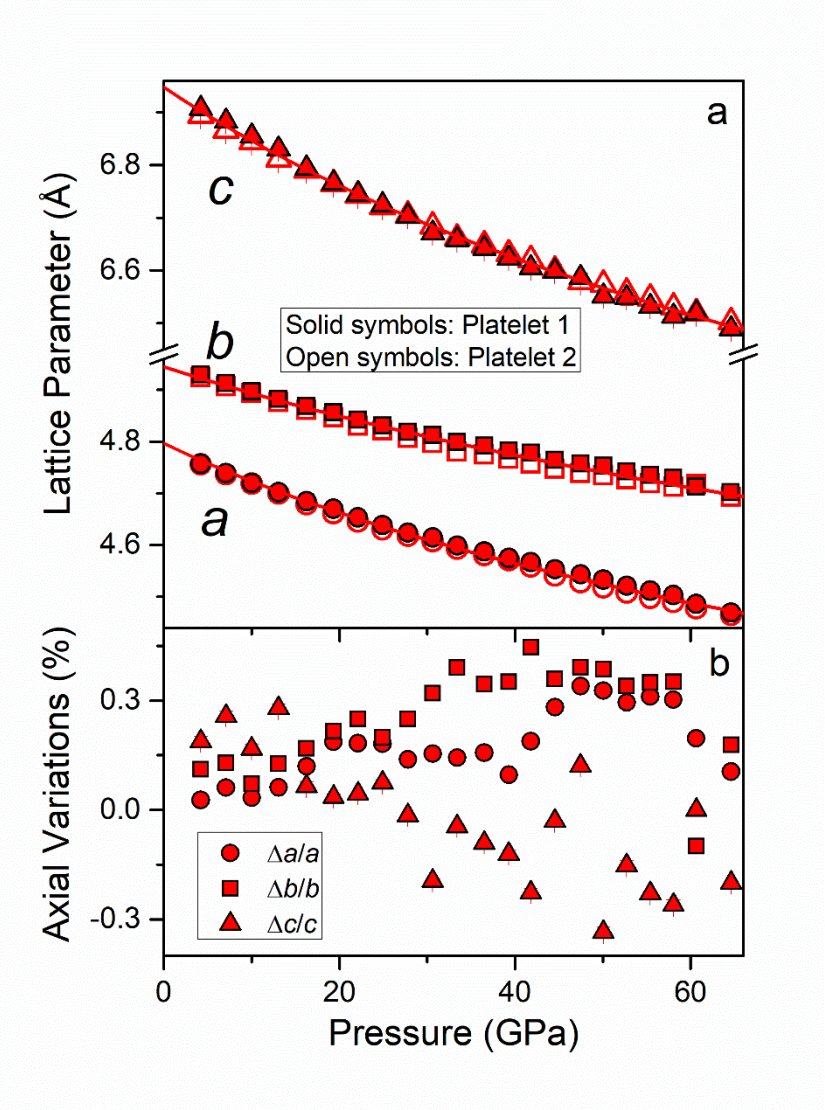

Figure S2. Lattice parameters of the two single-crystal Fe10-Al14-Bgm platelets obtained from analyses using CrysAlisPro software. **a** Lattice parameters (*a, b, c*) as a function of pressure. Solid and open symbols are for platelets 1 and 2, respectively. The solid lines are best fits to the dataset together using axial equation of state. **a** Axial variation (%) between the two platelets. Overall, the differences of the derived lattice parameters between the two platelets are less than 0.3%.

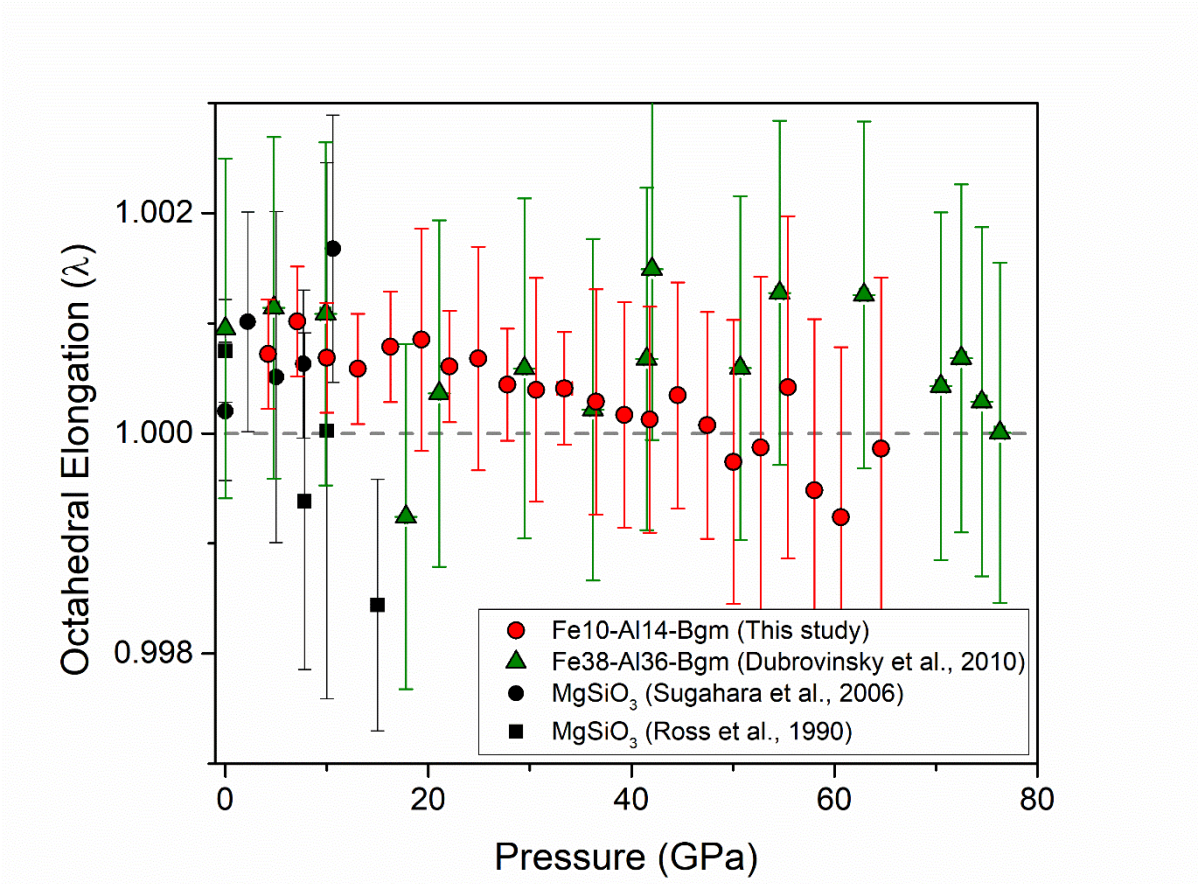

Figure S3. Octahedral elongation parameter (λ) of the single-crystal Fe10-Al14-Bgm as a function of pressure. λ is calculated by following a previous study (Robinson et al. 1971): $\lambda = \sum_{i=1}^{6}(l_i/l_0)^2/6$, where l_i and l_0 are B-O bond lengths under strained and unstrained states, respectively. Red circles are results from this study, and literature reports on bridgmanite with different compositions are plotted for comparisons (Ross and Hazen 1990; Sugahara et al. 2006; Dubrovinsky et al. 2010; Boffa Ballaran et al. 2012). The dashed gray line has a λ value of 1, indicating an ideal octahedron.

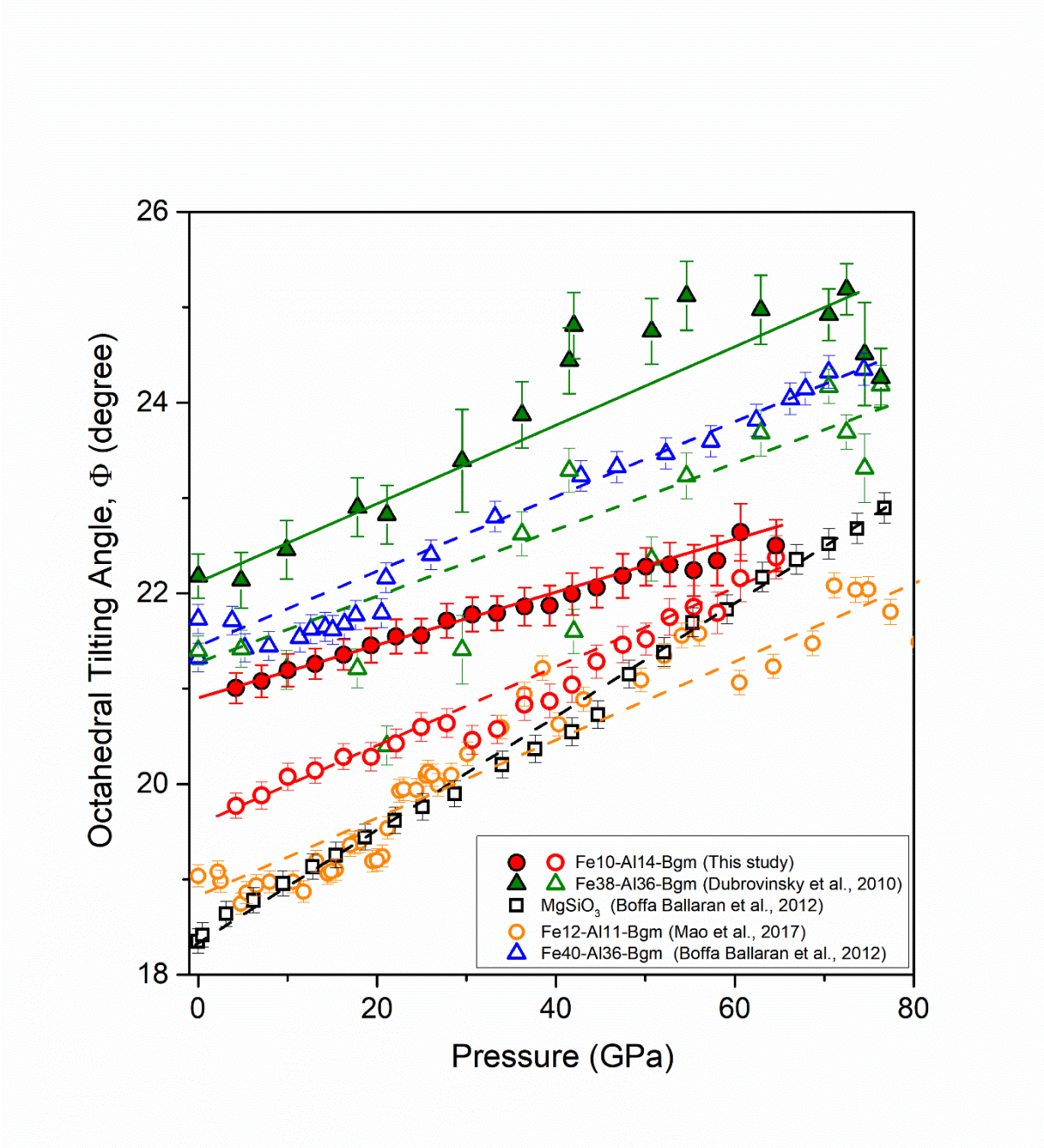

Figure S4. Octahedral titling angles in the single-crystal Fe10-Al14-Bgm as a function of pressure. Red circles are results of Fe10-Al14-Bgm in this study, and literature reports on bridgmanite with different compositions were plotted for comparisons (Dubrovinsky et al. 2010; Boffa Ballaran et al. 2012; Mao et al. 2017). Solid symbols are derived from the quantitatively refined atomic, while open symbols are calculations from unit-cell lattice parameters.

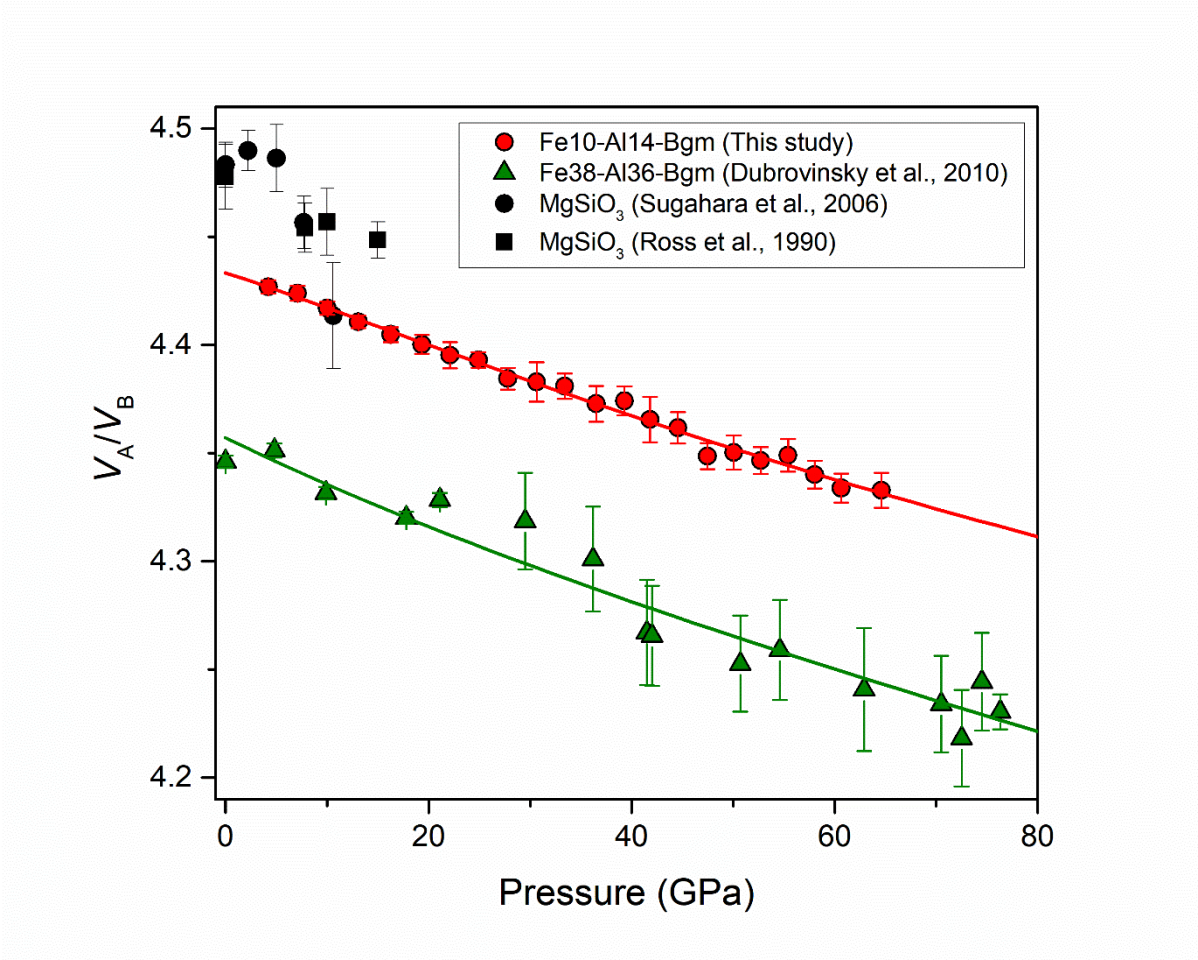

Figure S5. Volume ratios (V_A/V_B) between the AO_{12} pseudo-dodecahedra and BO_6 octahedra of Fe10-Al14-Bgm at high pressure. Red circles are results from this study, and literature reports on bridgmanite with different compositions are plotted for comparisons (Ross and Hazen 1990; Sugahara et al. 2006; Dubrovinsky et al. 2010; Boffa Ballaran et al. 2012). The lines are calculated from best-fits to volumes of AO_{12} pseudo-dodecahedra and BO_6 octahedra using the Birch-Murnaghan equation.

Table S1. Refined unit-cell parameters of single-crystal Fe10-Al14-Bgm at high pressures. Au was used as a pressure calibrant. 1σ uncertainty was shown in parentheses.

Pressure (GPa)	*a* (Å)	*b* (Å)	*c* (Å)
4.2(1)	4.7564(11)	4.9266(3)	6.9005(19)
7.1(2)	4.7378(4)	4.9098(3)	6.8742(13)
10.0(2)	4.7191(4)	4.8949(4)	6.8492(14)
13.1(2)	4.7007(4)	4.8792(4)	6.8205(15)
16.3(2)	4.6816(4)	4.8648(4)	6.7918(17)
19.3(2)	4.6658(5)	4.8512(4)	6.7650(18)
22.1(3)	4.6491(4)	4.8362(4)	6.7435(19)
24.9(3)	4.6342(5)	4.8257(4)	6.722(3)
27.8(3)	4.6208(4)	4.8127(4)	6.703(2)
30.6(3)	4.6107(5)	4.8047(5)	6.677(3)
33.4(7)	4.5955(6)	4.7895(5)	6.660(2)
36.5(4)	4.5835(12)	4.7832(11)	6.645(4)
39.3(4)	4.5725(14)	4.7743(40)	6.627(5)
41.8(4)	4.5624(47)	4.7674(14)	6.612(5)
45.6(5)	4.5467(6)	4.7557(5)	6.599(5)
47.5(5)	4.5353(7)	4.7480(6)	6.582(5)
50.1(4)	4.5254(12)	4.7435(45)	6.562(6)
52.7(4)	4.5142(9)	4.7341(9)	6.553(6)
55.4(5)	4.5044(8)	4.7269(7)	6.540(6)
58.0(5)	4.4962(10)	4.7206(9)	6.522(6)
60.6(6)	4.4814(8)	4.7150(7)	6.519(6)
64.6(6)	4.4668(7)	4.6972(6)	6.496(6)

Table S2. The values of evaluation parameters (*wR* and GoF) in different models with a certain amount of Fe fixed in the B site during single-crystal refinements at the lowest experimental pressure of 4.2 GPa.

	A-site Fe ions (mol%)	B-site Fe ions (mol%)	A-site Al^{3+} (mol%)	B-site Al^{3+} (mol%)	*wR* value (%)	GoF
Model 1(best-fit)	10	0	3	11	3.2	1.49
Model 2	5 (fixed)	5 (fixed)	8	6	11.6	4.38
Model 3	0 (fixed)	10 (fixed)	13	1	22.4	8.67

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