Supporting information

Exploring the high-pressure behavior of 2D and quasi-3D boron layers in MoB_2

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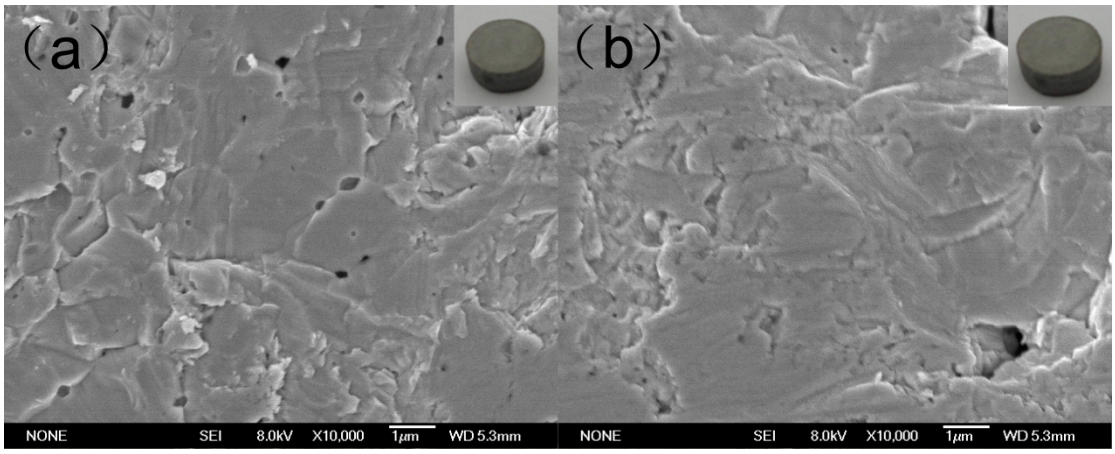

Fig. S1 (a): SEM of α-MoB_2; (b): SEM of β-MoB_2. The insert patterns in (a) and (b) are samples after high pressure and high temperature experiments, respectively. High pressure makes the samples to be bulk materials, and both the bulk samples and SEM results have no distinct difference.

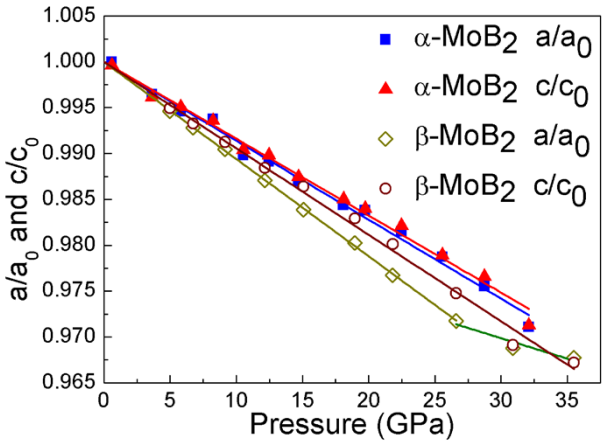

Fig. S2 MoB_2 fractional lattice parameters plotted as a function of pressure.

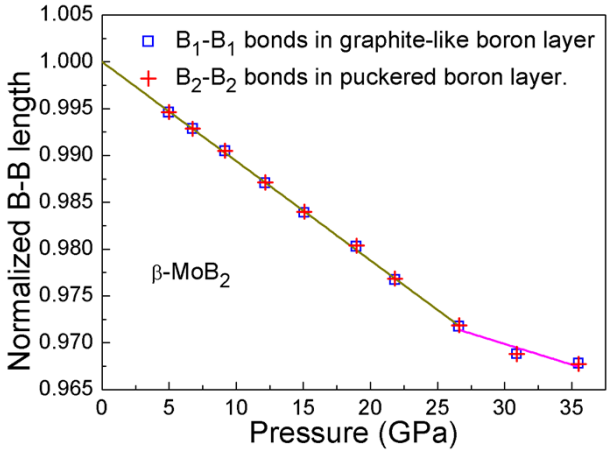

Fig. S3 Normalized B-B bonds length as a function of pressure in β-MoB_2. The changed rules of B_1-B_1 bonds length in graphite-like boron layer are same with B_2-B_2 bonds length in puckered boron layer.

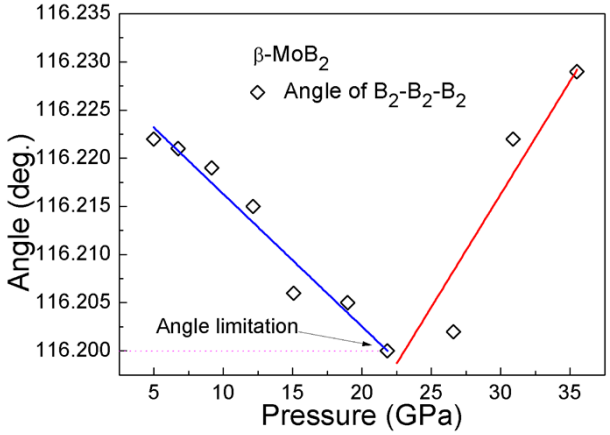

Fig. S4 Angle of B_2-B_2-B_2 as a function of pressure in puckered boron layer of β-MoB_2.

Table S1[a] The Calculated MoB_2 Elastic Constants Cij, Bulk Modulus B, Shear Modulus G, Young's Modulus E, calculated Vickers hardness Hv_{cal} and experimental Vickers hardness Hv_{exp} (in units of GPa).

Compounds	C_{11}	C_{33}	C_{12}	C_{13}	C_{44}	B	G	E	Hv_{cal}	Hv_{exp}
α-MoB_2(P6/mmm)	613	391	120	220	168	304	186	463	15.9	15.2
β-MoB_2 (R-3m)	550	624	126	180	230	299	216	522	21.2	22.0

[a]Reference 1.

1 Q. Tao, X. P. Zhao, Y. L. Chen, J. Li, Q. Li, Y. M. Ma, J. J. Li, T. Cui, P. W. Zhu and X. Wang, *RSC Adv.*, 2013, **3**, 18317.