Supplementary Information

Boron Suboxide and Boron Subphosphide Crystals: Hard Ceramics that Shear without Brittle Failure

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Table S1. The predicted elastic moduli (GPa) for the boron suboxide crystal framework. The calculated elastic constants used a non-standard set of cell axes.

C_{ijkl}	XX	YY	ZZ	YZ	ZX	XY
XX	468.9	92.2	75.0	26.2	-16.4	-22.7
YY	92.2	531.5	91.1	-39.6	-6.6	-39.9
ZZ	75.0	91.1	571.1	-20.6	-34.1	-16.3
XY	-22.7	-39.9	-16.3	0.0	29.7	216.1
YZ	26.2	-39.6	-20.6	204.3	-7.5	0.0
ZX	-16.4	-6.6	-34.1	-7.5	196.5	29.7

Figure S1

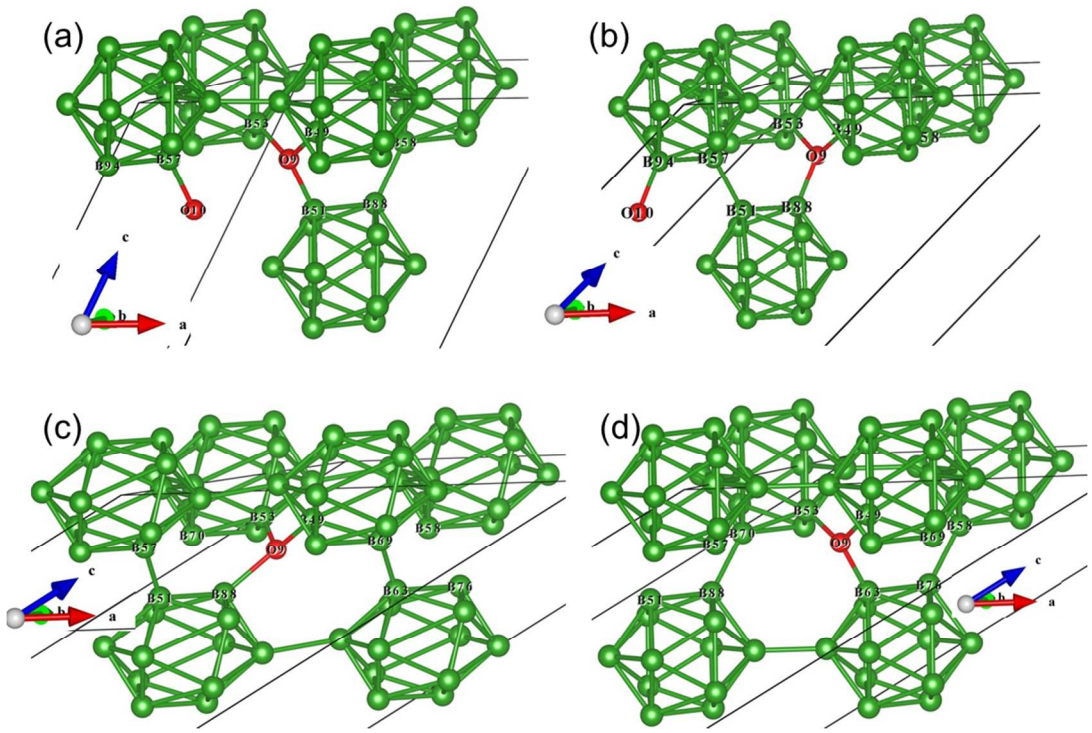

Figure S1. The local atomic structures for shearing along the $(0\bar{1}11)/<10\bar{1}1>$ slip system. (a) the intact structure. (b) the 0.565 strain, at which the structure recovers to the original structure, but with the "c" axis along $[111]_r$ direction. (c) the 1.13 strain, before the second recovery of the original structure. (d) the 1.16 strain, where the original structure is recovered the second time, but with the "c" axis along the $[101]_r$ direction. The boron and oxygen atoms are in green and red, respectively.

Figure S2

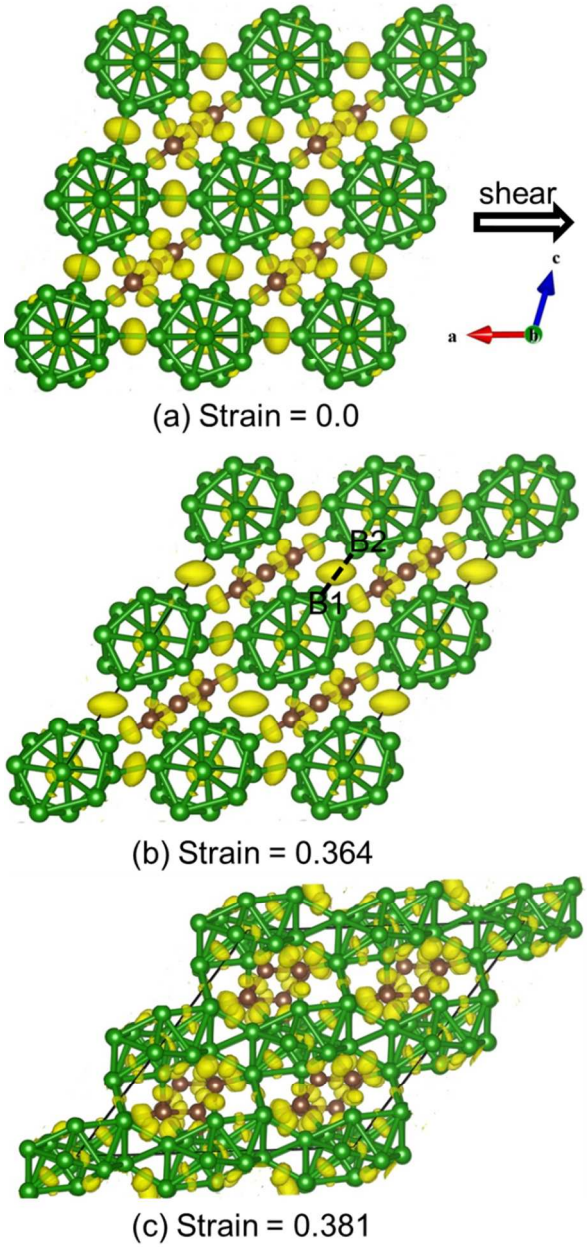

Figure S2. The atomic structures and ELFs for $(B_{12})(CCC)$ shearing along the $(0\bar{1}11)/<10\bar{1}1>$ slip system. (a) the intact structure. (b) the critical stain of 0.364 before failure where the B1-B2 bond still exits although it is stretched to 2.23 Å. (c) the 0.381 strain, the failure structure where the B_{12} icosahedra are broken and the middle C atoms bonded to the broken cages. The boron and carbon atoms are in green and brown, respectively.

Figure S3

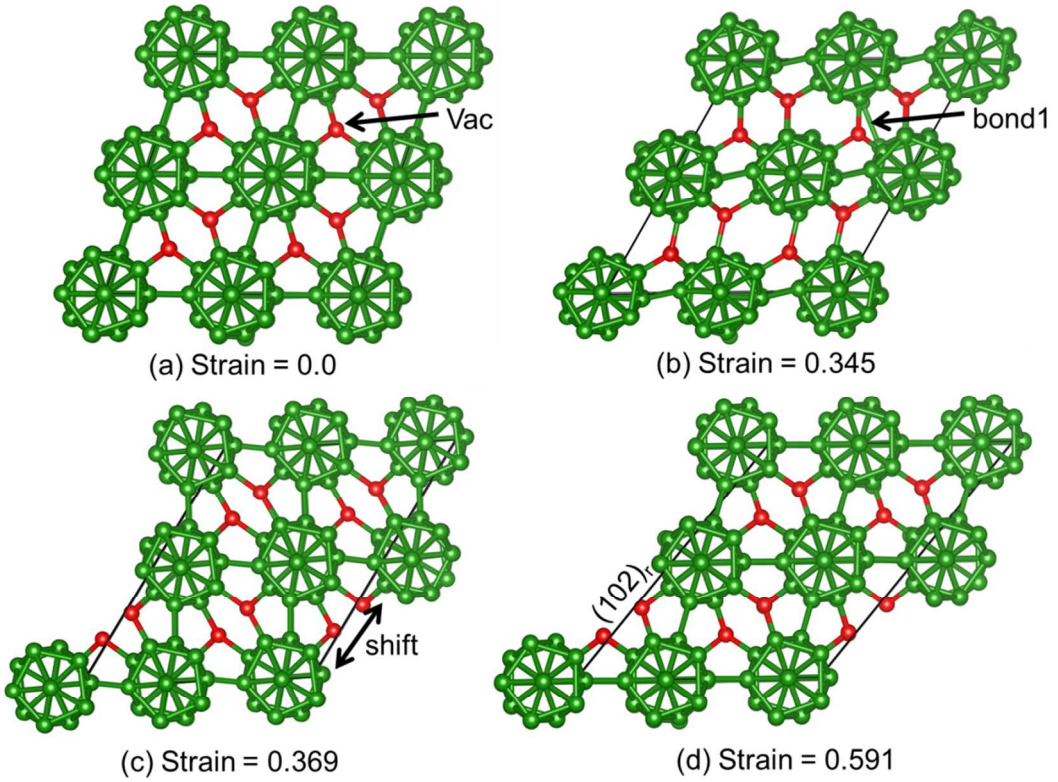

Figure S3. Deformation mechanism of B_6O crystal with O vacancy shearing along the $(0\bar{1}11)/<10\bar{1}1>$ slip system. (a) the intact structure. (b) the critical stain of 0.345 before structural change. (c) the 0.369 strain where the structure recovers to itself and the bottom two layers are shifted to each other. (d) the 0.591 strain where the transformed structure relaxes to ~0 pressure where the c axis along $[102]_r$ direction. The boron and oxygen atoms are in green and red, respectively.

Figure S4

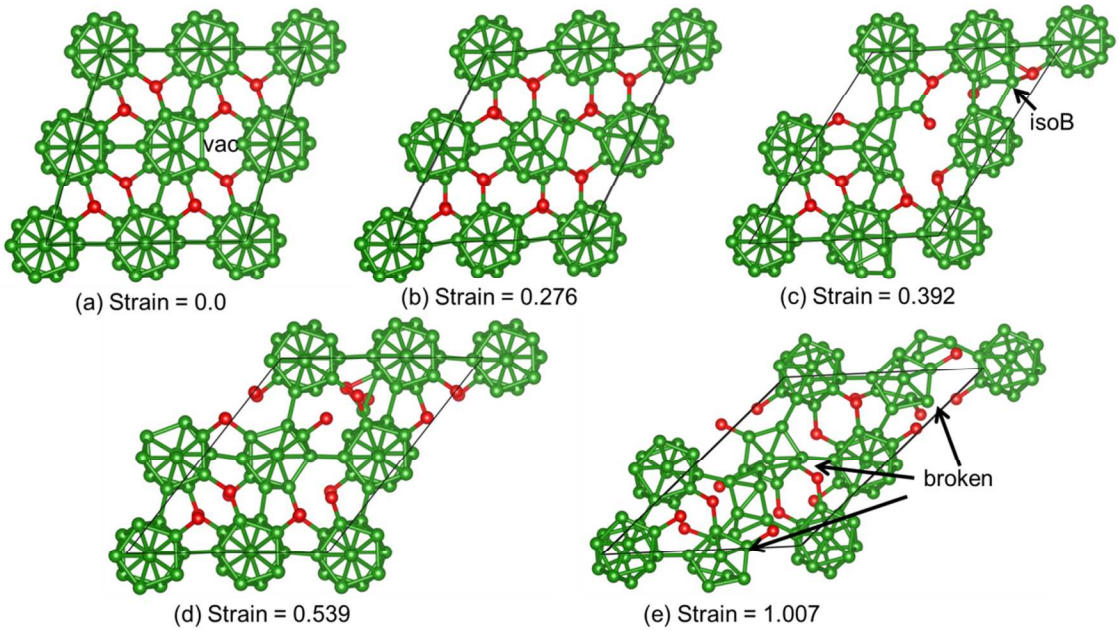

Figure S4. Deformation mechanism of B_6O crystal with B vacancy shearing along the $(0\bar{1}11)/<10\bar{1}1>$ slip system. (a) the intact structure. (b) the critical stain of 0.276 before structural change. (c) the 0.392 strain where one B atom is stretched out of the previous B_{11} cluster. (d) the 0.539 strain the structure relaxed. (e) the 1.007 strain for the second stress relax where several cages are broken. Only one layer of B_{12} icosahedra including B vacancy is shown. The boron and oxygen atoms are in green and red, respectively.

Figure S5

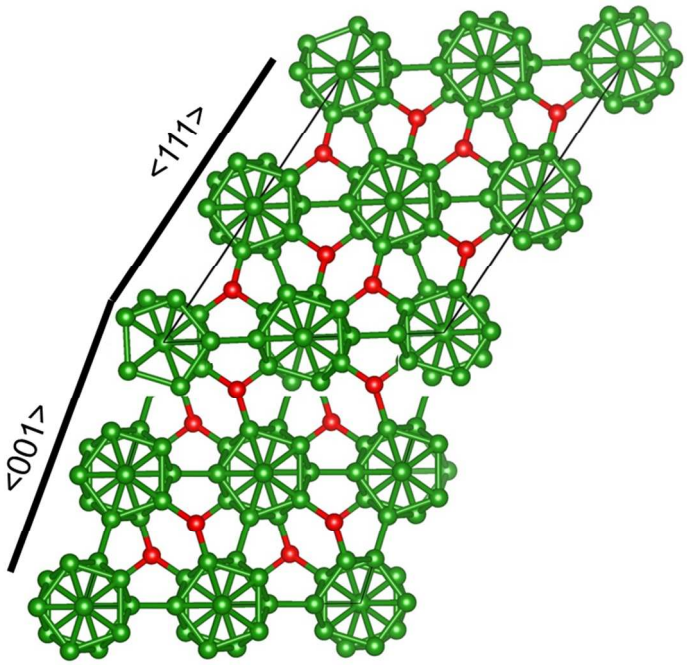

Figure S5. The proposed atomistic twining structure in boron suboxide. The boron and oxygen atoms are in green and red, respectively.