Supporting Information

Vanadium Diboride VB_2 Synthesized at High Pressure: Elastic, Mechanical, Electronic, and Magnetic Properties and Thermal Stability

Pei Wang,[*,†] Ravhi Kumar,[†] Esakki Muthu Sankaran,[†] Xintong Qi,[‡] Xinyu Zhang,[§] Dmitry Popov,[‖] Andrew L. Cornelius,[†] Baosheng Li,[‡] Yusheng Zhao,[†] and Liping Wang[*,†]

[†] *High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Las Vegas, Nevada 89154, United States*

[‡] *Department of Geosciences, Stony Brook University, Stony Brook, New York 11794, United States*

[§] *State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao 066004, People's Republic of China*

[‖] *High Pressure Collaborative Access Team, Geophysical Laboratory, Carnegie Institution of Washington, Argonne, Illinois 60439, United States*

*Email: pei.wang@unlv.edu (P.W.); liping.wang@unlv.edu (L.W.).

Table S1. The bond lengths, and lattice constants in VB_2 in comparison with that of honeycomb AlB_2-type borides (Ref. 1).

Table S2. The calculated single-crystal elastic constants (C_{ij} in GPa) for VB_2. Previous first-principles calculations results for TiB_2, CrB_2, ZrB_2, ReB_2, WB_3, and B_6O listed for comparison.

Figure S1. Calculated formation enthalpy as a function of pressure for vanadium diboride.

Figure S2. Selected high-pressure synchrotron x-ray diffraction patterns for VB_2. Peaks with arrows are from MgO (capsule material).

Figure S3. (a) Three-dimensional Electron Localization Function (ELF) isosurface in VB_2. The red and green spheres represent vanadium and boron atoms, respectively. Three-dimensional illustrations of isosurface of ELF for different lattice: (b) (110) and (c) (010).

Table S1.

Compounds	Bond lengths (Å)		Lattice constants (Å)			
	B–B	M–B	*a*	*b*	*c*	*c*/*a*
VB_2	1.727	2.30	2.998	2.998	3.060	1.020
TiB_2	1.748	2.38	3.028	3.028	3.228	1.064
TaB_2	1.788	2.41	3.097	3.097	3.225	1.041
HfB_2	1.813	2.51	3.141	3.141	3.470	1.105
NbB_2	1.790	2.43	3.110	3.110	3.270	1.050
ZrB_2	1.830	2.54	3.169	3.169	3.530	1.114
CrB_2	1.714	2.30	2.969	2.969	3.066	1.030

Table S2.

Compounds	C_{11}	C_{33}	C_{12}	C_{13}	C_{44}	References
VB_2	685	494	113	123	226	This study
	683	462	111	127	229	[4]
TiB_2	656	461	66	98	259	[5]
CrB_2	601	345	162	206	154	[4]
ZrB_2	541	422	56	111	253	[4]
ReB_2	631	1015	158	134	257	[2]
WB_3	639	470	106	169	262	[2]
B_6O	603	459	109	50	179	[2]

Figure S1.

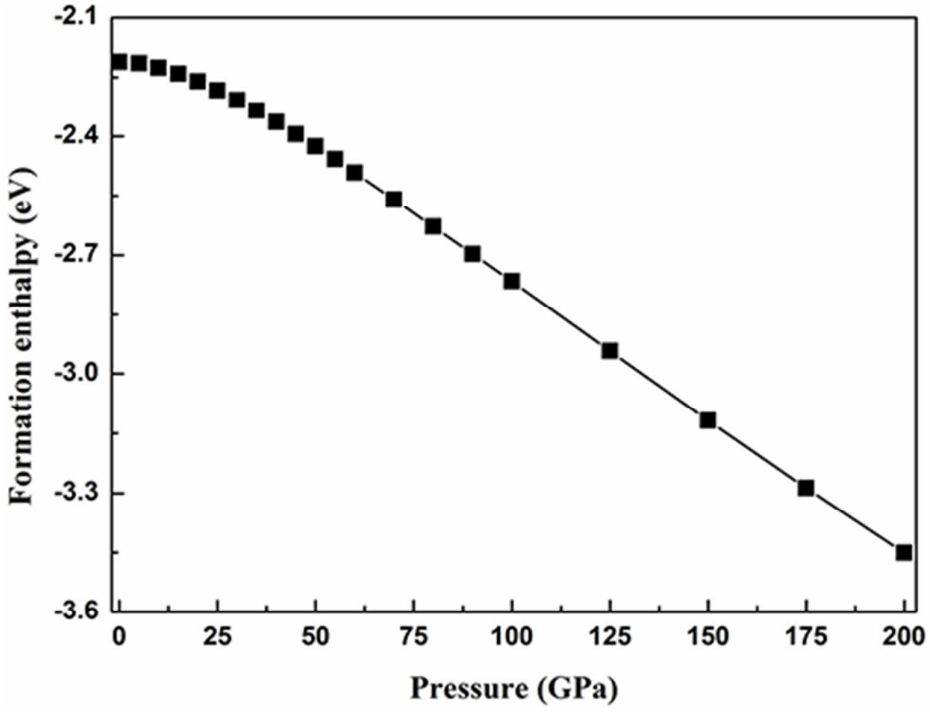

-2.1
-2.4
-2.7
-3.0
-3.3
-3.6
Formation enthalpy (eV)
0
25
50
75
100
125
150
175
200
Pressure (GPa)

Figure S2.

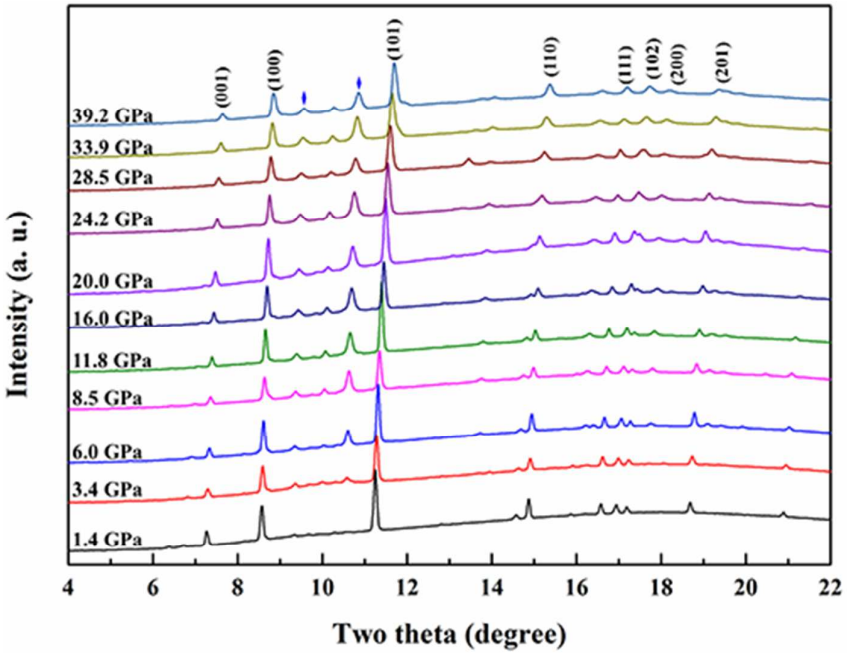
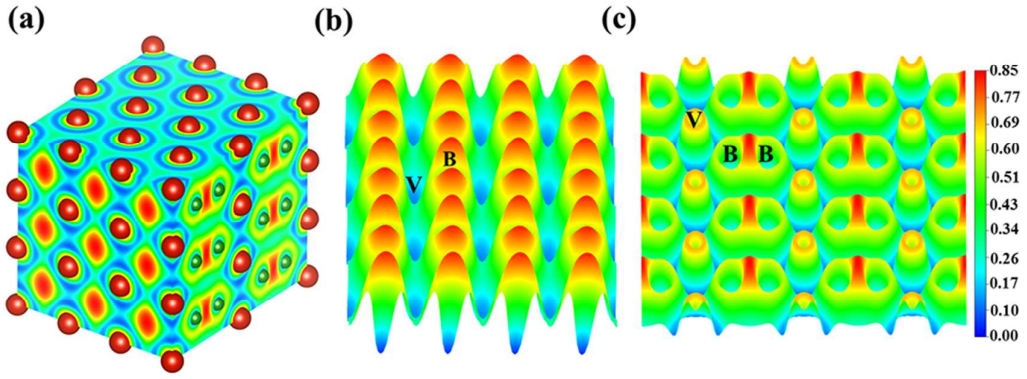

(001)
(100)
(101)
(110)
(111)
(102)
(200)
(201)
39.2 GPa
33.9 GPa
28.5 GPa
24.2 GPa
20.0 GPa
16.0 GPa
11.8 GPa
8.5 GPa
6.0 GPa
3.4 GPa
1.4 GPa
Intensity (a. u.)
4
6
8
10
12
14
16
18
20
22
Two theta (degree)

Figure S3.



■ REFERENCES

1. Fahrenholtz, W. G.; Hilmas, G. E.; Talmy, I. G.; Zaykoski, J. A. Refractory diborides of zirconium and hafnium. *J. Am. Ceram. Soc.* **2007**, 90, 1347-1364.
2. Zhang, R. F.; Legut, D.; Lin, Z. J.; Zhao, Y. S.; Mao, H. K.; Veprek, S. Stability and strength of transition-metal tetraborides and triborides. *Phys. Rev. Lett*. **2012**, 108, 255502.
3. Zhou, W.; Wu, H.; and Yildirim, T. Electronic, dynamical, and thermal properties of ultra-incompressible superhard rhenium diboride: A combined first-principles and neutron scattering study. *Phys. Rev. B* **2007**, 76, 184113.
4. Shein, I. R.; Ivanovskii, A. L. Elastic properties of mono-and polycrystalline hexagonal AlB_2-like diborides of *s*, *p* and d metals from first-principles calculations. *J. Phys. Condens. Matter.* **2008**, 20, 415218.
5. Milman, V.; Warren, M. C. Elastic properties of TiB_2 and MgB_2. *J. Phys. Condens. Matter.* **2001**, 13, 5585.