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Unexpectedly low indentation strength of WB3 and MoB3 from first principles

DOI: 10.1103/physrevb.86.180101  
Physical Review B, 2012, 86, .

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**Version:** 2024-04-09

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#	Paper	IF	Citations
48	Fundamental constraints on the strength of transition-metal borides: The case of CrB <sub>4</sub> . <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	35
47	Unexpectedly hard and highly stable WB <sub>3</sub> with a noncompact structure. <i>Chemical Physics Letters</i> , <b>2013</b> , 580, 48-52	2.5	39
46	Global structural optimization of tungsten borides. <i>Physical Review Letters</i> , <b>2013</b> , 110, 136403	7.4	216
45	Phase stability, mechanical properties, hardness, and possible reactive routing of chromium triboride from first-principle investigations. <i>Journal of Chemical Physics</i> , <b>2013</b> , 139, 234503	3.9	7
44	Interstitial-boron solution strengthened WB <sub>3+x</sub> . <i>Applied Physics Letters</i> , <b>2013</b> , 103, 171903	3.4	62
43	The structural and elastic properties of TMB <sub>4</sub> (TM = V, Cr, Mn) under pressure: A first-principles study. <i>International Journal of Modern Physics B</i> , <b>2014</b> , 28, 1450202	1.1	1
42	Unexpected structural softening of interstitial boron solid solution WB <sub>3+x</sub> . <i>Applied Physics Letters</i> , <b>2014</b> , 105, 211901	3.4	7
41	Lattice stress states of superhard tungsten tetraboride from radial x-ray diffraction under nonhydrostatic compression. <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	29
40	A semiconductive superhard FeB <sub>4</sub> phase from first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 22008-13	3.6	13
39	First-principles calculation of the indentation strength of FeB <sub>4</sub> . <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	32
38	Computational materials discovery: the case of the W-B system. <i>Acta Crystallographica Section C, Structural Chemistry</i> , <b>2014</b> , 70, 85-103	0.8	70
37	Crystal Structure of W <sub>1-x</sub> B <sub>3</sub> and Phase Equilibria in the Boron-Rich Part of the Systems Mo-Rh-B and W-{Ru,Os,Rh,Ir,Ni,Pd,Pt}-B. <i>Journal of Phase Equilibria and Diffusion</i> , <b>2014</b> , 35, 384-395	1	21
36	Exploring Hardness and the Distorted sp <sup>2</sup> Hybridization of B-B Bonds in WB <sub>3</sub> . <i>Chemistry of Materials</i> , <b>2014</b> , 26, 5297-5302	9.6	59
35	Polytypism in superhard transition-metal triborides. <i>Scientific Reports</i> , <b>2014</b> , 4, 5063	4.9	13
34	Materials discovery via CALYPSO methodology. <i>Journal of Physics Condensed Matter</i> , <b>2015</b> , 27, 203203	1.8	63
33	Structure of superhard tungsten tetraboride: a missing link between MB <sub>2</sub> and MB <sub>12</sub> higher borides. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2015</b> , 112, 3223-8	11.5	63
32	Exploring hardness enhancement in superhard tungsten tetraboride-based solid solutions using radial X-ray diffraction. <i>Applied Physics Letters</i> , <b>2015</b> , 107, 041903	3.4	14

31	Structural stability and elastic properties of WB4 under high pressure. <i>International Journal of Modern Physics B</i> , <b>2015</b> , 29, 1550103	1.1	4
30	Strength of tungsten triboride under pressure up to 86 GPa from radial X-ray diffraction. <i>Journal of Alloys and Compounds</i> , <b>2015</b> , 621, 116-120	5.7	5
29	The structural stabilities, mechanical properties and hardness of chromium tetraboride: Compared with low-B borides. <i>International Journal of Modern Physics B</i> , <b>2016</b> , 30, 1650201	1.1	14
28	Strong covalent boron bonding induced extreme hardness of VB3. <i>Journal of Alloys and Compounds</i> , <b>2016</b> , 688, 1101-1107	5.7	9
27	Structural optimization and physical properties of TcB3 and MoB3 at high-pressure: First-principles. <i>International Journal of Modern Physics B</i> , <b>2016</b> , 30, 1650131	1.1	4
26	Discovery of elusive structures of multifunctional transition-metal borides. <i>Nanoscale</i> , <b>2016</b> , 8, 1055-65	7.7	17
25	Ultraincompressible, Superhard Materials. <i>Annual Review of Materials Research</i> , <b>2016</b> , 46, 465-485	12.8	73
24	Extraordinary Indentation Strain Stiffening Produces Superhard Tungsten Nitrides. <i>Physical Review Letters</i> , <b>2017</b> , 119, 115503	7.4	108
23	Influence of Re Concentration on the Mechanical Properties of Tungsten Borides from First-Principles Calculations. <i>Jom</i> , <b>2017</b> , 69, 2009-2013	2.1	17
22	Ultrastrong Boron Frameworks in ZrB : A Highway for Electron Conducting. <i>Advanced Materials</i> , <b>2017</b> , 29, 1604003	24	50
21	DFT prediction of a novel molybdenum tetraboride superhard material.. <i>RSC Advances</i> , <b>2018</b> , 8, 18008-18015	9.7	15
20	First-principles design of strong solids: Approaches and applications. <i>Physics Reports</i> , <b>2019</b> , 826, 1-49	27.7	17
19	Revealing the Unusual Rigid Boron Chain Substructure in Hard and Superconductive Tantalum Monoboride. <i>Chemistry - A European Journal</i> , <b>2019</b> , 25, 5051-5057	4.8	7
18	Nonrandomly Distributed Tungsten Vacancies and Interstitial Boron Trimers in Tungsten Tetraboride. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 29314-29323	3.8	4
17	Unravelling the structure and strength of the highest boride of tungsten WB4.2. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	16
16	Elastic anisotropy and physical properties of semi-transition-metal borides: first-principles calculation. <i>Applied Physics Express</i> , <b>2020</b> , 13, 015501	2.4	4
15	Toughening a superstrong carbon crystal: Sequential bond-breaking mechanisms. <i>Physical Review B</i> , <b>2020</b> , 102,	3.3	2
14	Elucidating Stress-Strain Relations of ZrB from First-Principles Studies. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 9165-9170	6.4	50

13	Atomistic Mechanisms for Contrasting Stress-Strain Relations of BCN and BC. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 10454-10462	6.4	3
12	Mechanical properties of tantalum carbide from high-pressure/high-temperature synthesis and first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 5018-5023	3.6	7
11	Indentation Strengths of Zirconium Diboride: Intrinsic versus Extrinsic Mechanisms. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 2848-2853	6.4	32
10	Crystal structures and formation mechanisms of boron-rich tungsten borides. <i>Physical Review B</i> , <b>2021</b> , 104,	3.3	3
9	Progress in functional studies of transition metal borides. <i>Chinese Physics B</i> ,	1.2	0
8	Indentation-strain stiffening in tungsten nitrides: Mechanisms and implications. <i>Physical Review Materials</i> , <b>2020</b> , 4,	3.2	35
7	Structure-strength relations of distinct MoN phases from first-principles calculations. <i>Physical Review Materials</i> , <b>2020</b> , 4,	3.2	36
6	Unusual suppression of tungsten 5electron depletion in superhard tungsten tetraboride solid solution with chromium under compression. <i>Journal of Physics Condensed Matter</i> , <b>2021</b> , 34,	1.8	0
5	Superhard metallic compound TaB <sub>2</sub> via crystal orientation resolved strain stiffening. <i>Physical Review B</i> , <b>2022</b> , 105,	3.3	1
4	Macroscale Robust Superlubricity on Metallic NbB <sub>2</sub> . <i>Advanced Science</i> , <b>2022</b> , e2103815	13.6	0
3	Effect of pressure on anisotropy in elasticity, sound velocity, and thermal conductivity of vanadium borides. <i>Advanced Composites and Hybrid Materials</i> ,	8.7	2
2	Exceptional strain strengthening and tuning of mechanical properties of TiN. <b>2022</b> , 106,		1
1	Macroscale superdurable superlubricity achieved in lubricant oil via operando tribochemical formation of fullerene-like carbon. <b>2022</b> , 101130		0