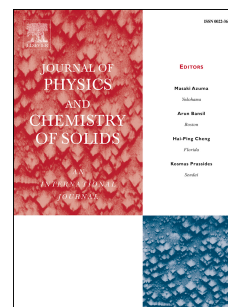


Accepted Manuscript

Mechanical behavior, electronic and phonon properties of ZrB_{12} under pressure

Xiao-Hong Li, Yong-Liang Yong, Hong-Ling Cui, Rui-Zhou Zhang



PII: S0022-3697(18)30014-3

DOI: [10.1016/j.jpcs.2018.02.033](https://doi.org/10.1016/j.jpcs.2018.02.033)

Reference: PCS 8448

To appear in: *Journal of Physics and Chemistry of Solids*

Received Date: 4 January 2018

Revised Date: 1 February 2018

Accepted Date: 12 February 2018

Please cite this article as: X.-H. Li, Y.-L. Yong, H.-L. Cui, R.-Z. Zhang, Mechanical behavior, electronic and phonon properties of ZrB_{12} under pressure, *Journal of Physics and Chemistry of Solids* (2018), doi: 10.1016/j.jpcs.2018.02.033.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Mechanical Behavior, Electronic and Phonon Properties of ZrB_{12} under Pressure

Xiao-Hong Li^{a,b,†}, Yong-Liang Yong^a, Hong-Ling Cui^a, Rui-Zhou Zhang^a

^a College of Physics and Engineering, Henan University of Science and Technology, Luoyang 471023, China

^b Henan Key Laboratory of Photoelectric Energy Storage Materials and Applications, Luoyang, 471023, China

Abstract: The mechanical, phonon and electronic properties of ZrB_{12} under pressure are investigated by first-principles calculations. The research shows that ZrB_{12} is mechanically and dynamically stable up to 100 GPa. The elastic constants, bulk modulus B , shear modulus G , hardness H_v , B/G ratio, Debye temperature under different pressures are systematically investigated. The calculation of electronic properties shows that ZrB_{12} has metallic character. The Zr-d states dominate the DOS at the Fermi level, and the total DOS and PDOS change slightly with the increasing pressure. DOS (E_f) first decreases, then increases with the increasing pressure. At 50 GPa, ZrB_{12} has less electron carriers. The analysis of electron localization function shows that the strong B-B and Zr-B covalent bonds may be responsible for the high hardness and stability.

Keywords: first-principles calculation; mechanical properties, electronic properties; phonon dispersion

[†] Corresponding author. Email: lorna639@126.com

Download English Version:

<https://daneshyari.com/en/article/7920342>

Download Persian Version:

<https://daneshyari.com/article/7920342>

[Daneshyari.com](https://daneshyari.com)