Accepted Manuscript

Study of the electronic, bonding, elastic and acoustic properties of covellite via first principles

Zhenlong Lv, Hongling Cui, Haiming Huang, Xiaohong Li, Hui Wang, Guangfu Ji

PII: S0925-8388(16)32847-X

DOI: 10.1016/j.jallcom.2016.09.095

Reference: JALCOM 38929

To appear in: *Journal of Alloys and Compounds*

Received Date: 8 May 2016

Revised Date: 15 July 2016

Accepted Date: 9 September 2016

Please cite this article as: Z. Lv, H. Cui, H. Huang, X. Li, H. Wang, G. Ji, Study of the electronic, bonding, elastic and acoustic properties of covellite via first principles, *Journal of Alloys and Compounds* (2016), doi: 10.1016/j.jallcom.2016.09.095.

Study of the electronic, bonding, elastic and acoustic properties of covellite via first principles

Zhenlong Lv [a,*], Hongling Cui [a], Haiming Huang[a], Xiaohong Li [a], Hui Wang [a,*], Guangfu Ji [b]

[a] School of Physics and Engineering, Henan University of Science and Technology, Luoyang 471003, China

[b] Institute of Fluid Physics, Chinese Academy of Engineering Physics, Mianyang 621900, China

Abstract: Covellite (CuS) is a compound with a simple chemical formula but a rather complex crystal structure. In this work, we studied the electronic, bonding, elastic and acoustic properties of covellite by first principles calculation. Electronic property calculations reveal that the p-d hybridization between S-3p and Cu-3d is responsible for the metallic behavior of covellite, which makes it a challenge to construct an accurate ionic model for this compound. The calculated partial density of states reproduce the experimental XPS and XAS well and the theoretically obtained Fermi surface verifies the experimentally found two-dimensional electronic transport characteristic of covellite. Calculated elastic constants demonstrate that covellite is mechanically stable but anisotropic. Investigation reveals that elastic constant C_{44} has a close correlation with the easy-cracked property of *c* axis of covellite. Besides, bulk modulus, shear modulus, Poisson's ratio, velocities of acoustic waves and Debye temperature were also predicated. Proceeding from the Christoffel equation of hexagonal crystal, we also discussed the propagation properties of acoustic waves in covellite to give a theoretical guidance for the related measurement.

* Corresponding authors. E-mail addresses: 9902883@haust.edu.cn (Z. Lv), nkxirainbow@gmail.com (H. Wang)