Current Applied Physics 18 (2018) 799–802

Contents lists available at ScienceDirect

Current Applied Physics

journal homepage: www.elsevier.com/locate/cap

First-principles study on the Poisson's ratio of transition-metal dichalcogenides

Yongmin Yoo, Jin-Hoon Yang, Joo-Hyoung Lee*

School of Materials Science and Engineering, Gwangju Institute of Science and Technology, 123, Cheomdangwagi-ro, Buk-gu, Gwangju, 61005, Republic of Korea

ARTICLE INFO

Keywords:
Transition-metal dichalcogenides
Poisson's ratio
Density functional theory
Anisotropy

ABSTRACT

In this study, we investigate the Poisson's ratio of transition-metal dichalcogenides (TMDCs) with a chemical formula of MX_2, where M = Mo, W and X = S, Se, respectively, from first-principles. Through density functional theory calculations, it is demonstrated that the Poisson's ratio of MX_2 exhibits not only a substantial difference between the planar and vertical values but also a systematic dependence on the chalcogen species. Among the TMDCs, MoS_2 displays the strongest anisotropy, which entails a distinctive contracting response under a planar strain. We find that such pronounced anisotropy in the Poisson's ratio of the TMDCs originates from the different filling of the in- (p_x, p_y, d_{xy}, and $d_{x^2-y^2}$) and out-of-plane (p_z, d_{yz}, d_{zx}, and d_{z^2}) electronic orbitals depending on the transition-metal elements. These findings shed a new light on the elastic properties of TMDCs which continue to be interesting and show intriguing phenomena.

1. Introduction

Successful isolation of graphene from graphite through mechanical exfoliation has brought about tremendous interest in layered materials such as group-IV or -V elemental structures [1–5] and transition-metal-based compounds including transition-metal dichalcogenides (TMDCs) [6,7]. The interest in these reduced-dimensional materials is primarily due to their rich and fascinating physics such as unique electronic structures, high mechanical strength and enhanced optical absorption, which also holds great promise for technological applications. Among them, TMDCs, which are denoted as MX_2 with M and X being transition-metal and chalcogen elements, respectively, have drawn particular attention because diverse electronic states, ranging from, for instance, semiconducting, metallic to superconducting ones, can be realized simply by varying chemical compositions [8]. In addition, within a given TMDC the electronic structure shows a distinctive layer-dependence in that the band gap of a semiconducting TMDC can be tuned by modifying the number of component X-M-X layers [9–13], which, together with the layer-dependent transition from indirect to direct gap, makes TMDCs particularly attractive for optoelectronic as well as electronic applications.

Mechanical aspects of TMDCs are of great interest as well since the electronic and optical properties can be controlled by applying external strain as is shown with the indirect-direct band gap transition, band gap modulation and enhanced photoemission phenomena [14–17]. Moreover, a high potential for nanoscale electro-mechanical energy conversion applications has been demonstrated with enhanced piezoelectricity in a single layer TMDCs [18,19], and even an auxetic behavior, negative Poisson's ratio, has been reported [20]. Certainly, all these efforts have significantly advanced our understanding of novel and exciting properties in these low dimensional materials and demonstrated promise towards development of next-generation high-performance devices.

However, it should be noted that the reported results have been focused exclusively on the two-dimensional (2D) form of TMDCs, either monolayer or few-layer structures. The corresponding bulk counterpart, in spite of its important role in technological applications such as solid lubricant, has not been paid as much attention on a fundamental side as the 2D allotropes until recently. In fact, it is highly interesting materials characteristics manifested in the mono- and few-layer structures of TMDCs that have generated renewed interest in the physical properties of the bulk phase at a microscopic level. Electronic properties including charge density waves [21–23], metal-insulator transition driven either electronically [24] or mechanically [25] and magnetic properties such as ferromagnetism, large magnetoresistance and spin-polarized states [26–29] have been subjects of intensive study for bulk TMDCs.

In contrast with the high interest in the electronic and magnetic attributes, the elastic properties of the bulk have not yet been examined as much although they constitute an important characteristic in the property space [30]. In particular, while the layered arrangement of TMDCs may well give rise to an anisotropy in various materials properties, only the electrical and optical properties [31] and the magnetic

* Corresponding author.
E-mail address: jhyoung@gist.ac.kr (J.-H. Lee).

https://doi.org/10.1016/j.cap.2018.03.018
Received 30 January 2018; Received in revised form 10 March 2018; Accepted 21 March 2018
Available online 06 April 2018