Physics Letters A 381 (2017) 3167–3172

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Effects of topological edge states on the thermoelectric properties of Bi nanoribbons

L. Cheng [a,b], H.J. Liu [a,*], J.H. Liang [a], J. Zhang [a], J. Wei [a], P.H. Jiang [a], D.D. Fan [a]

[a] Key Laboratory of Artificial Micro- and Nano-Structures of Ministry of Education and School of Physics and Technology, Wuhan University, Wuhan 430072, China

[b] Institute of Mineral Engineering, Division of Materials Science and Engineering, RWTH Aachen University, Aachen 52064, Germany

ARTICLE INFO

Article history:
Received 7 June 2017
Received in revised form 30 July 2017
Accepted 5 August 2017
Available online 16 August 2017
Communicated by R. Wu

Keywords:
First-principles
Boltzmann transport theory
Thermoelectric properties
Nanoribbons
Topological insulators

ABSTRACT

Using first-principles calculations combined with Boltzmann transport theory, we investigate the effects of topological edge states on the thermoelectric properties of Bi nanoribbons. It is found that there is a competition between the edge and bulk contributions to the Seebeck coefficients. However, the electronic transport of the system is dominated by the edge states because of its much larger electrical conductivity. As a consequence, a room temperature ZT value exceeding 3.0 might be achieved for both p- and n-type systems by fine tuning the relaxation time ratio between the edge and the bulk states.

1. Introduction

Searching for thermoelectric materials with high performance is one of the most important topics in the community of materials science. The efficiency of a thermoelectric material is quantified by the so-called figure of merit, defined as $ZT = S^2\sigma T/(\kappa_e + \kappa_l)$, where S is the Seebeck coefficient, σ is the electrical conductivity, κ_e and κ_l are respectively the electronic and lattice thermal conductivity, and T is the absolute temperature. For conventional thermoelectric materials, the electronic transport coefficients (S, σ and κ_e) are usually coupled in a way which makes it very challenging to obtain higher ZT values. During the past decades, a few promising strategies were proposed to enhance the thermoelectric performance including increasing the power factor ($S^2\sigma$) via band engineering [1–3], as well as decreasing the lattice thermal conductivity by phonon scattering [4,5]. It is interesting to find that low-dimensionalization combines both advantages and significantly larger ZT values can thus be expected [6,7]. Even so, it is still far from the target value ($ZT > 3.0$) to compete with the traditional power generation or cooling methods.

Recently, both theoretical predictions [8–10] and experimental studies [11–14] have shown that some of good thermoelectric materials such as Bi_2Te_3, Bi_2Se_3, and $Bi_{1-x}Sb_x$ are also known as topological insulators (TIs). Such a new kind of quantum materials exhibit insulating bulk gaps but topologically protected gapless surface or edge states [15,16], and they share some similar material features with good thermoelectric materials such as containing heavy elements and having small band gaps. However, whether these two classes of materials are inherently connected remains mysterious and conceptually perplexing. In particular, it is still controversial whether the topologically protected surface/edge states could be utilized to enhance the thermoelectric performance. For example, Ghaemi et al. [17] investigated the in-plane transport of Bi_2Te_3 and Bi_2Se_3 thin films and found that the surface states from top and bottom layers mix with each other, and the usual diffusive transport suggests that the tunable hybridization-induced gap leads to enhanced thermoelectric performance at low temperatures. However, Rittweger et al. [18] concluded that a reduction to metallic behavior of the thermopower and electrical conductivity in the Bi_2Te_3 films would be expected, which means that the presence of topological surface states may reduce the thermoelectric performance. Osterhage et al. [19] showed that the parallel contributing channels of bulk and surface states tend to cancel each other out, while Sun et al. [20] suggested that the thermoelectric performance of Bi_2Se_3 can be elevated substantially by utilizations of its gapless conducting surface. It should be noted that most of these works are focused on three-dimensional (3D) TIs with surface states. Recently, Xu et al. demonstrated that the topologically protected edge states in an idealized two-dimensional (2D) model system of TI lead to large and anomalous Seebeck ef-

* Corresponding author.
E-mail address: phlhj@whu.edu.cn (H.J. Liu).

http://dx.doi.org/10.1016/j.physleta.2017.08.013
0375-9601/

fect and the ZT value could be improved to be significantly larger than 1 by optimizing the geometric size [21]. It is thus natural to explore the effects of topological edge states on the thermoelectric performance of a realistic 2D TI. One example is graphene, which is believed to be the prototype of 2D TIs [22]. In fact, the thermoelectric properties of graphene and related structures have been recently studied theoretically. For example, Sevinçli et al. [23] found that edge disorder in zigzag graphene nanoribbons can dramatically reduce phonon transport while being only weakly detrimental to electronic conduction. Gunst et al. [24] calculated the electronic and thermal transport properties of graphene antidot lattices and found that the ZT values are highly sensitive to the atomic arrangement of the antidot edges. Chang and Nikolić [25] analyzed the electronic and phononic transport in zigzag and chiral graphene nanoribbons perforated with an array of nanopores. Xie et al. [26] studied the thermoelectric properties of graphene nanoribbons modulated with stub structures. They found that the phonon transport is dramatically suppressed by the elastic scattering of the stub structure, while the Seebeck coefficient can be enhanced by a few times of magnitude, and thus leads to a strong enhancement of the ZT value. Zhou and Chen [27] suggested that the thermoelectric properties of graphyne nanoribbons can be enhanced observably by introducing defects. All these works offer us some fundamental information about the thermoelectric properties of nanoribbons from which one can go further to discuss the effects of topological edge states. In this work, using first-principles calculations combined with Boltzmann transport theory, we explore the possibility to enhance the thermoelectric properties of Bi nanoribbon by utilization the topologically protected edge states. It is expected that our design strategy may prove to be instrumental in the experimental search of high-performance thermoelectric materials and devices.

2. Computational methods

Our first-principles calculations are performed by adopting the projector-augmented-wave method [28,29] within the framework of density functional theory (DFT) [30–32]. The exchange-correlation energy is treated with generalized gradient approximation (GGA) in the form of Perdew–Burke–Ernzerhof [33]. The vacuum space perpendicular to and along the nanoribbon width is set as 20 Å and 25 Å, respectively, which ensures that the nanoribbon and its periodic images can be treated as independent entities. During the structure optimization, the energy cutoff is set as 210 eV, and a uniform $1 \times 1 \times 20$ Monkhorst–Pack k-mesh is used the Brillouin zone. The structure is fully relaxed until the magnitude of the force acting on each atom is less than 0.01 eV/Å. As Bi is heavy atom, the spin–orbit coupling is considered in our calculations to correctly predict the TI nature. The electronic transport coefficients (S, σ and κ_e) are derived from the semi-classical Boltzmann theory [34], while the phonon transport coefficient (κ_l) can be obtained from molecular dynamics simulations [35]. It should be noted that the definition of electrical conductivity and thermal conductivity depends on the volume or cross-sectional area, which is in principle arbitrary for low-dimensional systems such as nanoribbons. However, this would not change the ZT value as long as the electronic transport coefficient (electrical conductivity σ, electronic thermal conductivity κ_e) and phonon transport coefficient (lattice thermal conductivity κ_l) are calculated with respect to the same vacuum distance.

3. Results and discussion

The Bi nanoribbon can be obtained by cutting the Bi (111) monolayer along a particular direction. In the present work, we

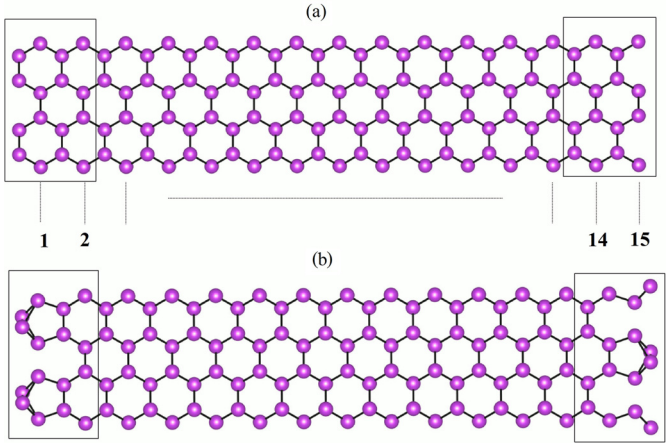

Fig. 1. Ball-and-stick model of (a) the initial, and (b) the fully relaxed structure of 15-ABNR.

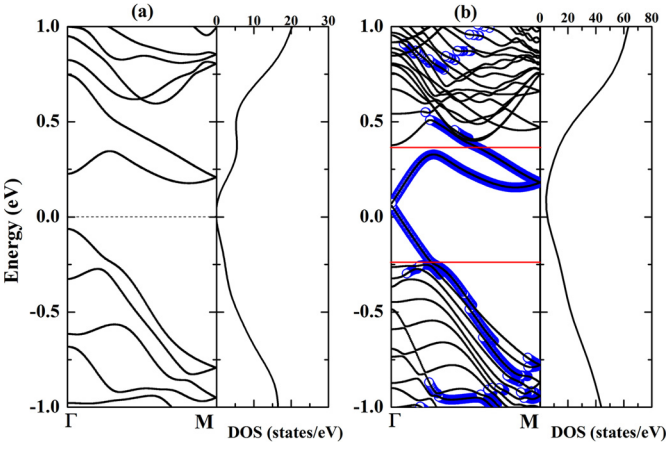

Fig. 2. Band structures and density of states of (a) 6-ABNR, and (b) 15-ABNR, where the edge states are indicated by blue circles. The red lines indicate the bulk gap, and the Fermi level is at 0 eV. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

only consider nanoribbons with armchair edges. Similar to the notation for graphene nanoribbons [36], the armchair Bi nanoribbon (ABNR) is classified by the number of dimer lines across the ribbon width (labeled as N-ABNR). The initial and optimized structures of 15-ABNR are illustrated in Fig. 1(a) and 1(b), respectively. Upon structure relaxations, we see there has an obvious edge reconstruction and all the dangling bonds are eliminated, which is very similar to those found in the BiSb nanoribbons [37].

Fig. 2 plots the band structures and density of states (DOS) of ABNR with two typical width ($N = 6, 15$), where the edge states (marked by blue circles) are identified by the wavefunction projection method [38,39]. For the 6-ABNR, we see it only possesses trivial edge states and has a direct band gap of 0.24 eV. In contrast, there is a single Dirac cone at the Γ point for the 15-ABNR, which indicates it has topologically protected edge states [8]. This can be also verified by simply counting the times of the edge states that across the Fermi level between time-reversal invariant momenta [8]. In fact, we have calculated the topological invariant number of Bi (111) monolayer by using the so-called "parity method" [8], and confirms that it is a 2D TI [39–43]. On the other hand, extensive calculations for a series ABNRs find that there is a transition from topological trivial to non-trivial edge states with increasing nanoribbon width. It is thus interesting to obtain the minimum width that required for the observation of non-trivial edge states, which is usually referred to as the penetration depth. Detailed analysis of the band structures reveals that the topolog-