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Ab-initio study of the structural, electronic and optical properties of BSb (110) and (100) surfaces

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ABSTRACT

In the present study, the structural, electronic and optical properties of BSb bulk, BSb (110) and (100) surfaces were investigated. The calculations were performed by using Full-Potential Linear Augmented Plane Wave (FP-LAPW) in Density Functional Theory (DFT) framework with various exchange-correlation functionals. Some surface properties such as surface energies, the work functions, surface relaxation, band structures and optical properties of cubic BSb (110) and (100) nano-slabs were studied. The (100) surface of cubic BSb has B- and Sb-terminations while the (110) surface has only one termination. The surface properties of all the terminations were presented and discussed. Moreover, some bulk properties such as structural, electronic, band structure and optical properties of BSb compound were investigated for comparison. The obtained band gaps for the BSb (110) nano-slab were 0.38 eV while the BSb (100) nano-slab showed a metallic behavior. Moreover, the surface states of the slabs were identified. The real and imaginary parts of the dielectric function of the BSb (110) nano-slab were also calculated and compared with bulk results.

1. Introduction

The group III–V semiconductors are widely used for electronic and optoelectronic tools. [1]. Among these compounds, the narrow band gap antimonide based compound semiconductors (ABCS) are widely considered as the first candidate materials for production of the third generation infrared photon detectors and ICs with ultra-high speed and ultra-low power consumption. Due to their unique band gap structure and physical properties, it makes a wide space to develop new varied devices [2]. However, III-Sb compounds have attracted more attention due to their potential usage in rechargeable lithium batteries. Among III-Sb compounds, boron antimonide exhibits a strong covalent character and shows an uncommon behavior because of small core and lack of "p" electrons in boron atom compared to other group III–V compounds. It makes this material a potential material for high temperature electronic and optical application [3]. The surfaces of group III–V semiconductors have a fundamental importance because their cleanness, geometry and photoelectric properties deeply affect the function of modern electronic devices [4]. The (110) nonpolar surface of III–V compounds has been broadly investigated and more concentration has been on their relaxed geometry, phonon vibrations and band structure [5–9]. Surface energy and work function are two important parameters for fully recognizing the surfaces [9,10]. Nowadays, various surfaces of group III–V compounds are developing owing to their applications in thin films. Regarding the fact that thin film process technology is firmly linked to the basic investigations on the surfaces and interfaces, their fundamental parameters including surface energy and work function must be specified first. Although they have wide applications, due to their difficulties in measurements few investigations are available [11–13]. Surface energy is defined as the difference of free energy between a surface atom and that of an inner one for a solid which is one of the most fundamental properties for expressing surfaces stabilities [14]. In the most experimental works, surface energy is achieved by extrapolating the value of liquid surface energies at high temperatures which give rise to less valid experimental data [15]. Another important property of surfaces is work function which was first introduced by Einstein when he was working on the photoelectric effect and is expressed as minimum required work to separate free electron from the inner of a solid away from the surface into the vacuum region [16]. Kelvin probe is proper device to calculate work function values from contact potential difference between the surface under study and a standardized surface [16,17]. Although this process is simple and nondestructive the work function value is easily affected by impurities, roughness and misorientation on the surfaces [18]. Some other issues such as polycrystallinity of the sample and absence of required ideal vacuum also lower the accuracy in experiments [12]. Regarding the abovementioned complications that occur in calculating the surface energy and work function in experimental studies, we believe that

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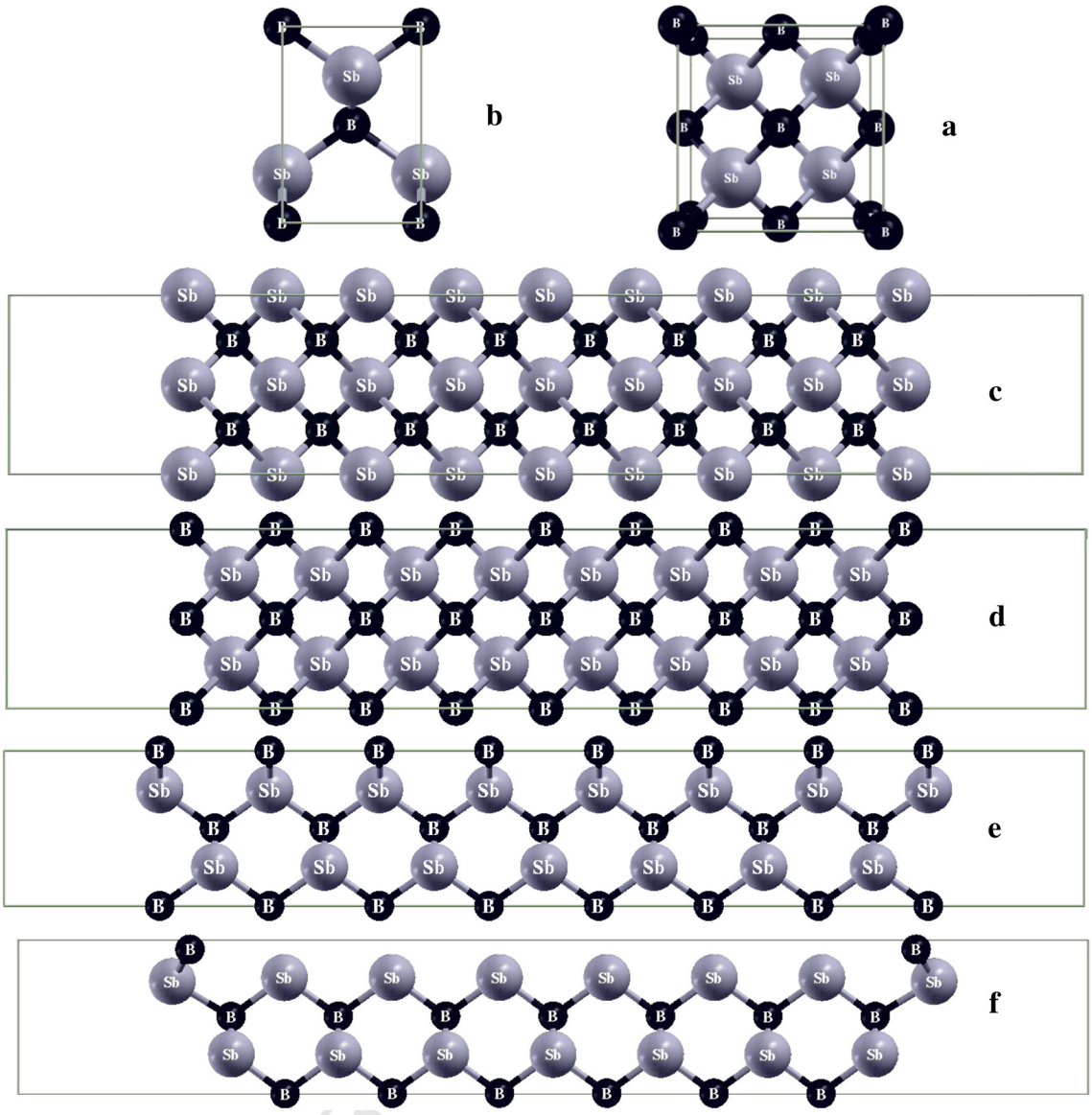

Fig. 1. (a) Bulk unit cell of BSb, (b) the top view of the BSb (110) slab, (c) symmetric 17 layer BSb (100) slab in the *z* direction (Sb-termination), (d) symmetric 17 layer BSb (100) slab in the *z* direction (B-termination), (e) symmetric 15 layer BSb (110) slab and (f) fully relaxed symmetric 15 layer BSb (110) slab.

theoretical studies can overcome these deficiencies. Over the last few decades, surface energy and work function of some pure elements and many other compounds have been calculated using DFT method. Most of the investigations on the BSb compound have been theoretical. Bagci and et al. reported pseudopotential study of structural, electronic and vibrational properties of the BSb (110) surface in 2008 [19]. To the

Table 1
Calculated lattice constant, a_0 (Å), bulk modulus, B_0 (GPa) and its pressure derivative B' of the BSb compound in the ZB phase using different functionals.

Approximations	**a**(**Å**)	**B**(**GPa**)	**B′**(**GPa**)
GGA-PBE	5.2809	98.9264	4.7660
LDA	5.1954	115.0498	5.0570
PBEsol	5.2316	108.2133	4.9070
WU-Chen	5.2354	107.7334	4.8818
Other results	5.278[a], 5.279[b], 5.278[c], 5.191[d], 5.201[e], 5.145[f], 5.21[g], 5.252[h], 5.177[i]	100[a], 96[b], 100[c], 111[d], 116[e], 118[f], 110[g], 103[h], 110[i]	4.40[a], 4.55[b], 4.40[c], 4.36[d], 4.16[e], 4.31[f], 4.07[g], 3.62[h], 4.237[i]

[a] FP-GGA Ref. [28].
[b] FP-GGA Ref. [3].
[c] FP-GGA Ref. [29].
[d] FP-LDA Ref. [3].
[e] FP-LDA Ref. [29].
[f] PP-GGA Ref. [30].
[g] PP-GGA Ref. [31].
[h] FP-GGA Ref. [32].
[i] FP-GGA Ref. [33].

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