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Research paper

Theoretical investigation of structural, electronic and optical properties of $(BeS)_1/(BeSe)_1$, $(BeSe)_1/(BeTe)_1$ and $(BeS)_1/(BeTe)_1$ superlattices under pressure

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HIGHLIGHTS

- $(BeS)_1/(BeSe)_1$, $(BeSe)_1/(BeTe)_1$ and $(BeS)_1/(BeTe)_1$ superlattices investigated by *Ab-initio*.
- Lattice parameters obtained by total energy are in good agreement with *Ab-initio* method by MET.
- $(BeS)_1/(BeSe)_1$ has indirect bandgap and $(BeSe)_1/(BeTe)_1$ and $(BeS)_1/(BeTe)_1$ have direct bandgap.
- The direct and indirect band gaps decrease with increasing pressure for all superlattices.
- Maximum anisotropy for $(BeS)_1/(BeTe)_1$ which has a large mismatch between BeS and BeTe.

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ABSTRACT

The influence of hydrostatic pressure on structural, electronic and optical properties of short period $(BeS)_1/(BeSe)_1$, $(BeSe)_1/(BeTe)_1$ and $(BeS)_1/(BeTe)_1$ superlattices, has been investigated. The lattice parameters a and c for the tetragonal unit cell obtained by total energy calculations are in good agreement with the values calculated by macroscopic elasticity theory. The $(BeS)_1/(BeSe)_1$ superlattice possesses an indirect band gap while $(BeSe)_1/(BeTe)_1$ and $(BeS)_1/(BeTe)_1$ superlattices possess a direct band gap. The pressure ranges from 0 to 47 GPa for $(BeS)_1/(BeSe)_1$, 0 to 39 GPa for $(BeSe)_1/(BeTe)_1$, and 0 to 45 GPa for $(BeS)_1/(BeTe)_1$, meanwhile the pressure dependence of the energy band gap along different symmetry directions obey the equation $E_g(p) = E_g + ap + bp^2$. The pressure coefficient of the indirect band gap for $(BeS)_1/(BeSe)_1$ is -22.5675×10^{-3} eV(GPa)$^{-1}$, while that of the direct band gap is estimated as -25.8581×10^{-3} eV(GPa)$^{-1}$ and -24.4695×10^{-3} eV(GPa)$^{-1}$ for $(BeSe)_1/(BeTe)_1$ and $(BeS)_1/(BeTe)_1$, respectively. The variation of the static dielectric constant with pressure is discussed.

1. Introduction

It has recently been possible by the development of crystal growth techniques to produce a new category of semiconductor heterostructures and superlattices of good quality. Semiconducting strained superlattices (SLs) are potential materials for wide range of applications in optical communications involving switching, amplification and signal processing [1]. The formation of SLs is generally controlled by strain caused by the lattice mismatch between two semiconductor compounds forming heterostructure. These strains can cause profound changes in the electronic properties, and by controlling the strain, one can expect exotic and rich physical properties which are absent in original bulk materials. Additional technological interest to study SLs is due to their unique transport properties along the growth direction.

Additionally, heterostructures based on II-VI compounds have attracted much attention because of their optical properties and their

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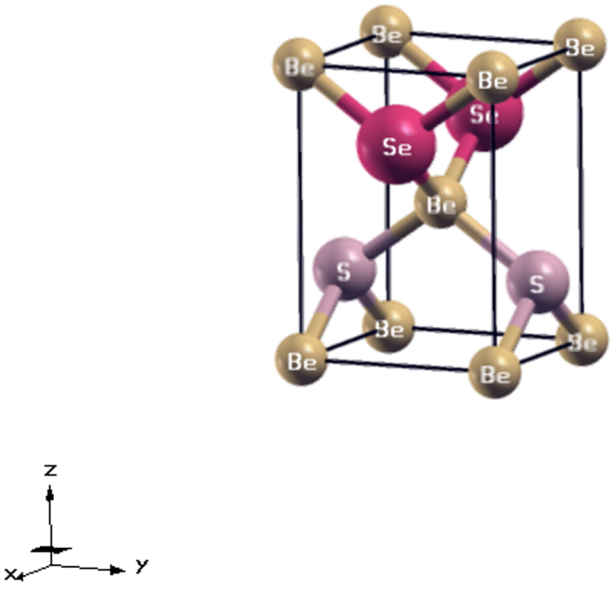

Fig. 1. Unit cell of $(BeS)_1/(BeSe)_1$ superlattice with a (0 0 1) growing direction.

Table 1
Calculated Structural parameters of $(BeS)_1/(BeSe)_1$, $(BeSe)_1/(BeTe)_1$ and $(BeS)_1/(BeTe)_1$ superlattices, lattice parameters a and c in (Å), bulk modulus B in (GPa) and the bulk modulus pressure derivative (B').

Superlattices	Parameters	Present work	Lattice constants by MET
$(BeS)_1/(BeSe)_1$	a	3.499	3.486
	c	4.933	4.955
	B	91.584	
	B'	3.624	
$(BeSe)_1/(BeTe)_1$	a	3.775	3.739
	c	5.307	5.361
	B	72.529	
	B'	3.643	
$(BeS)_1/(BeTe)_1$	a	3.687	3.602
	c	5.135	5.276
	B	78.861	
	B'	3.625	

applications in numerous optoelectronic devices [2]. Many experimental and theoretical works were reported for these artificial materials, such as ZnTe/CdTe [2], ZnS/ZnSe [3], ZnSe/BeTe [4] and BeTe/CdS [5].

It is known that II-VI compounds are characterized by different degrees of covalent, ionic and metallic bonding and thus offer a wide range of remarkable physical properties. Among them, beryllium chalcogenides BeS, BeSe and BeTe have attracted increasing interest because they exhibit covalent bonding [6], which is quite unique among II–VI semiconductor materials. In fact, they can be considered as "new materials" rediscovered recently in the context of the efforts to fabricate green and blue light emitting structures on the basis of II–VI compounds. Besides, these semiconductors are potentially a good choice for other technological applications due to their hardness. Only few experimental studies [7–13] have been performed on these compounds, presumably because of their very high toxic nature and consequently, only limited theoretical studies are available in literature [14–24].

It is well known, that beryllium chalcogenides BeX (X = S, Se and Te) are stable in cubic zinc blend structure. The rest of the group II_A-VI adopt the cubic rock-salt (NaCl) structure except BeO and MgTe which crystallize in the hexagonal wurtzite structure. It was found that these compounds are semiconductors with large and indirect band gap associated with (Γ-X) transitions. Note that BeTe is p-type semiconductor with a small gap; meanwhile BeS has a very high hardness. The lattice constants of BeSe and BeTe are close to those of GaAs and ZnSe [25]. The beryllium compounds BeS, BeSe and BeTe can be grown on various substrates by Molecular Beam Epitaxy (MBE) [10].

In this research work, to the best knowledge of the authors, for the first time, the structural, electronic, and optical properties of II–VI SLs system ($(BeS)_1/(BeSe)_1$(0 0 1), $(BeSe)_1/(BeTe)_1$(0 0 1) and $(BeS)_1/(BeTe)_1$(0 0 1)) are investigated by using first principle calculations. The influence of hydrostatic pressure on these properties is also studied.

The paper is organized as follows. In Section 2, we briefly describe the method used for the determination of physical properties. The results obtained for the structural, electronic, and optical properties at normal and high pressures of $(BeS)_1/(BeSe)_1$, $(BeSe)_1/(BeTe)_1$ and $(BeS)_1/(BeTe)_1$ are presented and discussed in Section 3. Finally, the results are summarized in Section 4.

2. Computational details

All calculations have been performed within the framework of the density functional theory (DFT) [26]. At present, it is considered as one of the most accurate method to determine the structural and electronic properties of the ground state of solids. We have employed the all-electron full-potential linear augmented plane wave plus local orbitals (FP-LAPW + lo) method [27] as implemented in WIEN2K code [28] within the local density approximation (LDA) [26,29]. In this method, the space is divided into non-overlapping muffin-tin (MT) spheres separated by an interstitial region. The basis functions are expanded into spherical harmonic functions inside the muffin-tin sphere and Fourier series in the interstitial region. During calculations, the Be ($2s^2$), S ($3s^23p^4$), Se ($3d^{10}4s^24p^4$) and Te ($4d^{10}5s^25p^4$) states are treated as valence electrons. The MT sphere radius is chosen to be 1.6, 2.0, 2.1 and 2.3 Bohr for Be, S, Se and Te respectively. The basis functions are expanded up to $R_{mt}K_{max} = 8$, (where R_{mt} is the smallest of the MT sphere radii and K_{max} is the largest reciprocal lattice vector used in the plane wave expansion). The potential and charge density representations inside the MT spheres are expanded using $L_{max} = 10$. Perdew and Wang functional [30] are used for the exchange and correlation potential. For the Brillouin zone, integration 5 × 4 × 4 k point mesh is used for all calculations. The self-consistent calculations were considered to be convergent when the total energy is stable within 0.1 mRy.

The optical properties of solid materials can be described by means of the complex dielectric function $\varepsilon(\omega)$. It is important to highlight that the contributions to the complex dielectric function $\varepsilon(\omega)$ mainly originate from the intraband and the interband transitions. The contribution from intraband transitions is significant for metallic materials. The interband transitions can be divided into direct and indirect transitions; where the direct transitions play an important role in the process of optical response, whereas indirect transitions have a small contribution as scattering of phonons is involved. Therefore, the intraband transitions and indirect interband transitions are neglected in our calculations.

In the limit of linear optics in the visible to ultraviolet regions, the