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Electronic and optical properties of mixed Be-chalcogenides

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ABSTRACT

The electronic and optical properties of BeS_xSe_{1-x}, BeS_xTe_{1-x} and $BeSe_xTe_{1-x}$, $(0 \leq x \leq 1)$ are studied using the highly accurate modified Beck and Johnson (mBJ) potential. The binary Be-chalcogenides are wide and indirect band gap semiconductors and hence they are not efficient materials for optoelectronics. In order to modify them into optically active materials, the anion chalcogen atoms are partially replaced by other chalcogen atoms like BeS_xSe_{1-x}, BeS_xTe_{1-x} and $BeSe_xTe_{1-x}$ $(0 \leq x \leq 1)$. The modified ternary compounds are of direct band gap nature and hence they are optically active. Some of these direct band gap materials are lattice matched with silicon and can possibly replace Si in semiconductor devices. Keeping in view the importance of these materials in optoelectronics, the optical properties of BeS_xSe_{1-x}, BeS_xTe_{1-x} and $BeSe_xTe_{1-x}$ in the full composition range are investigated. It is found that these materials are transparent in the IR, visible and near UV spectral regions. The alloys for the most of the concentrations have band gaps larger than 3 eV, so it is expected that they may be efficient materials for blue, green and UV light emitting diodes.

1. Introduction

Alkaline earth chalcogenides (AECs) have attracted scientific and technological attention due to their wide applications in luminescent devices [1]. Most of them are wide band gap semiconductors and are effectively used in optoelectronics. In the chalcogenides of group IIA (Be, Mg, Ca, Sr, Ba), BeS, BeSe and BeTe crystallize in the zinc-blende structure [1,2], while BeO and MgTe crystallize in the wurtzite structure and the rest exist in the rocksalt structure [3]. Among the AECs family, beryllium chalcogenides are more attractive because they exhibit stronger covalent bond nature, exist in high symmetric zinc-blende structure, and are effectively used in blue-green laser diodes [1,3–7].

Silicon is the backbone of semiconductor device technology, while its oxide (SiO_2) is also used in many devices. However, silicon and SiO_2 weakly respond to optical transitions because of their indirect band gap nature. Indirect band gap of a material constrains its applications in photonic devices. So, keeping in view the needs and importance of the optoelectronic industry, it is important to identify Si lattice and band gap matched semiconductors which can replace this optically inactive semiconductor. In this regard beryllium chalcogenides have closer lattice constant to Si. The lattice constant of BeTe is 3.6% larger than Si, while the lattice constant of BeSe is 5.2% smaller than Si [4]. These two compounds can be engineered by alloying them with proper concentration, into Si lattice matched compounds. The partial substitution of anions in BeS, BeSe and BeTe by S/Se/Te will not only provide Si-lattice matched semiconductors but will also provide band gap engineering of these systems for their possible effective use in optoelectronics. From Vegard's law the lattice constant of $BeS_{0.25}Te_{0.75}$ is 5.45 Å, and $BeSe_{0.50}Te_{0.50}$ is 5.43 Å. These two compounds are expected to be lattice matched with Si, and can hopefully replace Si.

Be-chalcogenides have toxic nature [8] and therefore few experimental studies are reported on these compounds [9–13], while no work has been reported on the ternary compounds—BeS_xSe_{1-x}, BeS_xTe_{1-x} and $BeSe_xTe_{1-x}$ $(0 \leq x \leq 1)$. However similar type of toxic materials like BeZnSe and BeZnTe are synthesized [14–18] using the molecular beam epitaxy (MBE) technique and they are stable materials which predict that these materials would also be stable. A number of theoretical attempts are made to investigate the structural, electronic, elastic and optical properties of binary Be-chalcogenides [1,5,6,8,19–28]. Though the band gap engineering of these compounds is reported by Hassan [2] using the electronic structure and bowing parameters of BeS_xSe_{1-x}, BeS_xTe_{1-x} and $BeSe_xTe_{1-x}$ $(x=0,\ 0.50,\ 1)$, the calculations were carried out with the density functional theory (DFT). But in the reported work the author has not clarified the direct band gap nature of the ternary alloys, which underestimates the importance of these compounds in optoelectronic industry. Bouamama et al. [29] studied the structural and elastic properties of BeS_xSe_{1-x}

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under high pressure using virtual-crystal approximation. Sandu and Kirk [4] investigated the electronic and optical properties of $BeSe_{0.41}Te_{0.59}$ using the tight binding (TB) model.

As these theoretical works are not focused on the direct band gap nature of the ternary Be-chalcogenides, none of these researchers have focused on the optoelectronic properties of these important compounds. The motivation behind the present work is the search for Si-lattice matched wide and direct band gap semiconductors in the ternary Be-chalcogenides. The full potential linearized augmented plane wave (FP-LAPW) method with the modified Beck and Johnson (mBJ) potential is used to investigate the electronic band structures, band gap bowing and optical properties of the ternary Be-chalcogenides.

2. Theory and calculations

The ground state calculations are performed with the FP-LAPW method using a recently developed modified Beck and Johnson (mBJ) [30] potential, implemented in the wien2k package [31]. The alloys BeS_xSe_{1-x}, BeS_xTe_{1-x} and $BeSe_xTe_{1-x}$ $(0 \leq x \leq 1)$ are modeled at various compositions with a step of 0.25 using eight atoms per unit cell. In the full potential scheme, the potential and charge density are expanded by spherical harmonics inside non-overlapping spheres (muffin–tin spheres) and by plane waves basis set in the remaining space of the unit cell (interstitial region). For the wave function expansion inside the atomic spheres the value of l is confined to $l_{max}=10$. The muffin–tin radii are selected as 2.06, 2.19, 2.27 and 2.35 a.u. for Be, S, Se and Te respectively, so that no leakage of charge occurs from the core and the total energy is converged. For wave function in the interstitial region the plane wave cut-off value of $K_{max}=7/R_{MT}$ is taken while the charge density is Fourier expanded up to $G_{max}=12$ Ryd. The Brillouin zone integration is performed using a mesh of 2000 special k points and convergence was checked through self-consistency.

Optical properties describe the interaction of electromagnetic radiations with a material and dielectric function plays key role in the investigation of the optical properties of a compound. Dielectric function has a complex nature and can be written as

$$\varepsilon = \varepsilon_1 + i\varepsilon_2 \tag{1}$$

Table 1
Calculated band gap energies (eV) compared with other calculations and experiments.

X	Symmetry	Present	Experimental	Other calculations
BeS_xSe_{1-x}				
0	$\Gamma-\Gamma$	5.62	5.55[j], 5.15[q]	4.19[p], 5.19[p], 4.37[a], 5.47[b], 4.72[d]
	$\Gamma-X$	3.55	4.00[o]	2.63[a], 3.61[h], 2.39[d], 3.61[n], 2.66[n], 3.12[s]
1/4	$\Gamma-\Gamma$	3.60		
1/2	$\Gamma-\Gamma$	3.68		3.83[n], 2.78[n]
3/4	$\Gamma-\Gamma$	4.00		
1	$\Gamma-\Gamma$	5.64		5.66[p], 6.06[p],5 0.65[a], 5.51[d], 5.50[k], 5.397[f]
	$\Gamma-X$	4.20	>5.5[o]	3.14[p], 4.26[p], 3.12[n], 4.23[n], 3.13[a]Se_1, 2.75[d], 4.17[h], 3.78[s]
BeS_xTe_{1-x}				
0	$\Gamma-\Gamma$	4.20	4.1[r], 4.53[g]	3.62[a], 3.68[c,d,e], 3.64[p], 3.82[p]
	$\Gamma-X$	2.60	2.8[h,l] 2.7[i],Se_1[o]	1.98[a], 1.80[d], 1.81[c], 2.89[h], 2.6[b,g], 2.03[p], 2.81[p], 2.17[s]
1/4	$\Gamma-\Gamma$	2.46		
1/2	$\Gamma-\Gamma$	2.80		2.96[n], 2.04[n]
3/4	$\Gamma-\Gamma$	3.42		
1	$\Gamma-\Gamma$	5.64		5.66[p], 6.06[p], 5.65[a], 5.51[d], 5.50[k], 5.397[f]
	$\Gamma-X$	4.20	>5.5[o]	3.14[p], 4.26[p], 3.12[n], 4.23[n], 3.13[a], 2.75[d], 4.17[h], 3.78[s]
$BeSe_xTe_{1-x}$				
0	$\Gamma-\Gamma$	4.20	4.1[r], 4.53[g]	3.62[a], 3.68[c,d,e], 3.64[p], 3.82[p]
	$\Gamma-X$	2.60	2.8[h,l] 2.7[i], Se_1[o]	1.98[a], 1.80[d], 1.81[c], 2.89[h], 2.6[b,g], 2.03[p], 2.81[p], 2.17[s]
1/4	$\Gamma-\Gamma$	2.45		
1/2	$\Gamma-X$	2.69		2.78[n], 1.91[n]
3/4	$\Gamma-\Gamma$	3.15		
1	$\Gamma-\Gamma$	5.62	5.55[j], 5.15[q]	4.19[p], 5.19[p], 4.37[a], 5.47[b], 4.72[d]
	$\Gamma-X$	3.55	4.00[o]	2.63[a], 3.61[h], 2.39[d], 3.61[n], 2.66[n], 3.12[s]

[a] Ref. [3],
[b] Ref. [21],
[c] Ref. [25],
[d] Ref. [8],
[e] Ref. [38],
[f] Ref. [24],
[g] Ref. [28],
[h] Ref. [23],
[i] Ref. [39],
[j] Ref. [40],
[k] Ref. [27],
[l] Ref. [45],
[n] Ref. [2],
[o] Ref. [34],
[p] Ref. [42],
[q] Ref. [43],
[r] Ref. [44],
[s] Ref. [26].