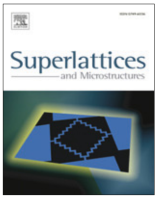
Superlattices and Microstructures 44 (2008) 794–801

Contents lists available at ScienceDirect

Superlattices and Microstructures

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



Electronic structure and optical properties of $CdSe_xTe_{1-x}$ mixed crystals

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ARTICLE INFO

Article history:
Received 12 May 2008
Received in revised form
22 September 2008
Accepted 22 September 2008
Available online 26 October 2008

Keywords:
Electronic structure
Dielectric constants
$CdSe_xTe_{1-x}$
Pseudopotentials

ABSTRACT

The band structure and optical properties of the $CdSe_xTe_{1-x}$ ternary mixed crystals have been studied using the pseudopotential formalism under an improved virtual crystal approximation approach. Quantities such as, energy gaps, band-gap bowing parameters, electron effective mass and dielectric constants are calculated. Our results agree well with the available data in the literature. The composition dependence of all studied quantities has been expressed by quadratic polynomial forms.

1. Introduction

The II–VI ternary semiconductor alloys are used in optoelectronic devices ranging from blue to near-ultraviolet spectral region [1]. These materials are also used to fabricate X-ray and γ-ray detectors [2,3]. Cadmium chalcogenides CdTe, CdSe and their mixed ternary crystals $CdSe_xTe_{1-x}$ have semi-conducting properties, which are especially suitable for the conversion of solar energy to electrical energy in photovoltaic or photo electro-chemical devices. The materials are also be used for the photo-assisted decomposition of water [4,5]. In addition, Cd-based compounds such as CdSeTe/Si can be used as an alternative material for short and medium wavelength infrared focal plane arrays [6]. Besides, $CdSe_xTe_{1-x}$/ZnSe quantum dots structures have the large conduction- and valence-band offsets at an appropriate composition and are expected to be a highly efficient light-emitting material in green region [7].

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doi:10.1016/j.spmi.2008.09.013

CdTe and CdSe exhibit both hexagonal wurtzite and cubic zinc-blende structures. While the common form of CdTe is known to have the zinc-blende structure, it is possible to produce thin crystals with the zinc-blende phase for CdSe as well [8]. For $CdSe_xTe_{1-x}$, Uthanna and Reddy [9], Mangalhara et al. [10] and Islam et al. [11] have observed the presence of only cubic phase over the entire composition range, whereas a number of other investigations [12–15] have revealed that $CdSe_xTe_{1-x}$ crystallizes in either cubic or hexagonal structure. In the present study, the crystal structures of CdTe and CdSe semiconductor compounds and their related ternary alloys $CdSe_xTe_{1-x}$ are assumed to have the cubic zinc-blende structure.

The electronic structure and optical properties of semiconductor alloys are important for guiding the successful design and fabrication of optoelectronic devices. Although some experimental and theoretical studies have been performed on $CdSe_xTe_{1-x}$ mixed crystals [4–7,9–18], many fundamental properties of these materials remain to be determined precisely.

To enhance the understanding of physical properties of $CdSe_xTe_{1-x}$ for device applications, a theoretical study has been undertaken. The electronic structure and optical properties of $CdSe_xTe_{1-x}$ alloys are calculated. The calculations are based on the empirical pseudopotential method (EPM) within the virtual crystal approximation (VCA). To include the compositional disorder, a correction to the alloy potential has been introduced. Traditionally, because of its simplicity, the VCA is preferred to treat the chemical disorder in semiconductor alloys. Together with the VCA, the EPM is the one of the effective and accurate schemes to obtain the overall band structure of multi-component semiconducting alloys [19–22]. Besides, the method is capable of exploring insights and it may be used to calculate other ground state quantities for semiconductors [23–25]. The first principles calculations are technically involved and computationally difficult to perform for ternary and quaternary alloys. Moreover, these calculations give accurate results for some typical cases [26] but normally underestimate the band gaps [27–29] depending upon the species. Quasiparticle calculations need a complicated and CPU-intensive process [30]. Comparatively, the empirical calculations are simple, rapidly converging and estimate band gaps in good agreement with experimental results [31–34]. In addition, using empirical methods, it is possible to perform a large number of calculations.

2. Computation methodology

The calculations are mainly based on the EPM. The Hamiltonian of the ternary alloy $CdSe_xTe_{1-x}$ is described by a component due to the virtual crystal, and another component in which the disorder effects are included as fluctuations around the virtual crystal [35,36]. In the EPM, the actual atomic potential is replaced by a pseudopotential. The pseudopotentials are characterized by a set of atomic form factors which are adjusted using a non-linear least-squares fitting procedure [37,38]. Our non-linear least-squares method requires that the root-mean-square deviation of the calculated level spacing (LS's) from the experiment defined as:

$$\delta = \left[\frac{\sum_{(i,j)}^{m} \left\{ \Delta E^{(i,j)} \right\}^2}{(m-N)} \right]^{\frac{1}{2}} \tag{1}$$

should be minimum. In Eq. (1), $\Delta E^{(i,j)} = E_{\exp}^{(i,j)} - E_{cal}^{(i,j)}$, where $E_{\exp}^{(i,j)}$ and $E_{cal}^{(i,j)}$ are the observed and calculated LS's between the ith state at the wave vector $k = k_I$ and the jth at $k = k_J$, respectively, in the m chosen pairs (i, j). N is the number of the empirical pseudopotential parameters. Good agreement with known band energies is required at some selected high-symmetry points in the Brillouin zone. In the present work, three pairs of states k_i and k_j : $(\Gamma\text{–}\Gamma)$, $(\Gamma\text{–}X)$ and $(\Gamma\text{–}L)$ which correspond to three band energy level spacing are used, with $k = (2\pi/a)(0, 0, 0)$ standing for the Γ point, $k = (2\pi/a)(1, 0, 0)$ for the X point and $k = (2\pi/a)(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ for the L point (a is the lattice constant). The band-gap energies of CdTe and CdSe fixed in the fits are : 1.505 [39] and 1.690 [40] for $\Gamma\text{–}\Gamma$, 3.480 [41] and 3.875 [42] for $\Gamma\text{–}X$, and 2.470 [41] and 3.612 eV [42] for $\Gamma\text{–}L$, respectively. The calculated energies given by solving the empirical pseudopotential secular