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Effects of in-plane tensile strains on structural, electronic, and optical properties of CdSe

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ABSTRACT

First-principles density functional theory was used to investigate effects of in-plane strains on the structural, electronic, and optical properties of wurtzite cadmium selenide (CdSe). The results of this work show some interesting properties of this material under finite strains that do not exist in the bulk unstrained regime. The structural deformation produced by increasing the in-plane strain, including the internal parameter *u*, was examined. The result shows that the structure undergoes a phase transition at a strain of 9.3% due to an extraordinary increase of the internal parameter *u*. By analyzing the electronic band structure using the modified Becke–Johnson approximation (mBJ), a direct–indirect band gap transition at an in-plane strain of 9.3% was found. Additionally, optical dielectric constants, reflectivity, and refractive index were calculated at different values of the strain. These results indicate that, by controlling the CdSe biaxial in-plane lattice constant (for example, by epitaxial growth on an appropriate substrate), the electronic and optical properties can be tuned for specific device applications.

1. Introduction

CdSe has received considerable attention because of its possible technological applications. Because CdSe has a direct band gap ~1.84 eV [1,2], it is utilized for a number of applications such as photo-detectors, photovoltaic devices, light-amplifiers, lasers, and sensors for gas detection [3–6]. The tunable synthesis of CdSe nanostructures suggests the possibility of enhancing their material properties, making them good candidates for new applications in nanotechnology in the areas of light emitting diodes, photovoltaic, photonic, and optoelectronic devices and sensors [7–12]. Nanostructures containing CdSe such superlattices and heterostructures have been grown by different deposition methods such as metal-lorganic chemical vapor deposition (MOCVD) [13], molecular beam epitaxy (MBE) [14], pulsed laser deposition (PLD) [15], and atomic layer deposition (ALD) [16].

Extensive theoretical and experimental studies have shown an enhancement of several properties of CdSe when it is used in core/shell QD nanocrystal. Peng and co-workers [17] have synthesized wurtzite CdSe/CdS core/shell nanocrystal with 3.4% bulk lattice mismatch. These nanocrystals show 50% increase of the photoluminescence quantum yield and an increase in the photostability. Zhan et al. [18] have synthesized CdSeS/ZnS core/shell QDs by employing microwave irradiation technique. They showed that CdSeS/ZnS core/shell QDs significantly enhanced luminescence and photostability than that of CdSeS core QDs. The large mismatch 12% between ZnS and CdSe lattice parameters causes an elastic deformation that changes their optical and structural properties [19,20].

In addition, the fabrication of a ternary alloy containing CdSe has gained the interests of many researchers as a successful technique to tailor the band gap. Firszt et al. [21] reported the possibility of tuning the band gap, the complex dielectric function, and refractive index of $Cd_{1-x}Be_xSe$ and $Cd_{1-x}Mg_xSe$ ternary alloy. Noor and Shaukat [22] calculated the electronic and optical properties of $Mg_xCd_{1-x}X$ (X = S, Se, Te) in zinc-blende structures. They showed that the band gaps of these alloys are direct and increase with increasing *x* composition.

Because this material can be fabricated and used under a large lattice mismatch, its electronic and optical properties are expected to change due to the deformation of the structure resulting from the strain. The effects of *a* lattice mismatch or biaxial in-plane strain on the properties of structures have motivated researchers to understand its roles on different structures of semiconductors. As demonstrated by Barruaud et al. [23], strain can be employed to enhance the electron mobility of silicon-on-insulator by a factor of 2. Tahini et al. [24] investigated the effects of strain on the band gap of Ge, and they found that strains can play important roles in introducing transformations of band gap energy from indirect to

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Table 1
Properties of CdSe in wurtzite structure compared to previous experimental and theoretical results, including lattice parameters (a, c/a and u) and the band gap energy E_g.

Parameter	This work	Experimental	Other cal.
a (Å)	4.2757	4.2985[a], 4.300[b]	4.2717[c]
c/a	1.6295	1.632[a], 1.630[b]	1.6336[c]
u	0.3759	0.375[a]	0.3756[c]
E_g (eV)	2.1	1.84[a], 1.83[b]	0.41[d]
B (GPa)	57.09	53[b]	57.58[d]

[a] Ref. [1].
[b] Ref. [35].
[c] Ref. [4].
[d] Ref. [38].

direct. Strained wurtzite ZnO, which has the same structure as CdSe, has been studied in detail in Ref. [25]. They showed that in-plane strains can play essential roles in affecting numerous properties such as structural response, polarization, band gap, and electron mobility. They reported a phase transformation at strain of 6.8% from direct to indirect band gap. A recent theoretical work by Guoqiang et al. [26] has further investigated the relaxation behavior of lattice and internal parameters of ZnO thin film under in-plane strains in the range of −3 to 3%. They showed that strains have a strong impact on the internal parameters and thus the electronic structure. Additionally, it was found that applying strain on the structure can reduce the Poisson ratio, decrease the piezoelectric effect, reshape the band dispersion at the Γ point, and reduce homogeneity of charge distribution between the two types of ZnO bonds [26]. Mandal [27] has reported full atomistic classical molecular dynamics simulations of strain induced phase transition in the wurtzite structure of CdSe nanowires. He showed that the wurtzite structure transforms into a five-fold coordinated h-MgO structure under uniaxial strain along the c-axis.

The influence of lattice strain on the properties of wurtize CdSe is still poorly understood. For example, it is unclear how the strain alters the chemical bonds of wurtzite structure of CdSe although the electronic properties strongly depend on these bonds. Additionally, the effects of in-plane strain on the electronic band structure are unknown though it is crucial for optical applications. Besides, to improve the optoelectronic applications of CdSe, more information about the variation of its optical properties under in-plane strain is required. Thus, analyzing the effects of in-plane strain on structural, electronic and optical properties of wurtzite CdSe is critical to enhance its use in several applications. In this work, the author has theoretically investigated the impact of biaxial in-plane tensile strains on wurtzite CdSe properties, including structural response, the electronic band structure, electronic charge density, optical functions, reflectivity, and refractive index. All electron full potential linearized augmented plane wave (FP-LAPW) was used in this work. The results of this work show some interesting properties of CdSe under finite strains that do not exist in the bulk unstrained regime and can lead to promising applications. The next section describes the calculated methods. The results of in-plane strain effects on structural and relative properties are illustrated in Section 3, and Section 4 summarizes the results of this work.

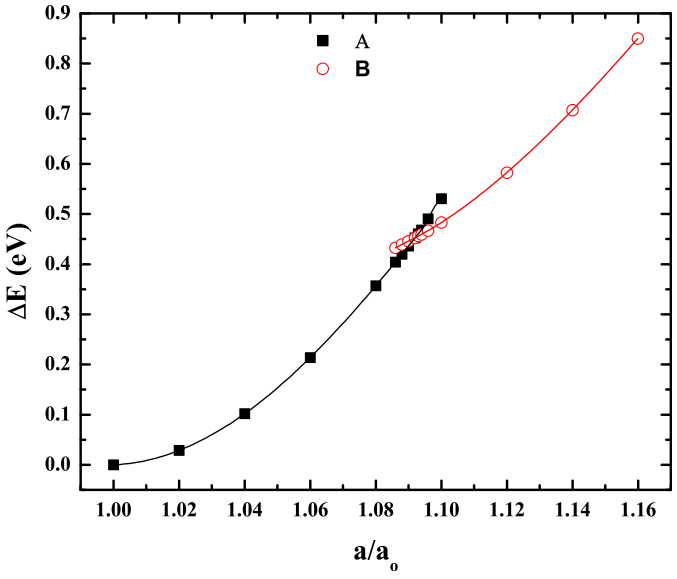

Fig. 2. The strain energy differences ΔE as a function of a/a_0.

2. Theoretical methods

The present results were obtained using density functional theory (DFT) [28] based on the all-electron FP-LAPW method and

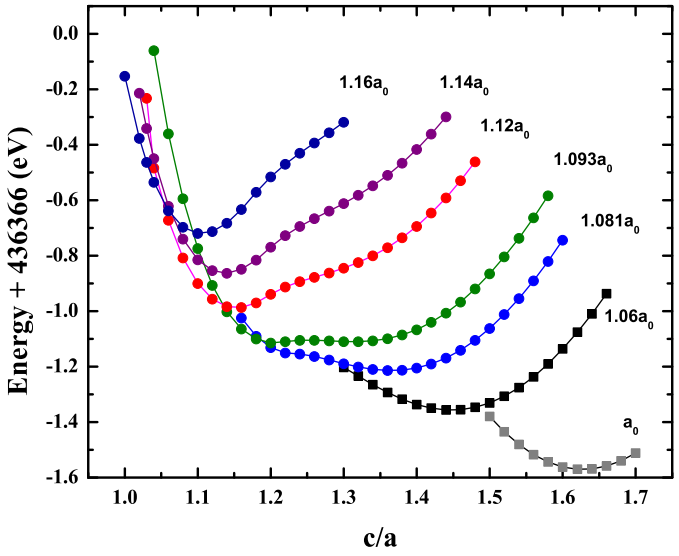

Fig. 1. Change in total energies with c/a ratio for different in-plane strains.

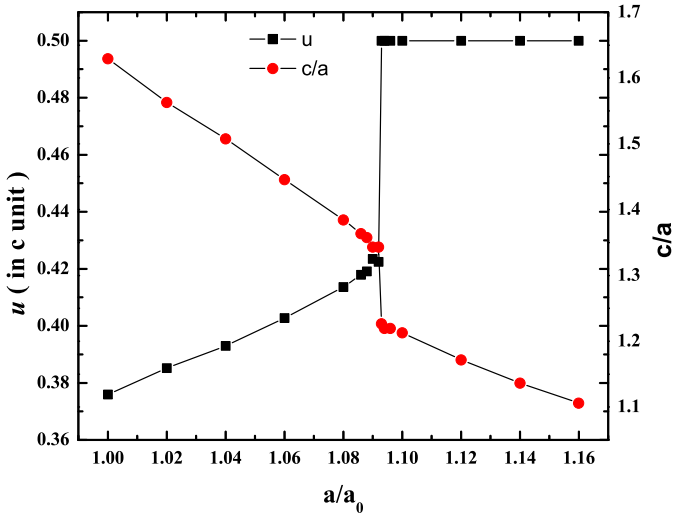

Fig. 3. The bond length u and c/a ratio versus in-plane strains.