

First-Principles Local Density Plus Virtual Crystal Approximations Study of HgCdTe

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Abstract: We have calculated the structural, elastic, mechanical and electronic properties of cubic $\text{Hg}_{0.5}\text{Cd}_{0.5}\text{Te}$ by using the first-principles density functional theory (DFT) within the local density approximation (LDA) plus virtual crystal approximation (VCA). Compared with the previous experimental and theoretical data of cubic $\text{Hg}_{0.5}\text{Cd}_{0.5}\text{Te}$, our calculated results demonstrate the adequacy of using the LDA+VCA for HgCdTe, which is expected to help people design new tellurium based multi-alloys using VCA.

Keywords: Density Functional Theory, Electronic Structure, Elastic Properties, HgCdTe

1. Introduction

Tellurium based II-VI alloys have received great attention due to their widespread use in high quality infrared detectors, gamma-ray detectors, high-speed multi-energy x-ray imaging devices, high energy astrophysics, room-temperature radiation detectors, modulators, etc. [1-10]. Among them HgCdTe (MCT) with a distinct narrow gap, has attracted the interest of a wide range of scientists [7, 11-18]. On the experimental side, the Bridgman method [5], the molecular-beam epitaxy (MBE) [5, 7, 11, 15, 16, 18-20], the metal organic vapor phase epitaxy (MOVPE) [13], the liquid phase epitaxy (LPE) [14, 17], have been used to fabricate MCT. Its infrared absorption spectra [5], infrared photoreflectance spectra [7], two-photon absorption (TPA) coefficient [11], minority carrier lifetime [12], negative luminescent properties [13, 20], Hall and photoconductive lifetime [15], carrier recombination lifetime [16], photoluminescence [17, 18], etc. have been investigated, which determine that MCT is the main material for high performance infrared photon detectors. Theoretically, the Monte Carlo treatment [21], the mathematical model [22], the first-principles calculation [23] and the finite-difference method [24] have been used to study the proton-energy

dependence of displacement damage mechanisms, the radiation defect profiles, the microstructures of the arsenic tetramer, dimer and singlet, and the interdiffusion processes of MCT, respectively. However, a clear theoretical research of MCT at the microscopic level on the structural and electronic properties seems to lack support and is necessary. As we know, CdTe and HgTe have been widely developed theoretically [25-31], and ZnCdTe_2 with chalcopyrite [32] as well as $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ alloys [33] have been calculated using the first-principles density functional theory. Hence, the bulk properties of MCT can be calculated by using the same method. Recently, $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ alloys have been investigated by using the local spin density approximation (LSDA) in the DFT with a $2\times 1\times 1$ super-cell with 16 atoms [34], whose calculated lattice constants satisfy Vegard's law and are close to the experimental results. It can be seen that the super-cell method is available for simulating MCT. Here, this paper aims to study $\text{Hg}_{0.5}\text{Cd}_{0.5}\text{Te}$ using another way, namely VCA [35], which allows us to model the $\text{Hg}_{0.5}\text{Cd}_{0.5}\text{Te}$ by defining the mixture Hg atom where half of the mixture is an atom of Cd.

2. Computational Method

The calculations were performed using the plane-wave pseudopotential DFT method implemented in the CASTEP (Cambridge Sequential Total Energy Package) code [36]. The LDA with a energy cutoff of 380 eV and the VCA method were applied. The Monkhorst-Pack k-point meshes [37] in the Brillouin zone were set to $7 \times 7 \times 7$. The Hg5d¹⁰6s², Cd4d¹⁰5s² and Te5s²5p⁴ electrons were treated as the valence electrons. The energy convergence threshold of 5.0×10^{-6} eV/atom, maximum force of 0.01 eV/Å and maximum displacement of 5.0×10^{-4} Å were carried out.

3. Results and Discussion

The crystal structure of Hg_{0.5}Cd_{0.5}Te has a cubic structure with space group $F\bar{4}3m$ and local symmetry T_d^2 [38]. In Table 1, we compare the calculated lattice constant for Hg_{0.5}Cd_{0.5}Te, HgTe and CdTe with zinc-blende structure by using the available experimental [34, 38-42] and theoretical data [25-27, 34, 43]. It can be seen that our calculated results of three compounds are in good agreement with the previous work. In particular, the optimized lattice parameter of Hg_{0.5}Cd_{0.5}Te is 6.4578 Å and agrees well with the experimental results of 6.478 Å [34] and 6.469 Å [38].

Table 1. Calculated lattice parameter (Å), elastic constants c_{ij} (GPa), bulk modulus B (GPa), shear modulus G (GPa), Young's modulus E (GPa), bulk modulus to shear modulus ratio (B/G) and Poisson's ratio ν of Hg_{0.5}Cd_{0.5}Te, HgTe and CdTe along with the available experimental [1, 25, 34, 38-42] and theoretical data [25-28, 34, 43].

	Present	Other theoretical data			Expt.				
	Hg _{0.5} Cd _{0.5} Te	HgTe	CdTe	Hg _{0.5} Cd _{0.5} Te	HgTe	CdTe	Hg _{0.5} Cd _{0.5} Te	HgTe	CdTe
a	6.4578	6.4534	6.4205	6.440 [34]	6.530 [25, 26],	6.430 [25],	6.478 [34],	6.492 [34],	6.467 [34]
					6.458 [34],	6.447 [26],	6.469 [38]	6.453 [39],	6.46 [41]
					6.486 [43]	6.421 [27, 34]		6.46 [40]	6.4827-6.492 [42]
c ₁₁ , c ₁₂ , c ₄₄	57.4, 39.4, 21.3	58.8, 42.3, 24.5	58.9, 40.4, 24.2			57.2, 39.5, 20.3 [28]		54.1, 37.4, 20.8 [1]	53.6, 37.0, 20.1 [1]
B	45.4	47.8	46.6		47.1 [25, 26]	29.5 [25], 34.3 [26], 46.179 [27], 44.7 [28]		47.6 [25]	44.5 [25]
G	15.1	15.9	16.5						
E	40.8	42.9	44.3						
B/G	3.007	3.006	2.824						
v	0.350	0.350	0.342						

The band structures of cubic HgTe, CdTe and Hg_{0.5}Cd_{0.5}Te along the high symmetry directions in the Brillouin zone are shown in Fig. 1. For cubic HgTe, there is no gap. The direct band gap is 0.623 eV in Γ point of CdTe, which is in agreement with the previous theoretical values 0.65 [25] and 0.566 eV [27]. However, these results are all smaller than the experimental data 1.645 eV [34] due to the use of DFT. Compared with the theoretical data 0.004 eV [34], the direct band gap 0.218 eV of Hg_{0.5}Cd_{0.5}Te at Γ point is close to the experimental value 0.592 eV [34]. Whatever, cubic

The deviations are less than 0.4% and 0.2%, respectively.

The elastic constants shown in Table 1 of Hg_{0.5}Cd_{0.5}Te, HgTe and CdTe are calculated with the energy-strain scheme. We can see that our calculated results of HgTe and CdTe are consistent with the experimental data [1], indicating that our calculated elastic constants of Hg_{0.5}Cd_{0.5}Te are believable. However, the c_{11} and c_{44} of Hg_{0.5}Cd_{0.5}Te are 57.4 and 21.3 GPa smaller than those of HgTe and CdTe, respectively, which lead to the lower resistance against the strain ϵ_{11} and the basal shear deformation, respectively. Moreover, cubic Hg_{0.5}Cd_{0.5}Te is mechanically stable due to our elastic constants satisfy the Born stability conditions [44]. Almost the same elastic constants of three compounds show that they have similar mechanical properties presented in Table 1. As we know, bulk modulus B , shear modulus G and Young's modulus E are associated with the resistance of a material to volume change, shape change and uniaxial tensions, respectively. The calculated B , G and E of Hg_{0.5}Cd_{0.5}Te are 45.4, 15.1 and 40.8 GPa all smaller than those of HgTe and CdTe, which shows that the mechanical properties of Hg_{0.5}Cd_{0.5}Te are decreased. The ductility of a material can be roughly obtained by using the value of bulk modulus to shear modulus ratio (B/G) [45], where large ratio (>1.75) shows ductile and lower ratio (<1.75) presents brittle. It is obvious that Hg_{0.5}Cd_{0.5}Te is characterized as a ductile material.

Hg_{0.5}Cd_{0.5}Te is a narrow gap semiconductor. In order to understand the alloying effect on the electronic states, the density of states (DOS) of three compounds has been shown in Fig. 2. The upper valence bands of three compounds are all mainly composed of Te-5p states which show hybridization with Hg-p or/and Cd-p states. Compared with the bottom of conduction bands of CdTe, the present of (Hg+Cd)-p states of Hg_{0.5}Cd_{0.5}Te induces red-shift.

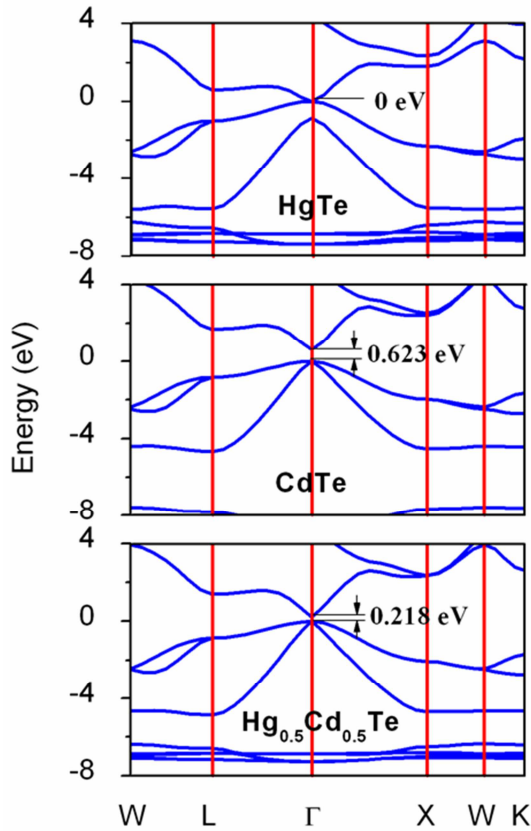


Fig. 1. Band structures of cubic HgTe, CdTe and $\text{Hg}_{0.5}\text{Cd}_{0.5}\text{Te}$ along the high symmetry directions in the Brillouin zone.

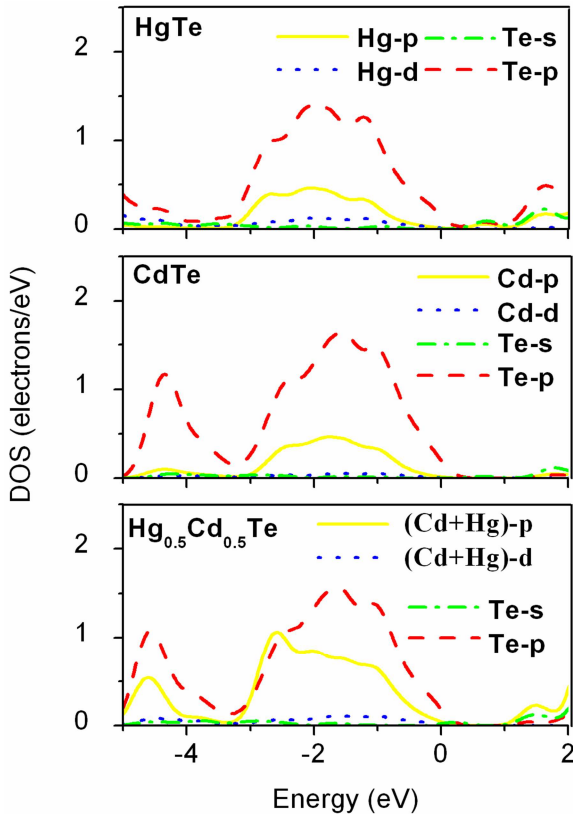


Fig. 2. DOS of cubic HgTe, CdTe and $\text{Hg}_{0.5}\text{Cd}_{0.5}\text{Te}$.

4. Conclusion

In conclusion, structural, elastic, mechanical and electronic properties of cubic $\text{Hg}_{0.5}\text{Cd}_{0.5}\text{Te}$ have been calculated using DFT-LDA plus VCA approach. The calculated lattice constant of $\text{Hg}_{0.5}\text{Cd}_{0.5}\text{Te}$ is in good agreement with the experimental data. The mechanical properties show that cubic $\text{Hg}_{0.5}\text{Cd}_{0.5}\text{Te}$ is mechanically stable and behaves in ductile manner. The calculated direct band gap is 0.218 eV which determines cubic $\text{Hg}_{0.5}\text{Cd}_{0.5}\text{Te}$ is a narrow gap semiconductor.

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