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Elastic properties of $CdTe_{1-x}Se_x$ (x = 1/16) solid solution: First principles study

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Abstract. Elastic properties of the $CdTe_{1-x}Se_x$ (x = 1/16) solid solution in the framework of the density functional theory calculations have been investigated. The structure of the sample has been constructed using that of the original binary compound CdTe, which crystallizes in the cubic phase. The Young modulus, shear modulus, bulk modulus and Poisson ratio have been calculated theoretically. On the results for elastic coefficients, value of acoustic velocity and Debye temperature have been obtained. The obtained values are in good agreement with experimental data.

Keywords: solid solution, elastic properties, acoustic velocity, Debye temperature.

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1. Introduction

The $A^{II}B^{VI}$ semiconductor compounds and their solid solutions, such as CdTeSe, have attracted considerable attention in both fundamental research and technological applications because of their wide use in fabrication of various optoelectronic devices [1-10]. This semiconducting solid solution demonstrates high values of the absorption coefficient and the possibility to adjust its band-gap by changing the content of Se for effective solar energy conversion [11].

CdTe compounds have a cubic (zinc blende) structure [12, 13], whereas CdSe compounds depending on the growth condition may have both sphalerite and wurtzite (hexagonal) structures under normal conditions [14-16], but the sphalerite CdSe structure is unstable and converts to the wurtzite form after moderate heating [17]. Taking into account its phase diagram [18], it was observed that CdTeSe crystallizes in the cubic structure with the concentration of CdSe compound below ~0.33 and wurtzite structure above ~0.55.

Up to now, we have found some information about physical properties of CdTeSe solid solution [9-11, 19-24]. Considerable attention of researchers is focused on the study of structural, optical, and electronic properties inherent to CdTeSe films [25] examined for different Se concentrations improving the performance of CdTe-based thin-film solar cells, the effectiveness of which is largely limited by the concentration of doping and the lifetime of minority carriers.

Despite the recent intensive experimental and theoretical study of these materials, some of the fundamental parameters remain currently unknown. One of the central problems of these solid solutions is their mechanical properties. This information is very important for modeling and developing parts for optical and electronic devices. Introduction of a small amount of Se into the CdTe structure should cause the appearance of impurity energy levels located inside the band gap of the host material. Since the band-energy structure of the material determines its main optical and electrophysical properties, this problem is quite relevant.

We found some works related with theoretical calculation of electron band structure [3, 7, 8, 13, 14, 21, 22, 26-28], optical parameters [13, 14, 22, 23] and effective mass [28-30]. But none of them used the $CdTe_{1-x}Se_x$ (x = 1/16; $Cd_{16}Te_{15}Se$) composition in cubic structure for the calculation. We didn't find any information about calculation of effective mass, sound velocity and elastic properties for $Cd_{16}Te_{15}Se$ solid solution.

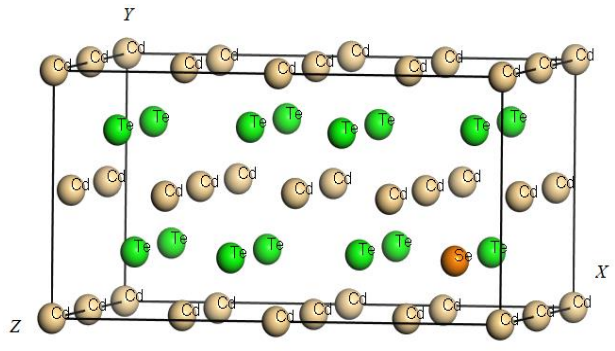
In this paper, we report elastic properties of the $Cd_{16}Te_{15}Se$ solid solution. The sample of $Cd_{16}Te_{15}Se$ was prepared using the parent compound CdTe (cubic structure), where Te atoms were substituted with Se. The acoustic velocity and Debye temperature of the sample were calculated using the obtained elastic modules.

2. Methods of calculation

The elastic properties of $Cd_{16}Te_{15}Se$ solid solutions have been calculated in the framework of the density functional theory (DFT) [31] by using CASTEP code [32]. In these calculations, the generalized gradient approximation (GGA) and the Perdew–Burke–Ernzerhof (PBESOL) exchange-and-correlation functional [33] were used. Within the method used, the electronic wave functions were expanded in a plane wave basis set with the energy cut-off at 310 eV. The electron configurations $4d^{10}5s^2$ for Cd, $5s^25p^4$ for Te and $4s^24p^4$ for Se atoms formed the valence electron states. The 4×2×2 Monkhorst–Pack mesh has been used for the Brillouin zone (BZ) sampling [34]. The self-consistent convergence of the total energy was taken as 5.0×10^{-7} eV/atom. For DFT calculations of $Cd_{16}Te_{15}Se$ solid solutions, the 2×1×2 supercell containing 32 atoms was created (see Figure). The triclinic symmetry *P*1 was used for the optimized structure of the crystal supercell $Cd_{16}Te_{15}Se$. Geometry optimization of the lattice parameters and atomic coordinates were performed using the Broyden–Fletcher–Goldfarb–Shanno (BFGS) minimization technique with the maximum ionic Hellmann–Feynman forces within 0.01 eV/Å, the maximum ionic displacement within 5.0×10^{-4} Å, and the maximum stress within 0.02 GPa. These parameters are sufficiently small to lead to a well-converged total energy of the studied structures.

3. Results and discussion

Elastic properties play an important role in providing valuable information about the bonding characteristics between adjacent atomic planes, they can determine how the material undergoes stress deformation and then recovers to its original shape after stress cessation. Also, these properties play an important role in providing valuable information on structural stability, anisotropic factors, Debye temperature, phonon spectra and specific heat. All this information is usually defined by the elastic constants C_{ij} [35]. The used calculation method allows obtaining the total energy *E* for arbitrary crystal structures.



View of $Cd_{16}Se_{15}Te$ crystal 2×1×2 supercell.

One can deform the calculated equilibrium crystal structure, determine the total energy of the strained crystal *E* and use the obtained results to estimate the elastic constants. They are proportional to the second-order coefficient in the polynomial expansion of the total energy *E* as a function of the strain parameter δ. Only small deformations that did not exceed the crystal elasticity limit were taken into consideration during calculations. Knowing the total crystal energy *E* and its variation caused by the strain δ, one can determine nine elastic constants from the following equations:

$$E(V,\delta)=E(V_0,0)+V_0\left(\tau_1\delta+\frac{C_{11}}{2}\delta^2\right),$$

$$E(V,\delta)=E(V_0,0)+V_0\left(\tau_2\delta+\frac{C_{22}}{2}\delta^2\right),$$

$$E(V,\delta)=E(V_0,0)+V_0\left(\tau_3\delta+\frac{C_{33}}{2}\delta^2\right),$$

$$E(V,\delta)=E(V_0,0)+V_0\left(2\tau_4\delta+2C_{44}\delta^2\right),$$

$$E(V,\delta)=E(V_0,0)+V_0\left(2\tau_5\delta+2C_{55}\delta^2\right),$$

$$E(V,\delta)=E(V_0,0)+V_0\left(2\tau_6\delta+2C_{66}\delta^2\right),$$

$$E(V,\delta)=E(V_0,0)+V_0\left[(\tau_1-\tau_2)\delta+\frac{1}{2}(C_{11}+C_{22}-2C_{12})\delta^2\right],$$

$$E(V,\delta)=E(V_0,0)+V_0\left[(\tau_1-\tau_3)\delta+\frac{1}{2}(C_{11}+C_{33}-2C_{13})\delta^2\right],$$

$$E(V,\delta)=E(V_0,0)+V_0\left[(\tau_2-\tau_3)\delta+\frac{1}{2}(C_{22}+C_{33}-2C_{23})\delta^2\right]. \quad (1)$$

In Eqs (1), *V* is the supercell volume. Here, the elastic constants C_{12}, C_{13}, and C_{23} were defined as linear combinations of the already obtained constants C_{11}, C_{22}, and C_{33}. The calculated elastic constants C_{ij} of $Cd_{16}Te_{15}Se$ are presented in Table 1.

The theoretical polycrystalline elastic modulus of $Cd_{16}Se_{15}Te$ solid solution can be determined using two approximation methods, namely: the Voigt and Reuss methods [36]. The Voigt method assumes the uniform strain throughout the polycrystalline aggregate, while the Reuss one assumes the uniform stress. The bulk modulus *B*, Young's modulus *E*, shear modulus *G* and Poisson's ratio σ were calculated directly by the Voigt–Reuss–Hill (VRH) method [37] (Table 2).

Table 1. Calculated elastic constants of $Cd_{16}Se_{15}Te$ solid solution.

Elastic constant C_{ij} (i, j = 1,2,…,6)	Value of C_{ij} (GPa)
C_{11}	35.80 ± 9.69
C_{22}	41.04 ± 5.75
C_{33}	35.88 ± 4.01
C_{44}	53.49 ± 9.06
C_{55}	52.57 ± 5.04
C_{66}	28.99 ± 2.87
C_{12}	47.87 ± 2.36
C_{13}	53.01 ± 3.06
C_{23}	46.34 ± 3.54

Table 2. The calculated values of shear modulus (G), bulk modulus (B), Young's modulus (E), and Poisson's ratio (σ) for $Cd_{16}Te_{15}Se$ solid solution.

	Voigt	Reuss	Hill
B, GPa	45.24	45.65	45.93
G, GPa	22.55	30.21	29.87
B/G	2.01	1.51	1.54
E, GPa	50.39	63.48	53.46
σ	0.31	0.27	0.30

Table 3. The calculated acoustic velocities in different directions of $Cd_{16}Te_{15}Se$ solid solution.

$\vartheta_l^{[100]}$, m·s^{-1}	$\vartheta_t^{[100]}$, m·s^{-1}	$\vartheta_l^{[111]}$, m·s^{-1}	$\overline{\vartheta}$, m·s^{-1}	θ_D, K
2440.6	2983.3	4377.5	3267.1	303.9

According to the elastic criteria, the material is brittle (ductile), if the B/G ratio is less (greater) than 1.75. The calculated values B/G of $Cd_{16}Te_{15}Se$ are smaller than 1.75 [38] when being obtained by the Reuss and Hill methods, hence, the studied material should probably behave in a brittle manner. The Poisson ratio of a stable, isotropic, linear elastic material must be between −1.0 and +0.5, because of the requirement for Young's modulus, the shear modulus and bulk modulus must have positive values [39]. According to Frantsevich rule [40], the critical value of the Poisson ratio for a material is 1/3 [41]. The value of Poisson's ratio σ, responsible for ductile ($\sigma > 1/3$) or brittle ($\sigma < 1/3$) character, corresponds in our case to the brittle one ($\sigma < 1/3$). The value of the Poisson ratio is indicative of the degree of directionality of the covalent bonds. This value is relatively small ($\sigma = 0.1$) for the covalent materials and relatively large ($\sigma = 0.25$) for the ionic ones. The calculated Poisson ratio σ for $Cd_{16}Te_{15}Se$ lies within the range 0.27…0.31.

Knowing the elastic constants C_{ij} of a material, one can calculate the corresponding acoustic velocities in certain directions. The values of acoustic velocity in different directions of $Cd_{16}Se_{15}Te$ crystal were calculated using the respective relations [42]:

$$\vartheta_l^{[100]} = \sqrt{\frac{C_{11}}{\rho}}, \tag{2}$$

$$\vartheta_t^{[100]} = \sqrt{\frac{C_{44}}{\rho}}, \tag{3}$$

$$\vartheta_l^{[111]} = \sqrt{\frac{C_{11} + 2C_{12} + 4C_{44}}{3\rho}}, \tag{4}$$

where ρ is the crystal density. The calculated value of density ρ is 6.01 g·cm^{-3}. This value is in good agreement with the experimental one for pure CdTe [43]. The calculated acoustic velocities in different directions are presented in Table 3.

The Debye temperature θ_D is one of the most important parameters that determines the thermal properties of material. The Debye temperature can be defined in terms of mean acoustic velocity and gives explicit information about lattice vibrations. This is the highest temperature that corresponds to the highest frequency normal vibration ν_D ($\theta_D = h\nu_D / k_B$, where $k_B = 1.380658 \cdot 10^{-23}$ J·K^{-1}). At relatively low temperatures, vibrational excitations arise mainly due to acoustic oscillations. Therefore, the value of θ_D, calculated from the elastic constants, is the same as that determined by specific heat measurements at relatively low temperatures.

Using the mean acoustic velocity, the Debye temperature is calculated from Eq. (5).

$$\theta_D = \frac{\hbar}{k_B}\left(\frac{6\pi^2 N}{V_0}\right)^{1/3} \overline{\vartheta}, \tag{5}$$

where N is the number of atoms in the supercell of $Cd_{16}Te_{15}Se$, V_0 – supercell volume. The obtained value of Debye temperature is in good correlation with other known θ_D values for binary compounds (295.6 K for CdTe and 317.6 K for CdSe at 298 K [44]).

3. Conclusions

In this work, elastic properties, Debye temperatures and acoustic velocity for $Cd_{16}Te_{15}Se$ solid solution are estimated using the first-principles calculations. The calculations were performed within the generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBESOL) exchange-and-correlation functional. Using the Voigt–Reuss–Hill approximation, the ideal polycrystalline aggregates bulk modulus, shear modulus, Young's modulus, and Poisson's ratio have been calculated and discussed. The obtained values are in good agreement with experimental data and correlate well with the values observed for binary compounds CdSe and CdTe.

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Пружні властивості твердого розчину $CdTe_{1-x}Se_x$ (x = 1/16): Дослідження з перших принципів

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Анотація. Досліджено пружні властивості твердого розчину $CdTe_{1-x}Se_x$ (x = 1/16) в рамках розрахунків теорії функціонала густини. Структура зразка побудована на вихідній бінарній сполуці CdTe, яка кристалізується в кубічній фазі. Модуль Юнга, модуль зсуву, об'ємний модуль та коефіцієнт Пуассона обчислено теоретично. За результатами коефіцієнтів пружності отримано значення акустичної швидкості та температури Дебая. Отримані значення добре узгоджуються з експериментальними даними.

Ключові слова: твердий розчин, пружні властивості, акустична швидкість, температура Дебая.