

AB INITIO STUDIES OF ELASTIC PROPERTIES OF THE CUBIC SOLID-STATE $\text{CdTe}_{1-x}\text{Se}_x$ SOLUTIONS

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Elastic properties of the solid-state $\text{CdTe}_{1-x}\text{Se}_x$ ($x = 0 - 0.5$, with $\Delta x = 0.125$) solutions within the framework of density functional theory calculations were investigated. The structures of the $\text{CdTe}_{1-x}\text{Se}_x$ samples are obtained by the substitution of tellurium with selenium atoms in cubic CdTe. Young's modulus, shear modulus, bulk modulus, and the Poisson ratio of $\text{CdTe}_{1-x}\text{Se}_x$ crystals were calculated from the first principles. The dependences of the elastic properties of the $\text{CdTe}_{1-x}\text{Se}_x$ solid solution on the content index x within the interval $0 \leq x \leq 0.5$ are analyzed. According to the Frantsevich rule and the value of the Poisson ratio, the materials have been classified as ductile. The Zener anisotropy factor and the Kleimann parameter are calculated on the basis of the elastic constants C_{ij} . Also, the concentration dependence of longitudinal elastic wave velocity, transverse elastic wave velocity, and average sound velocity, are calculated. Based on the average sound velocity the concentration behavior of the Debye temperature was calculated. The correlation analysis shows a good agreement between the calculation results (elastic modulus and Debye temperature) and known experimental data.

Key words: solid state solution, elastic properties, elastic modulus, Poisson ratio, Debye temperature.

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I. INTRODUCTION

CdTe and CdSe belong to the $A^{II}B^{VI}$ crystal family and show a typical semiconductor behavior. They are considered promising materials for various optoelectronic devices [1]. In particular, ternary solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions can demonstrate high values of the absorption coefficient and the possibility to adjust their band gap by changing the content of Se for effective solar energy conversion [2]. It is well known that the CdTe has a cubic (zinc-blende) structure [1, 3–7] whereas CdSe can be materialized in either zinc-blende or hexagonal (wurtzite) structures under normal conditions, depending on the growth conditions [8, 9]. According to the phase diagram [10], the $\text{CdTe}_{1-x}\text{Se}_x$ compounds at intermediate x are crystallized in either cubic (at the tellurium contents $x \leq 0.4$) or wurtzite (at $x \geq 0.7$) structures, while the concentration interval $0.4 \leq x \leq 0.7$ corresponds to a break of structural homogeneity. Therefore, we study only the concentrations ranging from 0 to 0.5, i.e. only the zinc-blende structures.

Despite the recent intensive experimental [11–16] and theoretical [1, 2, 15, 17–22] 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.

Some information on the concentration behavior of the elastic properties of the CdSe–CdTe system has already been reported in theoretical works [17, 18]. In particular, concentration dependences of Young's modulus, shear modulus, bulk modulus, and the Poisson ratio are calculated at some x values using the LDA [17] and LDA+U [18] methods. None of them has given

results of the calculation concentration dependence of the longitudinal elastic wave velocity, transverse elastic wave velocity, average sound velocity, and the Debye temperature.

Earlier, elastic properties of $\text{CdTe}_{1-x}\text{Se}_x$ with $x = 1/16$ and $15/16$ were reported using the same methods of calculation [1, 2]. Now, we study the concentration behavior of the elastic properties of the solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions. In particular, we have performed the elastic constants C_{ij} calculations for $\text{CdTe}_{1-x}\text{Se}_x$ to obtain the concentration dependences of Young's modulus, shear modulus, bulk modulus, the Poisson ratio, the Zener anisotropy factor, the Kleimann parameter, longitudinal elastic wave velocity, transverse elastic wave velocity, average sound velocity, and the Debye temperature.

II. MATERIALS AND METHODS

The density functional theory was used for the calculation of the elastic properties of the solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions with the content index x from 0 to 0.5 with the step of $\Delta x = 0.125$. The generalized gradient approximation (GGA) and the Perdew–Burke–Ernzerhof for solid (PBEsol) exchange-and-correlation functional [23] were utilized during the calculation. Ultrasoft Vanderbilt's pseudopotentials served as ionic potentials.

In this calculations, the value $E_{\text{cut-off}} = 310$ eV was taken for the cutting-off energy of the plane waves. The convergence of the total energy was about $5 \cdot 10^6$ eV/atom. Integration over the Brillouin zone



was performed on a $4 \times 2 \times 2$ grid of \mathbf{k} points, using a Monkhorst–Pack scheme. At the initial stage of our calculations, we optimized a starting CdTe structure for the case of $2 \times 1 \times 1$ supercell. The atomic coordinates and the unit-cell parameters were optimized following the Broyden–Fletcher–Goldfarb–Shanno technique. The optimization was continued until the forces acting on atoms became less than $0.01 \text{ eV}/\text{\AA}$, the maximum displacement less than $5 \cdot 10^{-4} \text{ \AA}$, and the mechanical stresses in the cell less than 0.02 GPa . In this work, we used almost the same parameters for calculations which were used in previous works [2, 22]. An exception was the choice of the $2 \times 1 \times 1$ supercell containing 16 atoms (Cd_8Te_8 — “parent” compound).

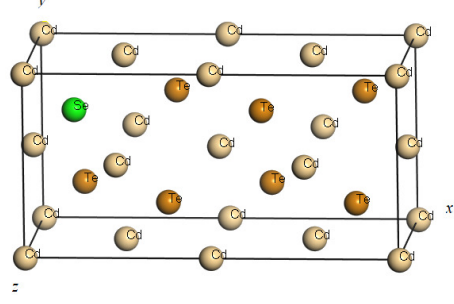


Fig. 1. View of $\text{CdTe}_{0.875}\text{Se}_{0.125}$ crystal $2 \times 1 \times 1$ supercell

III. RESULTS AND DISCUSSION

Elastic constants can be determined based on the results of the deformation of the calculated equilibrium crystal structure and the determined total energy of the strained crystal E . The elastic constants are proportional to the second-order coefficient in the polynomial expansion of the total energy E as a function of the strain parameter δ . The calculations took into account only small deformations that did not exceed the elastic limit of the crystal. One can determine nine elastic constants based on the known total energy of the crystal E and its change in deformation δ [2, 22, 25]. The calculated elastic constants C_{ij} of the solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions ($0 \leq x \leq 0.5$) are presented in Fig. 2.

The Voigt and the Reuss approximation methods can be used to determine the polycrystalline elastic modulus of solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions [26]. The Voigt method assumes a uniform strain throughout polycrystalline sample and the Reuss one assumes a uniform stress. Calculations of the actual effective constants using the Hill method show that they lie within the values obtained by the Voigt and Royce methods (the arithmetic mean of these two values is the Hill values). The bulk modulus B , Young’s modulus Y , shear modulus G , and Poisson’s ratio ν are calculated directly using the Voigt–Reuss–Hill (VRH) method [27]. The dependences of those quantities on the content x are shown in Fig. 3.

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 the solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions are higher than 1.75 (see Figs. 4) [28] when they are obtained using the VRH methods, hence, the materials studied should probably behave in a ductile manner.

Poisson’s ratio of a stable, isotropic, linear elastic material must be between -1.0 and $+0.5$ because of the requirement for Young’s modulus, and the shear and bulk modulus must be positive [29]. According to the Frantsevich rule [30], the critical value of the Poisson ratio of a material is $1/3$ [31]. The value of the Poisson ratio ν , responsible for the ductile ($\nu > 1/3$) or brittle ($\nu < 1/3$) character, corresponds in our case to the ductile one ($\nu > 1/3$). The value of Poisson’s ratio is indicative of the degree of directional of the covalent bonds. This value is relatively small ($\nu = 0.1$) for the covalent materials and relatively large ($\nu = 0.25$) for the ionic ones. The

Element	Atom Number	x/a	y/b	z/c
Cd	1	0.0	0.0	0.0
Cd	2	0.0	0.5	0.5
Cd	3	0.25	0.0	0.5
Cd	4	0.25	0.5	0.0
Cd	5	0.5	0.0	0.0
Cd	6	0.5	0.5	0.5
Cd	7	0.75	0.0	0.5
Cd	8	0.75	0.5	0.0
Te	1	0.125	0.25	0.25
Te	2	0.375	0.75	0.25
Te	3	0.375	0.25	0.75
Te	4	0.125	0.75	0.75
Te	5	0.625	0.25	0.25
Te	6	0.875	0.75	0.25
Te	7	0.875	0.25	0.75
Te	8	0.625	0.75	0.75

Concentration, x	Atom Number of Te used for substitution
0.125	4
0.25	4, 7
0.375	3, 4, 7
0.5	3, 4, 7, 8

Table 1. Atoms’ positions, in the solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions

The solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions were modeled as follows. First, we formed a $2 \times 1 \times 1$ supercell of the initial compound, CdTe, based on its already optimized structure (structure type ZnS, space group $F43m$, $Z = 4$). The next stage was the theoretical construction of solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions. In the optimization structure CdTe, Te atoms were gradually replaced with Se. For such substitution, the crystal structure of optimization structure CdTe was changed to a triclinic with symmetry $P1$. Finally, structures of $\text{CdTe}_{1-x}\text{Se}_x$ were optimized with finding a crystal structure. The obtained structure of $\text{CdTe}_{0.875}\text{Se}_{0.125}$ is drawn in Fig. 1 for visualization. The cell parameters of solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions were calculated using Vegard’s law from the known values for binary compounds ($a(\text{CdTe}) = 6.564376 \text{ \AA}$ [4] and $a(\text{CdSe}) = 6.166147 \text{ \AA}$ [24]). Atoms position are listed in Table 1.

calculated Poisson's ratio ν of solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions lies in the range of 0.360–0.405 (see Fig. 5). As a result, we confirm our assumption about the ductile behavior of the solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions.

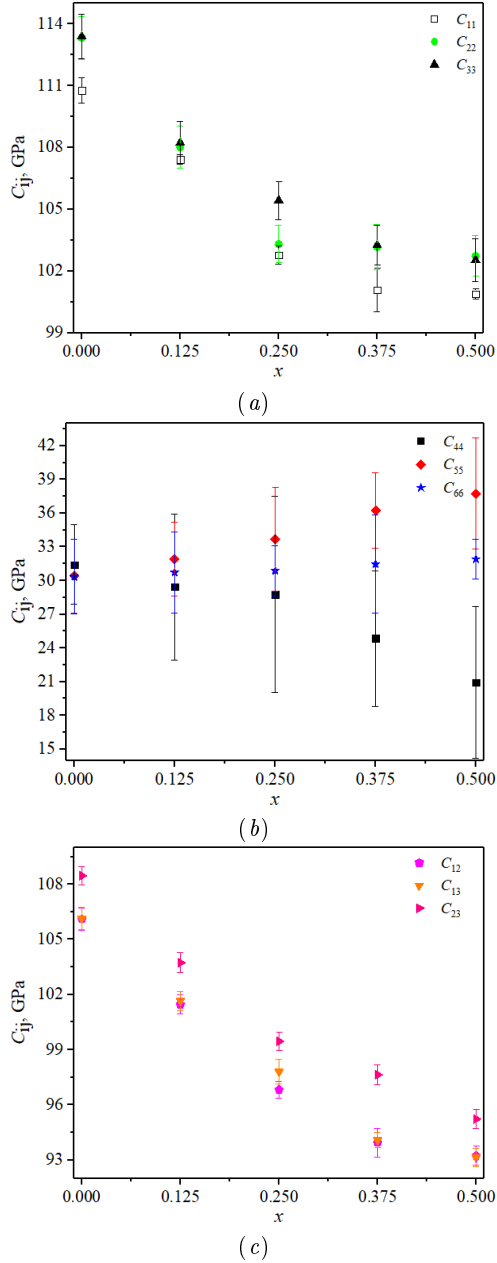


Fig. 2. Concentration dependence of elastic constants ((a) C_{11} , C_{22} and C_{33} ; (b) C_{44} , C_{55} and C_{66} ; (c) C_{12} , C_{13} and C_{23}) in the cubic solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions

Depending on the value of the Zener anisotropy coefficient, the material can be characterized as follows: elastically isotropic with uniform deformation along with all directions for $A = 1$; the stiffest along $\langle 111 \rangle$ diagonal for $A > 1$ and the stiffest along $\langle 100 \rangle$ cube axes for $A < 1$.

$$A = \frac{2C_{44}}{C_{11} - C_{12}}. \quad (1)$$

It is established that with an increase in the selenium concentration, there is a decrease in the calculated value of A for $\text{CdTe}_{1-x}\text{Se}_x$ from 14 to 6 (see Fig. 6). It indicates that solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions are the stiffest along $\langle 111 \rangle$ diagonal.

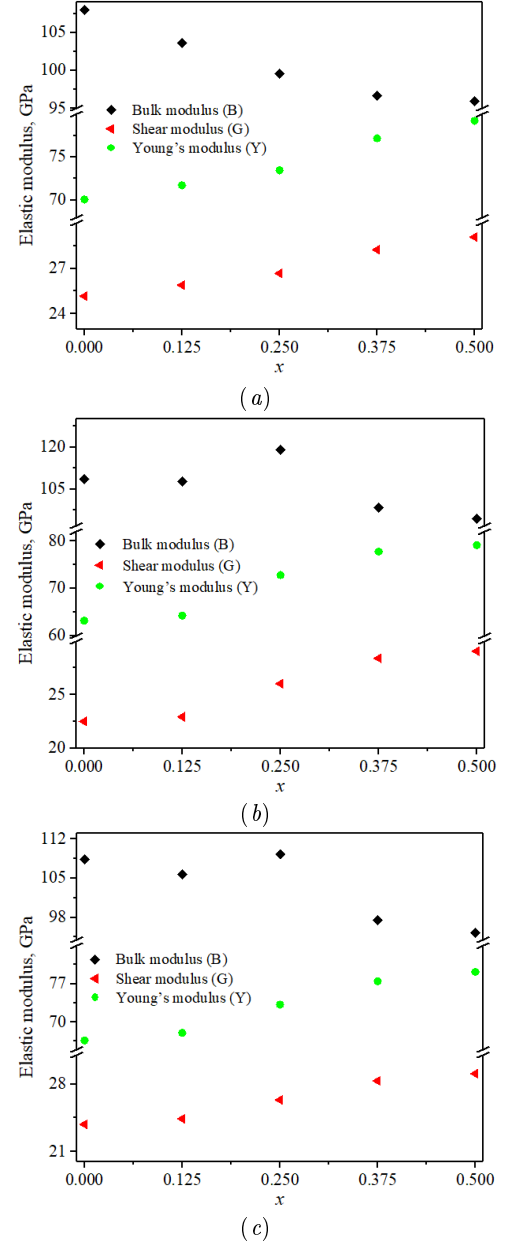


Fig. 3. Concentration dependence of the elastic modulus (see information in the legend to figures) calculation using the Voigt (a), Reuss (b) and Hill (c) approximation methods in the cubic solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions

The Kleimann parameter (ζ) indicates the relative ease of bond bending against the bond stretching and also implies resistance against bond bending or bond angle distortion [32]. For minimizing the bond bending, the value of the Kleiman parameter is $\zeta = 0$, and for minimizing the bond stretching $\zeta = 1$.

$$\zeta = \frac{C_{11} + 8C_{12}}{7C_{11} + 2C_{12}} \quad (2)$$

In the present study, ζ changed between 0.94 and 0.98 (see Fig. 6) for the solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions indicating shrinkage in bond-stretching. The value of ζ decreases with an increase in the selenium concentration.

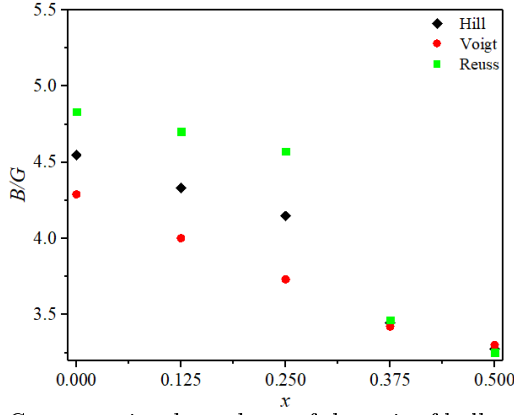


Fig. 4. Concentration dependence of the ratio of bulk modulus B to shear modulus G in the cubic solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions

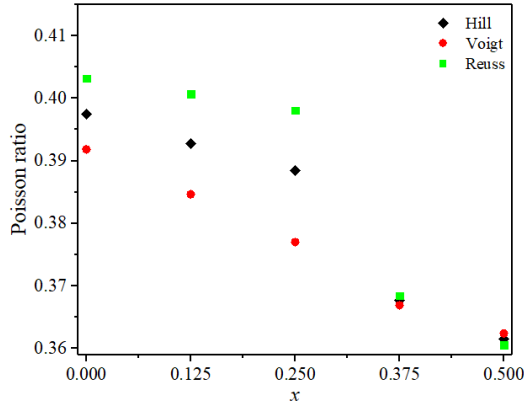


Fig. 5. Concentration dependence of the Poisson's ratio ν in the cubic solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions

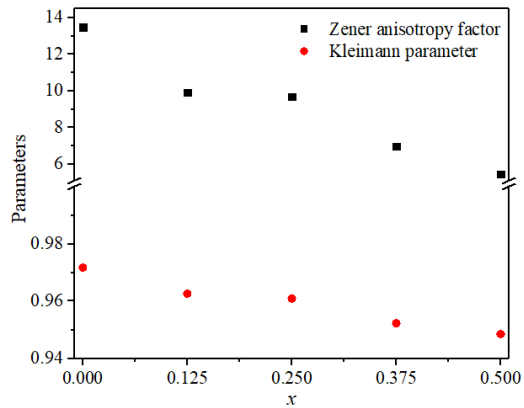


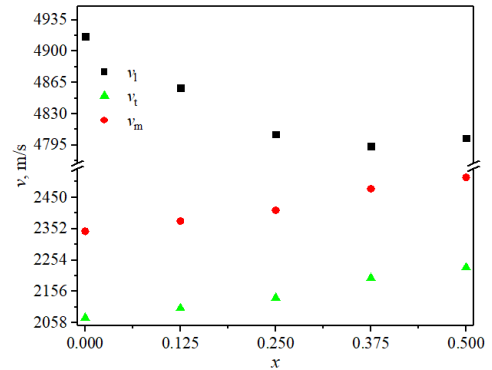
Fig. 6. Concentration dependence of the Kleimann parameter (ζ) and Zener anisotropy factor (A) in the cubic solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions

Longitudinal and transverse velocities of the elastic waves ϑ_l and ϑ_t can be calculated using the values of the obtained elastic modules [32]. The values of acoustic velocity in different directions of solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions were calculated using relations (3) and (4)

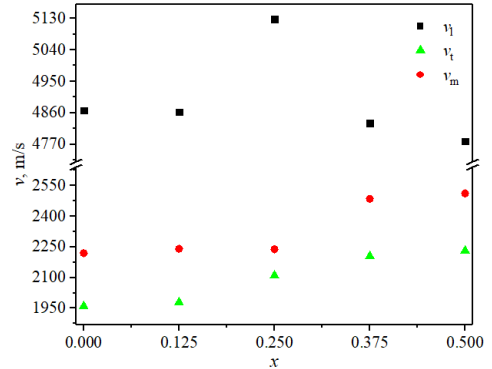
below, where ρ is the density of a sample. The density of the solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions was calculated according to Vegard's law [33] from the known values for binary compounds ($\rho(\text{CdTe}) = 5.85 \text{ g/cm}^3$ and $\rho(\text{CdSe}) = 5.81 \text{ g/cm}^3$). The calculated acoustic velocities are presented on Fig. 7.

$$\vartheta_l = \sqrt{\frac{3B + 4G}{3\rho}} \quad (3)$$

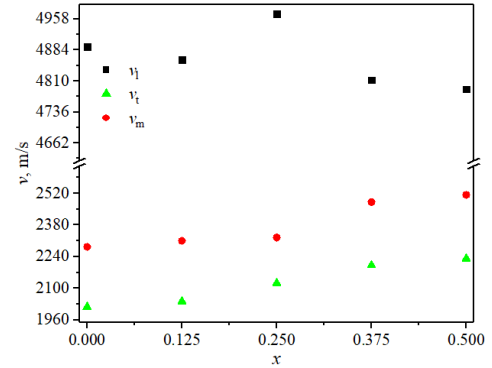
$$\vartheta_t = \sqrt{\frac{G}{\rho}} \quad (4)$$



(a)



(b)



(c)

Fig. 7. Concentration dependence of the acoustic velocity (see information in the legend to figures) calculated on the basis of the elastic modules estimated using the Voigt (a), Reuss (b), and Hill (c) approximation methods in the cubic solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions

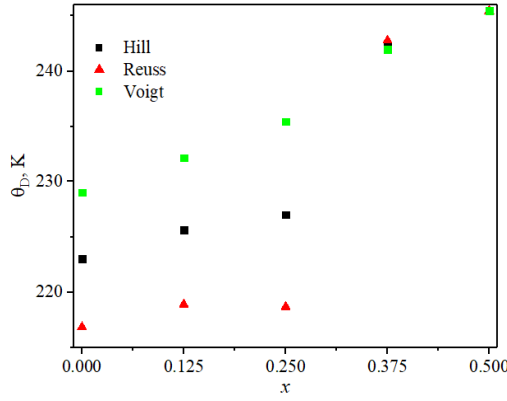


Fig. 8. Concentration dependence of the Debye temperature (θ_D) in the cubic solid-state CdTe_{1-x}Se_x solutions

The Debye temperature θ_D is one of the most important parameters which determine the thermal properties of the material. The Debye temperature gives information about the oscillations of the lattice and can be determined from the mean acoustic velocity [see Eq. (5)].

$$\theta_D = \frac{\hbar}{k_B} \left(\frac{6\pi^2 N}{V_0} \right)^{1/3} v_m. \quad (5)$$

In Eq. (5), N is the number of atoms in the supercell of CdTe_{1-x}Se_x, V_0 is the supercell volume, v_m is average sound velocity (see Fig. 7). The average sound velocity

is calculated by using the following Eq. (6).

$$v_m = \left(\frac{2}{3v_t^3} + \frac{1}{3v_l^3} \right)^{-1/3}. \quad (6)$$

Concentration dependence of the acoustic velocities $v_i(x)$ ($i = l, t, m$) of CdTe_{1-x}Se_x (see Fig. 7) calculated based on elastic modules estimated using different VRH methods reveal similar behaviors. Longitudinal elastic wave velocity v_l decreases on increase the selenium concentration x (except for the sample with concentration $x = 0.25$). Another behavior is observed for the transverse and mean sound velocities: these velocities, v_t and v_m , increase with an increase in the content index x .

The calculated Debye temperature θ_D is in good agreement with the corresponding experimental data of CdTe_{1-x}Se_x which are shown in Fig. 8. With an increase in the selenium concentration, we can see an increase in the Debye temperature. A relatively good comparison of the calculated and experimental Debye temperatures θ_D is observed for the binary compound of CdTe (see table. 2). Experimental values of the Debye temperatures θ_D are closer to the corresponding calculated ones, obtained by using the Hill method (see Fig. 8).

As a summary of all results obtained in this study, Table 2 gives comparisons of the known fundamental physical properties which are obtained experimentally and calculated using different methods. The obtained values show a small variation with other reference results.

Properties	Selenium concentration	This work	Reference data/ method of calculation
B/G	$x = 0$	4.55	2.67/LDA+ U [18]
	$x = 0.25$	4.15	2.88
	$x = 0.5$	3.28	3.29
ν	$x = 0$	$\nu_H = 0.40$ $\nu_R = 0.39$	0.33/LDA+ U [18], 0.41 [34] $\nu_H = 0.354$, $\nu_R = 0.364$ /LDA [17]
	$x = 0.25$	$\nu_H = 0.39$ $\nu_R = 0.38$	0.34/LDA+ U [18] $\nu_H = 0.360$, $\nu_R = 0.371$ /LDA [17]
	$x = 0.5$	$\nu_H = 0.36$ $\nu_R = 0.36$	0.35/LDA+ U [18] $\nu_H = 0.362$, $\nu_R = 0.375$ /LDA [17]
v_l , m/s	$x = 0$	4866.82–4916.47	3343.93/LDA [17] 3020 ([1 0 0]), 3440 ([1 1 1]) [35]
	$x = 0.25$	4807.09–5127.91	3408.36
	$x = 0.5$	4803.15–4778.56	3512.18
v_t , m/s	$x = 0$	1959.96–2073.34	1589.38/LDA [17] 1860 ([1 0 0]), 1450 ([1 1 1]) [35]
	$x = 0.25$	2110.04–2135.89	1592.62
	$x = 0.5$	2231.54–2231.37	1629.39
θ_D , K	$x = 0$	216.8–229	165.96/LDA [17], 295.6 (at 298 K) [36]
	$x = 0.25$	218.7–235.5	168.96
	$x = 0.5$	245.5	175.679

Table 2. Comparisons of the same fundamental elastic properties of the solid-state CdTe_{1-x}Se_x solutions. Bottom index corresponds to the VRH method of calculation. Boldface numbers are experimental data

IV. CONCLUSIONS

The elastic properties of solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions are determined by first-principles calculations. Using the VRH approximation, the ideal polycrystalline aggregates' bulk modulus, shear modulus, Young's modulus, and Poisson's ratio are calculated and discussed. The materials studied probably behave in a ductile manner. The Zener anisotropy factor shows that the solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions are the stiffest along $\langle 111 \rangle$ diagonal. The Kleimann parameter shows that the solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solutions shrink in bond-stretching.

Based on the elastic modules the longitudinal elastic wave velocity, transverse elastic wave velocity, and average sound velocity were calculated. The longitudi-

nal elastic wave velocity decreases with an increase in the selenium concentration. The transverse and average sound velocities increase with an increase in the selenium content in $\text{CdTe}_{1-x}\text{Se}_x$. The Debye temperature for solid-state $\text{CdTe}_{1-x}\text{Se}_x$ solution increases with an increase in the selenium concentration. The calculated properties for $\text{CdTe}_{1-x}\text{Se}_x$ show good agreement with the corresponding reference data.

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**AB INITIO РОЗРАХУНКИ ПРУЖНИХ ВЛАСТИВОСТЕЙ ТВЕРДИХ РОЗЧИНІВ
ЗАМІЩЕННЯ $\text{CdTe}_{1-x}\text{Se}_x$, КРИСТАЛІЗОВАНИХ У КУБІЧНІЙ СТРУКТУРІ**

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Пружні властивості твердих розчинів заміщення $\text{CdTe}_{1-x}\text{Se}_x$ ($x = 0-0.5$, з $\Delta x = 0.125$), кристалізованих у кубічній структурі, досліджено з використанням теорії функціонала густини. Структуру зразків $\text{CdTe}_{1-x}\text{Se}_x$ отримано заміщенням атомів телуру на атоми селену в кубічному кристалі CdTe .

Модуль Юнга, модуль зсуву, модуль усебічного стиску й коефіцієнт Пуассона кристалів $\text{CdTe}_{1-x}\text{Se}_x$ розраховано з використанням методики Фойгта–Ройсса–Гіл्ला (ФРГ). Згідно з отриманими даними встановлено, що модуль Юнга й модуль зсуву зростають зі збільшенням умісту селену. Проте модуль усебічного стиску, обчислений методом Ройсса і Гіл्ला, показує складну поведінку: він зростає з умістом селену для $x < 0.25$ і спадає для вищих концентрацій ($x > 0.25$).

Відповідно до правила Францевича та значення коефіцієнта Пуассона ($\nu > 1/3$) досліджувані матеріали були класифіковані як пластичні. Коефіцієнт анізотропії Зенера та параметр Клеймана розраховано на основі пружних констант C_{ij} . Обидва параметри зростають зі збільшенням умісту селену в досліджуваних зразках. Коефіцієнт анізотропії Зенера показує, що тверді розчини $\text{CdTe}_{1-x}\text{Se}_x$ є пружно ізотропними матеріалами з рівномірною деформацією в усіх напрямках.

Також обчислено концентраційну залежність поздовжньої, поперечної та середньої швидкостей звуку. Поперечна та середня швидкості звуку зростають зі збільшенням умісту селену, натомість значення поздовжньої хвилі виявляє концентраційну залежність, аналогічну до поведінки модуля усебічного стиску. На основі середньої швидкості звуку розраховано концентраційну поведінку температури Дебая. Концентраційна залежність температури Дебая, обчислена з використанням методики ФРХ, засвідчує розбіжність для зразків з умістом селену $x < 0.25$, натомість для вищих концентрацій усі методики показують аналогічні результати. Кореляційний аналіз виявляє значну збіжність розрахованих параметрів із відомими експериментальними й теоретичними даними. Найліпшу збіжність розрахованих параметрів отримано для значення коефіцієнта Пуассона.

Ключові слова: твердий розчин заміщення, пружні властивості, модулі пружності, коефіцієнт Пуассона, температура Дебая.