

## Ab initio Studies of Elastic Properties of CdSe<sub>1-x</sub>S<sub>x</sub> Solid State Solution

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The elastic properties of the CdSe<sub>1-x</sub>S<sub>x</sub> ( $x = 0 - 1$ , with  $\Delta x = 0.25$ ) solid state solution in the framework of density functional theory calculations were investigated. The structures of the CdSe<sub>1-x</sub>S<sub>x</sub> samples are obtained by the substitution of sulfur with selenium atoms in hexagonal CdS. The Young's modulus, shear modulus, bulk modulus and Poisson ratio of CdSe<sub>1-x</sub>S<sub>x</sub> crystals were calculated from first principles. The dependences of the elastic properties of the CdSe<sub>1-x</sub>S<sub>x</sub> solid solution on the content index  $x$  within the interval  $0 \leq x \leq 1$  are analyzed. According to Frantsevich rule and value of Poisson ratio the materials have been classified as ductile. Zener anisotropy factor and Kleimann parameter are calculated on the basis of the elastic constants  $C_{ij}$ . Also, 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 Debye temperature was calculated. The correlation analysis shows a good agreement of the calculation results (elastic modulus and Debye temperature) with known experimental data.

**Keywords:** Solid state solution, Elastic properties, Elastic modulus, Poisson ratio, Debye temperature.

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### 1. INTRODUCTION

Semiconductor materials of II-VI group (CdSe, CdS) are characterized by their wide band gap and some excellent properties, namely high quantum efficiency, large nonlinear susceptibility, narrow band edge, good photoconduction, and fast response times, therefore these materials are the basis of various optoelectronic devices. Cadmium selenide is widely used for optoelectronic devices [1] such as solar cells [2], light emitting devices [3], lasers, photodetectors and transistors [13]. Cadmium sulfide has wide band gap and is used extensively in solar cells as "window" material in connection with CdTe [5]. This photovoltaic technology, the previous six years have featured significant increases in efficiency, from 17.3 % to 22.1 %. Recent research has demonstrated that the combination of CdS with the incorporation of the CdSe layer can significantly improve the solar cell's photo-response at both short and long wavelength ranges, by the increasing short circuit current ( $J_{sc}$ ) and external quantum efficiency (EQE) [6].

The formation of CdSe<sub>1-x</sub>S<sub>x</sub> solid state solution improves the physical properties in comparison to the binary compounds, CdSe and CdS. The CdSe<sub>1-x</sub>S<sub>x</sub> solid state solution is characterized by a direct band gap which can be varied by the composition changes from 1.72 eV for  $x = 0$  (CdSe) to 2.44 eV for  $x = 1$  (CdS). It is known that binary compounds CdS and CdSe exist in both wurtzite [7] and zinc-blende (ZB) structures [8], which are observed also for CdSe<sub>1-x</sub>S<sub>x</sub>. By modifying of CdSe<sub>1-x</sub>S<sub>x</sub> composition an improvement of their physical properties and therefore widening of their practical applications in optoelectronic devices may be achieved [9].

Therefore, CdSe<sub>1-x</sub>S<sub>x</sub> has attracted interest from both experimental and theoretical points of view. In Ref. [10], the theoretical investigations of the electronic, structural, optical, thermodynamic properties of CdSe<sub>1-x</sub>S<sub>x</sub> have been reported, namely the composition dependence of the lat-

tice constant, bulk modulus, band gap, refractive index and dielectric function were studied. The investigation of the thermodynamic stability of CdSe<sub>1-x</sub>S<sub>x</sub> has allowed obtaining the critical temperature, which was found to be 314 K. It was shown also that the refractive index and dielectric constant vary none linearly with respect to the content index  $x$  (the bowing effect), that is a result of the compositional disorder [10]. Thermodynamic properties of CdSe<sub>1-x</sub>S<sub>x</sub> were also investigated in Ref. [11].

Band structure parameters of the solid state solution CdSe<sub>1-x</sub>S<sub>x</sub> were studied only in few papers. In Ref. [9], the electronic structure of CdSe<sub>1-x</sub>S<sub>x</sub> was studied by ultraviolet photoelectron spectroscopy. The corresponding theoretical investigations of the electronic structure are presented in our previous studies [12-14].

The elastic constants determine the response to applied macroscopic stress and help to understand the related physical problems, such as the elasticity, mechanical stability and stiffness of compounds. In Ref. [13], the results of theoretical studies in the framework of the local density approximation (LDA) of the structural, electronic, and elastic properties of CdSe<sub>1-x</sub>S<sub>x</sub> for zinc-blende modification are presented. The elastic constants  $C_{11}$ ,  $C_{12}$ ,  $C_{44}$ , Young Modulus, and Shear Modulus were also calculated, that permitted to conclude that CdSe<sub>1-x</sub>S<sub>x</sub> is rather a ductile compound [13].

As we can see, the electronic structure of CdSe<sub>1-x</sub>S<sub>x</sub> is not fully studied, among them, the elastic properties for the wurtzite structure of this solid solution are not known. Such theoretical data for these physical properties would be highly useful for comparison to the corresponding experimental ones, for simulation of the device performance and for searching the ways to improve its efficiency.

In this paper, we report on the elastic and related properties of the CdSe<sub>1-x</sub>S<sub>x</sub> solid state solution for the compound index  $x$  in the range of  $x = 0 - 1$ , changed with the step of  $\Delta x = 0.25$ . As the initial crystal structure of CdSe<sub>1-x</sub>S<sub>x</sub> solid state solution the structure of

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the hexagonal crystal CdSe has been taken, where one selenium atom has been changed by sulfur one.

## 2. MATERIALS AND METHODS

The density functional theory (DFT) was used for the calculation of the elastic properties of CdSe<sub>1-x</sub>S<sub>x</sub> solid state solutions with the content index  $x$  from 0 to 1 with the step of  $\Delta x = 0.25$  [15]. The generalized gradient approximation (GGA) and the Perdew–Burke–Ernzerhof (PBE) exchange-and-correlation functional [16] were utilized during the calculation. Within the method used, the electronic wave functions were expanded in a plane wave basis set with the cut-off energy of 290 eV. The electrons  $4d^{10}5s^2$  for Cd,  $3s^23p^4$  for S, and  $4s^24p^4$  for Se atoms have been taken as the valence ones. For the Brillouin zone (BZ) sampling has been used  $2 \times 2 \times 2$  Monkhorst–Pack mesh [17]. The self-consistent convergence of the total energy in the calculations was  $5.0 \times 10^{-6}$  eV/atom. The Broyden–Fletcher–Goldfarb–Shanno (BFGS) minimization technique was used for geometry optimization of the lattice parameters and atomic coordinates. The maximum ionic Hellmann–Feynman forces within  $0.01$  eV/Å, the maximum ionic displacement within  $5.0 \times 10^{-4}$  Å, and the maximum stress within 0.02 GPa were used during optimization. These parameters are sufficiently small to lead to the well-converged total energy of the structures studied.

## 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 and returns 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  $C_{ij}$  [18-20]. The calculation method used allows the calculation of the total energy  $E$  for arbitrary crystal structures.

Estimation of elastic constants can be performed based on the results of deformation 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  $\delta$ . 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  $\delta$  by the following equations:

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

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

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

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

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

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

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

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

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

where  $V$  – supercell volume. The elastic constants  $C_{12}$ ,  $C_{13}$ , and  $C_{23}$  were determined as linear combinations of the obtained  $C_{11}$ ,  $C_{22}$  and  $C_{33}$  constants. The calculated elastic constants  $C_{ij}$  of CdSe<sub>1-x</sub>S<sub>x</sub> solid solutions ( $0 \leq x \leq 1$ ) are presented in Fig. 1.

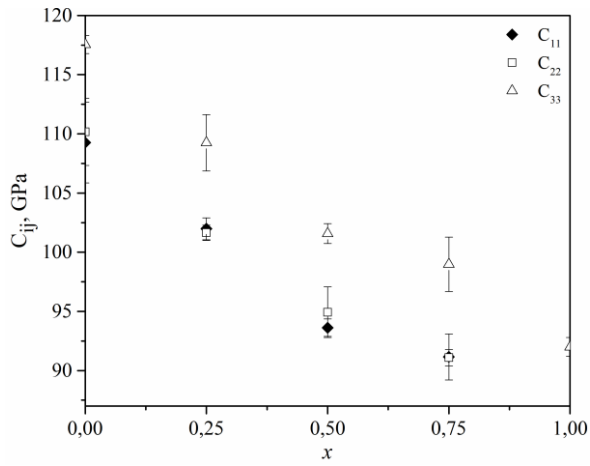
Note that, with the growth of the CdS component content, the elastic constants demonstrate qualitatively similar behavior. Hence, a conclusion can be drawn that the growth of the Se content in CdSe<sub>1-x</sub>S<sub>x</sub> solid state solution leads to the increase of the elastic constants  $C_{ij}$  in all directions.

The Voigt and the Reuss approximation methods can be used to determine the polycrystalline elastic modulus of CdSe<sub>1-x</sub>S<sub>x</sub> solid state solution [21]. Voigt method assumes the uniform strain throughout the polycrystalline sample and the Reuss one assumes the uniform stress. Calculations of the actual effective constants using the Hill method show that they lay 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  $E$ , shear modulus  $G$ , and Poisson's ratio  $\nu$  are calculated directly by the Voigt–Reuss–Hill (VRH) method [22]. The dependences of those quantities on the content  $x$  are shown in Fig. 2.

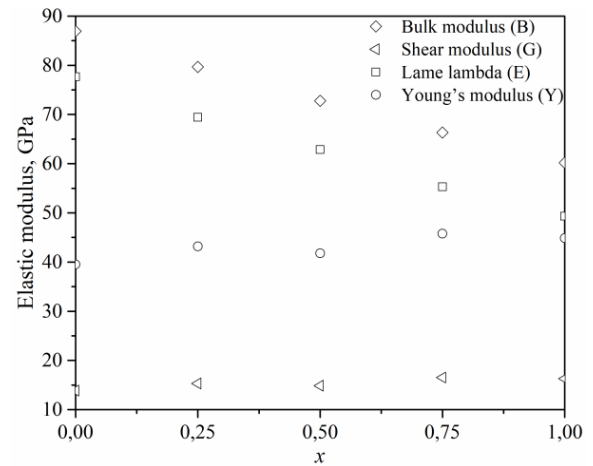
According to the elastic criteria, the material is brittle (ductile) if the  $B/G$  ratio is less (greater) than 1.75. The calculated values  $B/G$  of CdSe<sub>1-x</sub>S<sub>x</sub> solid state solution are higher than 1.75 (Fig. 3) [23] when they are obtained by the VRH methods, hence, the materials studied should probably behave in a ductile manner.

The 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 [24]. According to Frantsevich rule [25], the critical value of Poisson ratio of a material is  $1/3$  [26]. The value of the Poisson's ratio  $\nu$ , responsible for the ductile ( $\nu > 1/3$ ) or brittle ( $\nu < 1/3$ ) character, corresponds in our case to the brittle one ( $\nu < 1/3$ ). The value of Poisson's ratio is indicative of the degree of directionality 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 calculated Poisson's ratio  $\nu$  of CdSe<sub>1-x</sub>S<sub>x</sub> solid state solution lies in the range of 0.37–0.44 (Fig. 4). As result, we confirm our assumption about ductile behavior for CdSe<sub>1-x</sub>S<sub>x</sub> solid state solution.

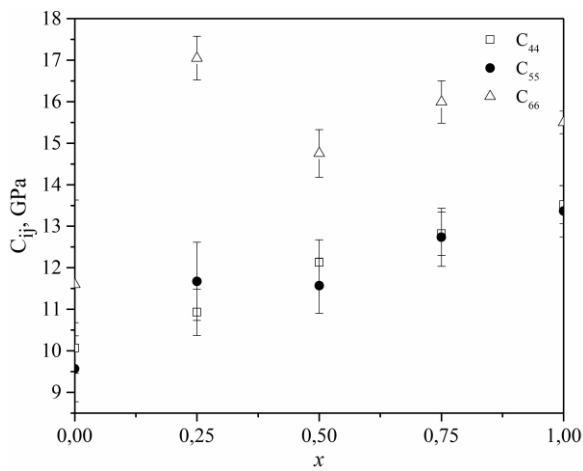
Comparisons of the elastic modulus with known values for binary compounds (CdSe and CdS) and solid state solutions based on them are listed in Table 1. We note that in other reference works [13, 27] were used cadmium chalcogenides crystallization in zinc-blende structure as an object of research. Also, we noted that in Ref. [13, 27] using standard calculation methods LDA [13, 27] and LDA + U [13] (in our case using GGA+PBEsol). As a result, the obtained values show small variation with other reference results.



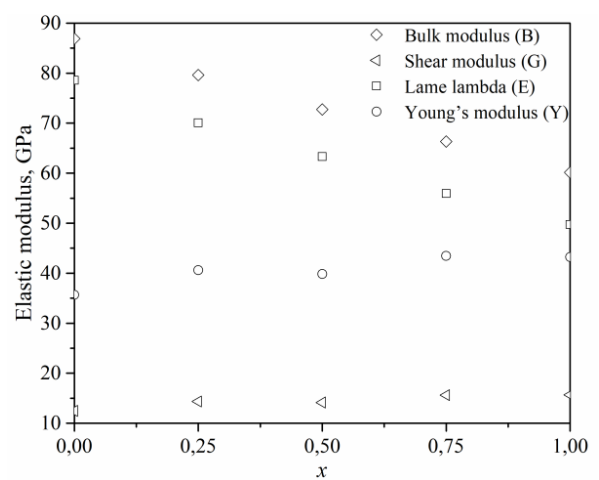
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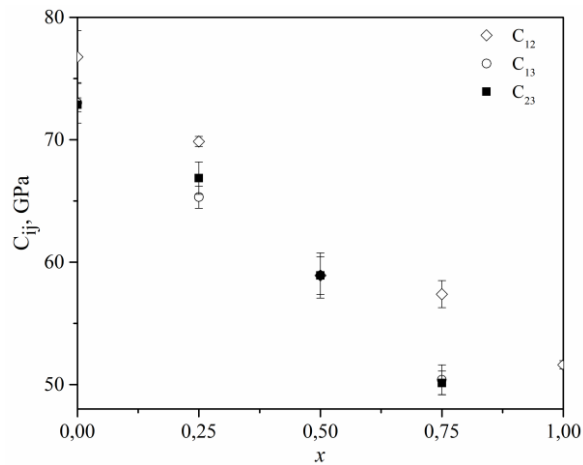
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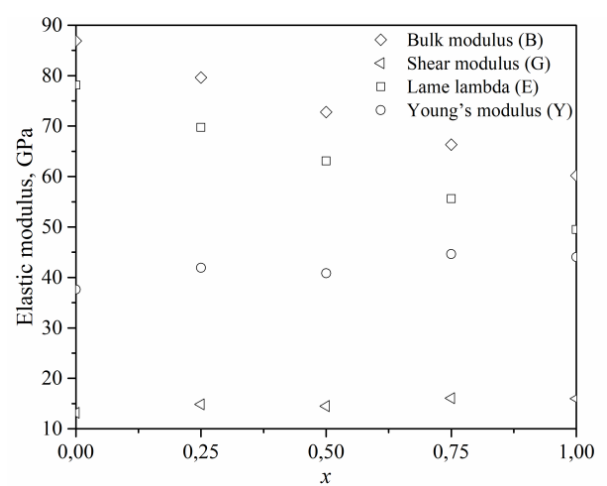
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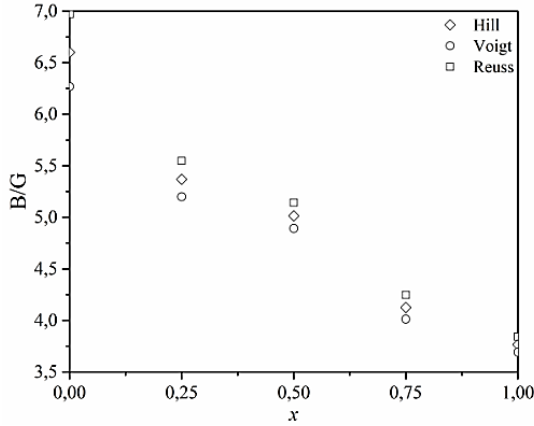
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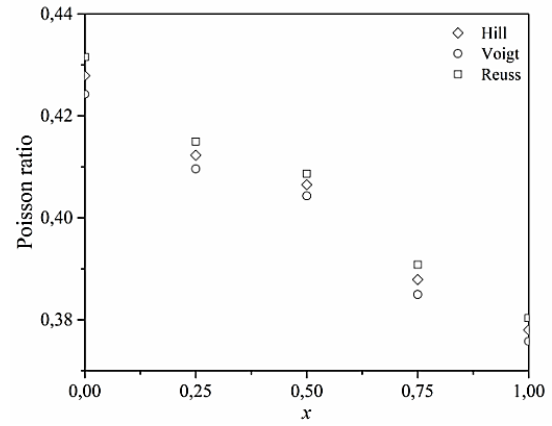
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**Fig. 1** – Dependences of elastic constants ((a)  $C_{11}$ ,  $C_{22}$  and  $C_{33}$ ; (b)  $C_{44}$ ,  $C_{55}$  and  $C_{66}$ ; (c)  $C_{12}$ ,  $C_{13}$  and  $C_{23}$ ) on the content index  $x$  in the  $\text{CdSe}_{1-x}\text{S}_x$  solid state solution

**Fig. 2** – Dependences of the elastic modulus (see information in legend to figures) calculation by Voigt (a), Reuss (b) and Hill (c) methods on the content index  $x$  in the  $\text{CdSe}_{1-x}\text{S}_x$  solid state solution



**Fig. 3** – Dependences of the ratio of bulk modulus  $B$  to shear modulus  $G$  on the content index  $x$  in the  $\text{CdSe}_{1-x}\text{S}_x$  solid state solution



**Fig. 4** – Dependences of the Poisson's ratio  $\nu$  on the content index  $x$  in the  $\text{CdSe}_{1-x}\text{S}_x$  solid state solution

**Table 1** – Present and reference data of elastic modulus and elastic constants (in GPa) for CdSe, CdS and  $\text{CdSe}_{1-x}\text{S}_x$  solid state solutions.

Compounds	Elastic modulus	This work	Reference
CdSe	Bulk modulus, $B$	86.87–86.92	65.12 [27], 53 [28], 58.1 [13]
	Young modulus, $Y$	35.68–39.51	61.20 [27], 52.00 [13]
	Shear Modulus, $G$	12.46–13.87	19.25 [13]
	Poisson ratio, $\nu$	0.42–0.43	0.345 [27]
	$C_{11}$	109.26	88.1 [27], 74.2 [13]
	$C_{12}$	76.76	53.6 [27], 49.9 [13]
	$C_{44}$	10.07	27.4 [27], 24.0 [13]
$\text{CdSe}_{0.75}\text{S}_{0.25}$	Bulk modulus, $B$	79.61–79.65	58.64 [13]
	Young modulus, $Y$	40.61–43.19	52.55 [13]
	Shear Modulus, $G$	14.35–15.32	19.45 [13]
	$C_{11}$	101.9	74.2 [13]
	$C_{12}$	69.9	50.9 [13]
	$C_{44}$	10.9	24.6 [13]
$\text{CdSe}_{0.5}\text{S}_{0.5}$	Bulk modulus, $B$	72.75–72.77	59.65 [13]
	Young modulus, $Y$	39.85–41.77	51.16 [13]
	Shear Modulus, $G$	14.14–14.87	18.85 [13]
	$C_{11}$	93.6	73.2 [13]
	$C_{12}$	58.9	54.0 [13]
	$C_{44}$	12.1	24.9 [13]
$\text{CdSe}_{0.25}\text{S}_{0.75}$	Bulk modulus, $B$	66.32–66.34	66.68 [13]
	Young modulus, $Y$	43.45–45.79	57.1 [13]
	Shear Modulus, $G$	15.62–16.53	27.1 [13]
	$C_{11}$	91.2	85.8 [13]
	$C_{12}$	57.4	57.1 [13]
	$C_{44}$	12.8	27.1 [13]
CdS	Bulk modulus, $B$	60.16–60.18	72.42 [27], 62 [28], 68.44 [13]
	Young modulus, $Y$	43.21–44.86	67.99 [27], 51.71 [13]
	Shear Modulus, $G$	15.65–16.31	18.82 [13]
	Poisson ratio, $\nu$	0.376–0.381	0.344 [27]
	$C_{11}$	82.9	97.8 [27], 91.1 [13]
	$C_{12}$	51.6	59.7 [27], 57.4 [13]
	$C_{44}$	13.5	30.6 [27], 26.8 [13]

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

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

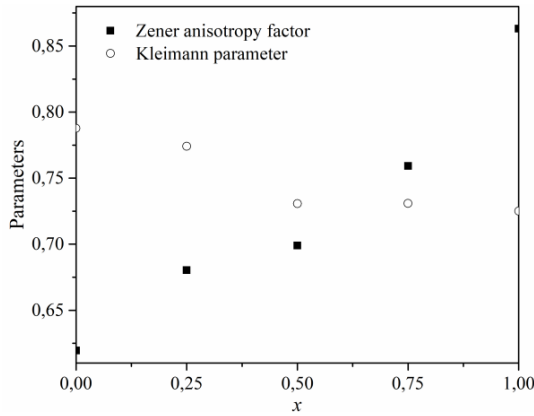
It is established that with increasing sulfur concentration there is an increase in the calculated value of  $A$  for  $\text{CdSe}_{1-x}\text{S}_x$  from 0.61 to 0.87 (Fig. 5). It indicates that

$\text{CdSe}_{1-x}\text{S}_x$  solid state solutions are not elastically isotropic materials but are the stiffest ones along  $\langle 100 \rangle$  cube axis.

The Kleimann parameter ( $\zeta$ ) indicates the relative ease of bond bending against the bond stretching and also implies resistance against bond bending or bond angle distortion [29]. For minimizing the bond bending, the value of the Kleiman parameter is  $\zeta = 0$ , and for minimizing the bond stretching  $\zeta = 1$ .

$$\zeta = \frac{C_{11} + 8C_{12}}{7C_{11} + 2C_{12}}. \quad (3)$$

In the present study  $\zeta$  changed between 0.72 and 0.79 for  $\text{CdSe}_{1-x}\text{S}_x$  solid state solution indicating shrinkage in bond-stretching (Fig. 5). The value of  $\zeta$  decreases with increase of sulfur concentration.



**Fig. 5** – Dependences of the Kleimann parameter ( $\zeta$ ) and Zener anisotropy factor ( $A$ ) on the content index  $x$  for  $\text{CdSe}_{1-x}\text{S}_x$  solid state solution

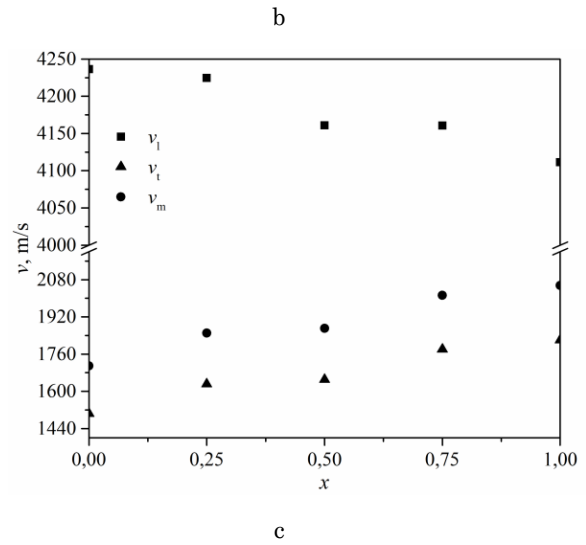
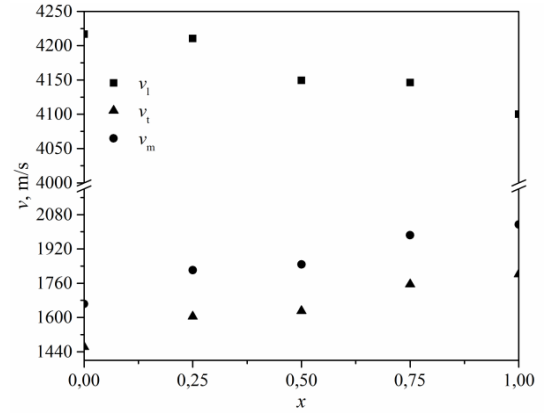
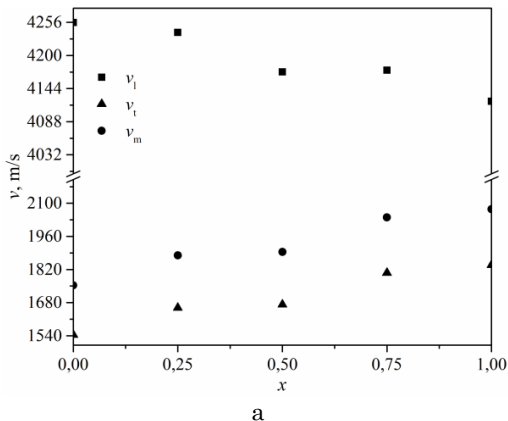
Longitudinal and transverse velocities of the elastic wave  $v_l$  and  $v_t$  can be calculated using the values of the obtained elastic modules. The values of acoustic velocity in different directions of  $\text{CdSe}_{1-x}\text{S}_x$  solid state solution were calculated using the following relations [29]:

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

$$v_t = \sqrt{\frac{G}{\rho}} \quad (5)$$

where  $\rho$  is the density of a sample. The density of  $\text{CdSe}_{1-x}\text{S}_x$  solid state solution was calculated by Vegard's law [30] from the known values for binary compounds ( $\rho(\text{CdSe}) = 5.82 \text{ g/cm}^3$  and  $\rho(\text{CdS}) = 4.82 \text{ g/cm}^3$ ). The calculated acoustic velocities are presented on Fig. 6.

The Debye temperature  $\theta_D$  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 by the mean acoustic velocity. This is the highest temperature that corresponded to the highest frequency normal vibration  $\nu_D$  ( $\theta_D = h\nu_D/k_B$ , where  $k_B = 1.380658 \cdot 10^{-23} \text{ J} \cdot \text{K}^{-1}$ ). At relatively low temperatures,



**Fig. 6** – Dependences of the acoustic velocity  $v$  on the content index  $x$  for  $\text{CdSe}_{1-x}\text{S}_x$  solid state solution calculated on the bases of the elastic modules estimated by Voigt (a), Reuss (b) and Hill (c) methods

vibrational excitations arise mainly due to acoustic oscillations. Therefore, the value of Debye temperature  $\theta_D$ , calculated through elastic constants, is similar to that determined by measuring the specific heat at low temperatures [19, 20].

Debye temperature can be calculated based on the mean acoustic velocity using equation:

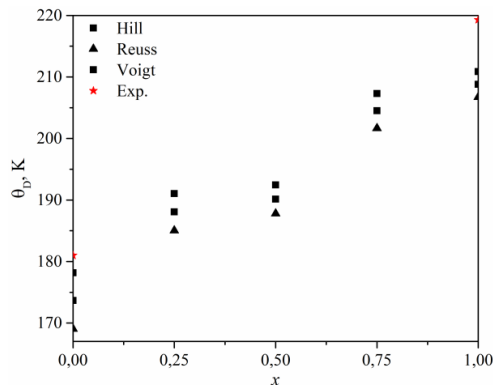
$$\theta_D = \frac{\hbar}{k_B} \left( \frac{6\pi^2 N}{V_0} \right)^{1/3} v_m \quad (6)$$

where  $N$  is the number of atoms in the supercell of  $\text{CdSe}_{1-x}\text{S}_x$ ,  $V_0$  – the supercell volume,  $v_m$  – average sound velocity (Fig. 6). The average sound velocity is calculated by using the following relation [29]:

$$v_m = \left[ \frac{1}{3} \left( \frac{2}{v_t^3} + \frac{1}{v_l^3} \right) \right]^{-1/3} \quad (7)$$

Concentration dependences of the acoustic velocities  $v_i(x)$  ( $i = l, t, m$ ) of  $\text{CdSe}_{1-x}\text{S}_x$  (Fig. 6) calculated on the basis of elastic modules estimated by different VRH methods reveal similar behaviors. Longitudinal elastic wave velocity  $v_l$  decreases with increasing sulfur concen-

tration  $x$ . Another behavior is observed for the transverse and mean sound velocities: these velocities,  $v_t$  and  $v_m$ , increase with increasing of the content index  $x$ .



**Fig. 7** – Dependences of the Debye temperature  $\theta_D$  on the content index  $x$  for  $\text{CdSe}_{1-x}\text{S}_x$  solid state solution calculated on the bases of the elastic modules estimated by Voigt (a), Reuss (b) and Hill (c) methods. Red stars – experimental results from Ref. [31] (CdSe) and Ref. [32] (CdS)

The increase of the content index  $x$  in  $\text{CdSe}_{1-x}\text{S}_x$  leads to the increase of the Debye temperature  $\theta_D$  obtained by using different VRH methods (Fig. 7). The calculated Debye temperature  $\theta_D$  is in good agreement with the corresponding experimental data of  $\text{CdSe}_{1-x}\text{S}_x$  are shown in Fig. 7. With increasing sulfur concentration, we can see decreases Debye temperature. The relatively good comparison of the calculated and experimental Debye temperatures  $\theta_D$  is observed for the binary compounds CdS and CdSe (Fig. 7). Experimental values of the Debye temperatures  $\theta_D$  are more close to the corresponding calculat-

ed ones, obtained by using the Hill method (Fig. 7). In general, the differences of the Debye temperatures  $\theta_D$  of  $\text{CdSe}_{1-x}\text{S}_x$  between the calculated by VRH methods and experimental values do not exceed 5.7-6.6 %.

#### 4. CONCLUSIONS

The elastic properties of  $\text{CdSe}_{1-x}\text{S}_x$  solid state solution are estimated by first-principles calculations. Using the Voigt-Reuss-Hill approximation, the ideal polycrystalline aggregates bulk modulus, shear modulus, Young's modulus, and Poisson's ratio, are calculated and discussed. The materials studied should probably behave in a ductile manner. Zener anisotropy factor shows that  $\text{CdSe}_{1-x}\text{S}_x$  solid state solutions are not elastically isotropic materials, but are stiffest along  $\langle 100 \rangle$  cube axis. The Kleimann parameter shows that  $\text{CdSe}_{1-x}\text{S}_x$  solid state solutions are shrinkage in bond-stretching. Based on the elastic modules the longitudinal elastic wave velocity, transverse elastic wave velocity and average sound velocity were calculated. The longitudinal elastic wave velocity decreases with increasing sulfur concentration. The transverse and average sound velocities increase with increasing sulfur content in  $\text{CdSe}_{1-x}\text{S}_x$ . The Debye temperature for  $\text{CdSe}_{1-x}\text{S}_x$  solid state solution increases with increasing sulfur concentration. Calculated Debye temperatures for  $\text{CdSe}_{1-x}\text{S}_x$  are in good agreement with the corresponding reference data for the binary compounds CdSe and CdS.

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### **Ab initio** дослідження пружних властивостей твердого розчину $\text{CdSe}_{1-x}\text{S}_x$

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Досліджено пружні властивості твердого розчину  $\text{CdSe}_{1-x}\text{S}_x$  ( $x = 0 - 1$ , при  $\Delta x = 0,25$ ) у рамках розрахунків теорії функціоналу густини. Структури зразків  $\text{CdSe}_{1-x}\text{S}_x$  отримані заміщенням сірки на атоми селену в гексагональному  $\text{CdS}$ . Модуль Юнга, модуль зсуву, об'ємний модуль і коефіцієнт Пуассона кристалів  $\text{CdSe}_{1-x}\text{S}_x$  були розраховані з перших принципів. Проаналізовано залежності пружних властивостей твердого розчину  $\text{CdSe}_{1-x}\text{S}_x$  від показника вмісту  $x$  на інтервалі  $0 \leq x \leq 1$ . Відповідно до правила Францевича та значення коефіцієнта Пуассона матеріали були класифіковані як пластичні. Коефіцієнт анізотропії Зенера та параметр Клеймана розраховуються на основі пружних констант  $C_{ij}$ . Також розраховано концентраційну залежність швидкості поздовжньої пружної хвилі, швидкості поперечної пружної хвилі та середньої швидкості звуку. На основі середньої швидкості звуку було розраховано концентраційну поведінку температури Дебая. Кореляційний аналіз показує збіг результатів розрахунку (модуль пружності та температури Дебая) з відомими експериментальними даними в рамках похибки.

**Ключові слова:** Твердий розчин, Пружні властивості, Модуль пружності, Коефіцієнт Пуассона, Температура Дебая.