Thermodynamic Properties of CDSE Crystals Using First Principles Calculations and Experiment

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Abstract: The cluster models have been built for calculation of the geometric and thermodynamic parameters based on the analysis of the crystal and electronic structure of CdSe crystals in the cubic phase. The temperature dependence of formation energy ΔE, formation enthalpy ΔH, Gibbs free energy ΔG, entropy ΔS, specific heat capacity at constant volume C_V and constant pressure C_P have been defined according to first principles calculations. Computer calculations of thermodynamic parameters carried out by density functional theory (DFT) and with using of the hybrid B3LYP valence base set. Also, in the work have been derived analytical expressions of temperature dependences of the presented thermodynamic parameters, which have been approximated by the first principles calculation data using mathematical package Maple 14. Theoretically calculated data of specific heat at constant pressure CP compared with the data of calorimetric measurements.

Index Terms—First Principles Calculations, Cadmium Selenide, Thermodynamic Properties, Heat Capacity.

I. INTRODUCTION

The commercial interest in CdSe crystals caused by the ability to use them as luminescent biolabels as components of regenerative solar cells [1], optical amplifiers and electroluminescence devices [2], thin film transistors with high efficiency, LEDs [3], radiation detectors and nonlinear optical devices [4]. Also, special attention recently attracted CdSe layers as one of the components of p-ZnTe-n-CdSe hetero junction, the interface of which is close to ideal. Such hetero junctions, in particular, can be used in integrated detectors of ionizing radiation. Should be noted, that CdSe semiconductor crystals, nanocrystals and films, as pure and admixtures are using with so high technological interest due to their stable properties at high temperatures and capacities. However, the available published data about changes in their values with temperature is controversial, and often, in general, uncertain. Therefore, it is important to study the parameters of the semiconductor at temperature range used for technical purposes. The dimorphism is typical for CdSe semiconductor crystals at normal pressure. Depending on the conditions of preparation, it crystallizes or as sphalerite (space group F43m) or as wurtzite (space group P63mc). In paper [5] reported that the transition from the cubic phase to hexagonal occurs at a temperature of 368 K. In the samples produced at higher temperatures saved hexagonal structure [5]. However, the variations of the lattice parameter in such crystals have been observed, what indicated the presence of impurities or packaging defects. Modification of zinc blende obtained at room temperature by deposition from solution [3]. Zinc blende structure becomes unstable at temperatures above 2000 K [6]. The authors of paper [3] reported that the cubic phase of CdSe is unstable It observed the partially transforms into the hexagonal modification at a temperature of 403 K Full transformation was going during 18 hours at temperatures above 973 K. That mean the question of polymorphic transition temperature between "sphalerite-wurtzite" modifications is quite ambiguous. The melting temperature is T = 1512 K [4]; in [11] indicated a slightly higher melting point - T = 1563 ± 10 K. Lattice constant for cadmium selenide which calculated by ab initio methods and investigated experimentally for sphalerite structure equal to a_{exp} = 6.052 Å and a_{calc} = 5.929 (±2%) Å, respectively. Band gap of CdSe is E_g = 1.7 eV [8], [9]. In work [10] a slightly different meaning of band gap which determined from electrical measurements equal to Eg = 1.88 eV, and optical studies give the value E_g = 1.83 eV. Usually conductivity of CdSe considered as n-type. Own donor centers are selenium vacancies [10]. In this paper, the analysis of the structure and physical-chemical properties of CdSe crystals has been done, and, based on first principle calculations, the temperature dependence of important thermodynamic parameters have been found. The experimental studies of isobaric heat capacity C_P have been spent.

II. CALCULATIONS OF THERMODYNAMIC PARAMETERS

A. Models of Clusters

In the CdSe sphalerite structure, the chemical bonding between two atoms Cd-Se, taking into account the configuration of the valence electrons Cd-5s^2, and Se-4p^4, carried out by the participation of three electrons of the selenium atom and one electron of the cadmium atom.
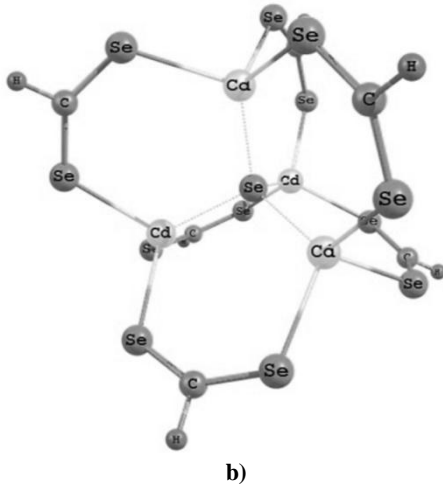

a)

b)
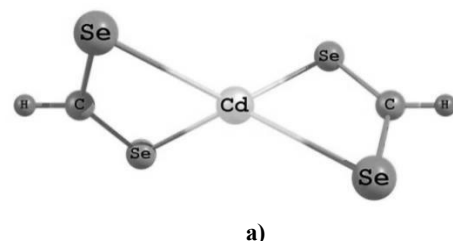
Fig. 1. Model of clusters A (CdC$_2$H$_2$Se$_4$) (a) and B (Cd$_4$C$_6$H$_6$Se$_{13}$) (b) respectively for CdSe cubic phase.

We proposed two cluster models for calculations of the thermodynamic parameters, namely, A – "small" (Fig. 1,a) and B – "large" (Fig. 1,b). At "small" cluster of CdSe sphalerite structure (Cd +4Se) the compensation of dangling bonds was implemented by four electrons of carbon atoms C and one electron of hydrogen atom H, which corresponds to the formula CdC$_2$H$_2$Se$_4$ (fig.1,a). Except of three structures of previous cluster the model of "large" cluster B (Fig. 1,b) includes Cd and Se atoms, which corresponds to the formula Cd$_4$C$_6$H$_6$Se$_{13}$ (fig.1,b). The saving of geometrical parameters after optimization (finding of minimum of potential energy) within 2% error defines the rationality of this choice. The application of presented cluster models allows the calculation of the thermodynamic properties with sufficient accuracy even with using of small clusters.

B. Calculation Methods

With using of the rigid molecule approximation [9] the formation enthalpy H of the crystals is defined as:

$$H \approx H_{elec} + H^0_{vib} + E_{vib}(T) + H_{rot}(T) + H_{trans}(T) + RT , \quad (1)$$

Where H_{elec} is electronic component of enthalpy, H_{vib} is vibrational component of enthalpy, H^0_{vib} is enthalpy of zero point vibrations, H_{rot} is rotational component of enthalpy, H_{trans} is translational component of enthalpy, R is universal gas constant, T is a temperature. Similarly, there was calculated formation energy ΔE.

The rotary and the translational components of enthalpy are presented as follows:

$$H_{rot} = \frac{3}{2} NkT , \quad (2)$$

where N is the total number of atoms, k is Boltzmann const

$$H_{trans} = \frac{5}{2} NkT . \quad (3)$$

Vibrational enthalpy is a function of $(3N-6)$ vibrational frequencies of the molecules. The enthalpy of zero points vibrations:

$$H^0_{vib} = \frac{1}{2} \sum_{i=1}^{3N-6} h\nu_i , \quad (4)$$

where h is Planck's constant, ν_i is frequency of i-th vibration.

Vibrational contribution to the enthalpy (depends on T) is:

$$H_{vib}(T) = \sum_{i=1}^{3N-6} \frac{h\nu_i}{\left(e^{\frac{h\nu_i}{kT}} - 1 \right)} . \quad (5)$$

The entropy of the crystal, in general, is the sum of the components:

$$\Delta S = S_{trans} + S_{rot} + S_{vib} + S_{elec} - nR \left[\ln(nN_0) - 1 \right] , \quad (6)$$

where N_0 is Avogadro constant, n is the number of moles of molecules, M is mass of the molecule.

Where the translational entropy component S_{trans} are showing as the next following:

$$S_{trans} = nR \left\{ \frac{2}{3} + \ln \left[\left(\frac{2MkT\pi}{h^2} \right)^{\frac{2}{3}} \left(\frac{nRT}{P} \right) \right] \right\} . \quad (7)$$

Rotary S_{rot} and vibrational S_{vib} components of the entropy calculated similarly to the components of the enthalpy.

After calculating contributions of zero point energy and entropy of certain members of the molecules of reagents A (Cd) and B (Se), we can calculate the Gibbs free energy of the crystal at a given temperature T.

$$\Delta G = H_A - H_B + \frac{1}{2} \sum_{i \in A} h\nu_i - \frac{1}{2} \sum_{j \in B} h\nu_j - \\ - T \left(S^A_{vibr} - S^B_{vibr} + S^A_{rot} - S^B_{rot} + S^A_{trans} - S^B_{trans} \right) . \quad (8)$$

Presented calculations theory has been successfully used in quantum-chemical calculation programs [13].

For calculations of ΔE, ΔH, ΔS, ΔG we used the following method of taking into account of the initial conditions, which is illustrated by the formation energy ΔE. At first was calculated the formation energy ΔE_A of the cluster A (fig.1,a) according [9]:

$$\Delta E_A = E - \sum E_{el} + \sum E_{at} , \quad (9)$$

Where E is the total energy of the system; E_{el} is electronic energy of the atoms that form the system (in atomic state); E_{at} is atomization energy of atoms. The total and electronic energy of the system were taken from the results of the quantum-chemical calculations, and all other values – from the reference materials [3,7, 11]. The formation energy ΔE_B of B cluster (Figure 1,b) was calculated similarly. So, from the formation energy of B cluster there are subtracted the triple value of the formation energy of A cluster, that mean, from the formation energy of the cluster consisting of sphalerite crystal fragment and three ligands are subtracted the formation

energy of three ligands. This value can be related to real crystal [9]:

$$\Delta E = \Delta E_B - 3 \cdot \Delta E_A . \qquad (10)$$

Based on the calculated vibrational spectrum, the calculation of the thermodynamic properties of CdSe crystals at different temperatures have been spent (Fig.2-4).

C. Details of the Calculation

The first step for the first principles calculations of the cluster properties was the determination of the lowest energy configuration. All calculations started with SCF convergence, geometry optimization and after obtaining a stable minimum, the frequencies were calculated. The calculations were carried out using density functional theory, using bases in Stevens-Basch-Krauss-Jasien-Cundari (SBKJC) [11] parameterization. In this basic set only the valence electrons which are directly involved in chemical bonding are considered. This basis set was chosen due to our previous experience with this basis set in several vibrational studies carried out in this group [13]-[15]. DFT calculations were performed with the use of Becke's three parameter hybrid method [16] with the Lee, Yang, and Parr (B3LYP) gradient corrected correlation functional [17] using the PCGamess program packages [18]. The visualization of spatial structures was carried out using Chemcraft.

III. RESULTS AND DISCUSSION

A. The thermodynamic Parameters

In Fig. 2, 3 are presented the change of the formation energy ΔE, formation enthalpy ΔH, Gibbs free energy ΔG and entropy ΔS of CdSe crystals as a function of the temperature from 20 K to 800 K. Their analytical expressions can be represented by dependences:

$$\Delta E(T) = 0.1697 \cdot T + 103.58 ; \qquad (11)$$

$$\Delta H(T) = 0.153 \cdot T + 103.58 ; \qquad (12)$$

$$\Delta G(T) = 0.7453 \cdot T + 76.174 ; \qquad (13)$$

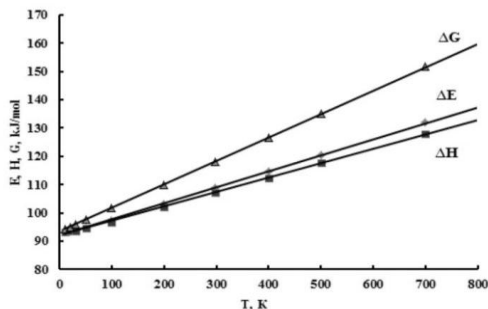$$\Delta S(T) = 130.037 \ln(T) + 26.541 . \qquad (14)$$

Fig. 2. Temperature dependences of the energy ΔE and enthalpy ΔH of formation and Gibbs free energy ΔG for CdSe crystals: lines - approximation of analytic functions (11-13), points - first principles calculation.

The Fig. 2 shows that formation energy ΔE and formation enthalpy ΔH of cadmium selenide uniformly increases in the whole studied range. And Gibbs free energy ΔG has a rapid change of temperature, which is logical for semiconductor crystals II-VI in cubic phase [11].
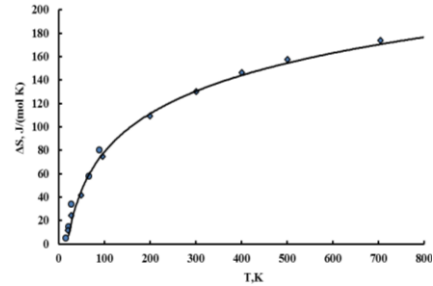

Fig. 3. Temperature dependence of entropy ΔS for CdSe sphalerite crystals. Squares - calculation from first principles, circles - calculation of work [19], line - approximation of analytic function (14).

Fig. 3 shows the temperature dependence of the entropy of CdSe crystals, and estimated data taken from paper [19]. From the figure it is evident that the entropy increases throughout all given temperature range, and that the temperature factor more effect on this parameter at high temperatures. The table shows known literature and calculated by us values of thermodynamic parameters for CdSe which are in good agreement, what is indicating the adequacy of the calculations.

Table 1. Thermodynamic properties of CDSE crystals

Parameter, units	Literatures date	Calculation
Lattice constant a, Å	5.929 [21]	6.03
Distance between oppositely atoms, Å	2.63 [22]	2.61
The enthalpy of formation, $-\Delta H_{298.15}$, kJ/mol	136.5 [23]; 143.1±1,9 [24]; 144.9 [25]	107.1
Gibbs free energy, $-\Delta_{G298.15}$, J/(mol·K)	96.7 [23]; 140.9±1,9 [24] 141.6 [25]	118.2
Entropy, $S_{298.15}$, J/(mol·K)	86,5±0,8 [24] 83.3 [25]	129.83
Heat capacity, $C_{V,298.15}$, J/(mol·K)	49.40424 [19]**Error ! Reference source not found.** 46.850292 [21]	52.06

B. Isobaric C_P and Isochoric C_V Heat Capacity

Temperature dependence of the heat capacity of crystal structures by classical laws are defined by the following function:

$$C = a + b \cdot 10^{-3} T - c \cdot 10^5 T^{-2} , \qquad (7)$$

Where a, b, c are the coefficients that depend on the structure and type of material.
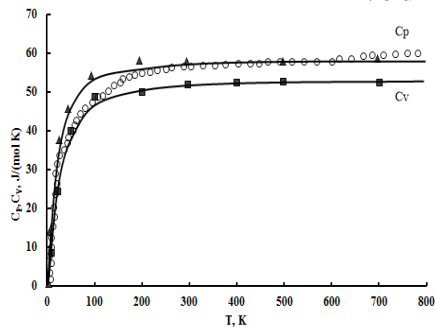
Fig. 4. Temperature dependence of isochoric C_V - ■ and isobaric C_P - ▲, heat capacities and experimental values C_P - ○ of CDSE crystals.

Obtained by us analytical expressions of temperature dependencies of heat capacity at constant volume, which were approximated by first principles calculation points using a mathematical package Maple 14, are shown by the following equations:

$$C_V = 41.608 + 21.009 \cdot 10^{-3} T - 0.036 \cdot 10^5 T^{-2} \quad (15)$$

$$C_P = 47.100 + 20.998 \cdot 10^{-3} T - 0.036 \cdot 10^5 T^{-2} \quad (16)$$

Synthesis of cadmium selenide was performed in quartz ampoules by fusion of elements cadmium and selenium (according to the certificate, the content of the basic substance not less than 99.9999% and 99.9996%, respectively) taken in stoichiometric ratios, up to 10^{-4} g. Preliminary elements further purified by zone melting. The concentration of background impurities in the source component does not exceed 10^{-5} weights. Received CdSe samples periodically checked by the contents of uncontrolled impurities by atomic absorption analysis, secondary ions, Auger- and laser mass spectrometry. Polycrystalline CdSe grew from the powder in a glass mortar and then inserted into quartz ampoule with 16 cm length and 12 mm diameter under the 133.32 Pa pressure. Growth was carried out in a two-zone furnace from melt by the Bridgman method in which the ampule slowly move at a speed of 1.5 mm/h using extractor with controlled speed engine. Originally the ampule heated at 1523 K within 24 hours. During melting the ampoule always stirred using a mechanical system to ensure homogeneity. Then the ampule with its contents moved into the area of crystallization (1323 K). During growth temperature was kept constant within ± 5 K. The ampule moved through two-zone tube furnace for eight days. Grown CdSe sample sticks to the plate and split in the direction of the sample line. Samples grown by this method were ideally in the direction {100}. Measurements of isobaric heat capacity at the temperature range 13-300 K were carried out on the CU-300 equipment. Temperature ranges (300 - 800 K) have been studied by differential cooling calorimeter Parkin-Elmer. The operation principle of which is based on a comparison of the heat flow of the sample and the standard. Calorimetric measurements were carried out on crystalline samples weighing 12 mg and dimensions of 2x2x4

mm. Temperature and energy calibration calorimeter were carried out in the melt of pure metals In, Sn, Bi, Al, Cu and with known exact temperature and enthalpy of melting. The investigation of the heat capacities C_V and C_P at 10-800 K temperatures is shown in Fig. 4. At high temperatures, the constant volume heat capacity CV tends to the Petit and Dulong limit which is common to all solids [10]. At sufficiently low temperatures, C_V is proportional to T^3 [11]. At intermediate temperatures, however, the temperature dependence of C_V and C_P are governed by the details of vibrations of the atoms and for a long time could only be determined from experiments. At 298 K, CV and CP are in the range of 48–59 J/(mol•K), respectively. Note, the experimental values of isobaric heat capacity coincide well from the calculated curve approximation at the low temperatures. A value at temperatures from 50 K till 300 K is too low relative to theory. The latter is due from un harmonic vibrations of real crystal, which it is difficult to take into account in the theoretical model [20]. Also, you should note that for the calculation of basic thermodynamic functions of the studied compound at 298.15 K, smoothed heat capacity values were extrapolated to 0 K using the model equations that include the phonon contribution to the specific heat as a combination of Debye and Einstein functions, and as electronic component. The presented expressions of the heat capacity temperature dependences (Fig. 4) are particularly important for the calculation of the Debye characteristic temperature. This, in turn, provides insight into the analysis of heat transfer processes and phonon interactions with each other and with defects in the crystal structure.

IV. CONCLUSION

1. The cluster models for calculating of the thermodynamic parameters of cadmium selenide have been proposed based on the crystal and electronic structure of cubic CdSe and paid attention on their physical and chemical properties.
2. Have been defined the temperature dependences of the thermodynamic parameters of the CdSe crystals, namely, formation energy ΔE, formation enthalpy ΔH, entropy ΔS and Gibbs free energy ΔG. These results can be used to predict properties of CdSe crystals during annealing.
3. From the first principles calculations there have been received the analytical expressions for the temperature dependences of the specific heat capacity of the CdSe crystals in cubic phases at constant volume CV and at constant pressure CP.
4. Experimental calorimetric study of the temperature dependence of heat capacity for CdSe crystals at constant pressure was carried out. These results were compared with quantum-chemical calculation results. We can conclude about the adequacy of the proposed cluster models based on the coincidence of theoretical and experimental points.

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