

Modeling of Structure, Thermodynamic Properties and Phase Transition Temperatures of II-VI Crystals

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The work is devoted to the theoretical calculations and experimental study of important thermodynamic parameters of II-VI crystals. Cubic sphalerite and hexagonal wurtzite cluster models of polymorphs for stoichiometric II-VI crystals (ZnX, CdX; X = S, Se, Te) have been proposed. In the work one carried out the calculations of thermodynamic parameters under normal conditions and defined the analytical expressions of temperature dependences for energy ΔE , enthalpy ΔH , Gibbs free energy ΔG , entropy ΔS for sphalerite phase stoichiometric crystals of zinc and cadmium chalcogenides. Using the results of DFT-calculations according to equality of Gibbs free energy for sphalerite and wurtzite phases ($\Delta G_S = \Delta G_W$) of zinc chalcogenides crystals we defined phase transition "sphalerite-wurtzite" temperatures, which decreased in the line ZnS (1454 K) – ZnSe (1427 K) – ZnTe (1382 K) and was found the specified region of stability for these polymorphs.

Keywords: Cluster models, Quantum chemical calculations, Chalcogenide crystals, Thermodynamic parameters.

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1. INTRODUCTION

The increasing interest of II-VI semiconductors are caused by their wide use in practice and in model studies. In particular, zinc chalcogenides used in semiconductor and quantum electronics – for solar-powered detectors of X - and γ -radiations, lasers, infrared receivers [1-3]. Cadmium chalcogenides are well-established in various areas of energy, solid-state electronics and radiation technology. In particular, CdTe, due to the unique set of physical properties, used for making a range of highly efficient devices, nuclear power, solar technics, optic and acoustic electronics, X - and γ -detectors, substrates for epitaxial growth. As for the cadmium sulfide and selenide, in addition to the above, on their base for a long time are forming thin-film transistors, elements for solar cells and photoelectronics, rulers for injection lasers, etc. [1-3].

For the effective implementation of the described application requires a large amount of information about the properties of crystals. Namely, for the growing of crystals and their appliance are necessary data about the thermodynamic properties in the stoichiometric state. The research of these parameters in semiconductors is important for understanding of the phonon heat transfers processes in solids. They also important for finding of the information about the crystal lattice dynamics, for the calculations of the elasticity parameters at stresses and variable temperature. Despite the long practical use of the studied materials, an actual problem at present is the determination of the thermodynamic parameters and their temperature changes.

The development of theoretical methods for study of the structure, electron and phonon subsystems which are based on first principles calculations allowed to calculate number of crystals characteristics with good accuracy, to spend the theoretical interpretation of their physical and chemical properties. However, de-

spite the fact that today developed a range of powerful computer programs for the practical implementation of these methods, they are not universal. For each compound and for each task are necessary to develop a unique approach. That's why the use of such computational complexes refers to the priority tasks of modern physics and chemistry of solids.

2. CALCULATIONS OF THERMODYNAMIC PARAMETERS

2.1 Models of Clusters

In the paper, based on the ideas of the crystal and electronic structure the cluster models of sphalerite and wurtzite phase of II-VI semiconductors have been proposed. Based on the developed models of "small" (A) and "large" (B) clusters for sphalerite phases (Fig. 1) using first principle approaches we calculated the temperature dependence of energy ΔE , enthalpy ΔH , Gibbs free energy ΔG , entropy ΔS for ZnS, ZnSe, ZnTe and CdS, CdSe, CdTe crystals.

Let's consider the nature of bonds in II-VI crystals: ZnS, ZnSe, ZnTe, CdS, CdSe, CdTe, taking into account configuration of valence electrons of the constituent atoms: Zn – $3d^{10}4s^2$, Cd – $4d^{10}5s^2$, S – $3s^23p^4$, Se – $4s^24p^4$, Te – $5s^25p^4$. The electronic structure of II-VI compounds highlighted in paper [2]. The system Me-X has two valence electrons of the metal and four valence electrons of the chalcogen. In the cubic phase of II-VI crystals each atom of the metal (chalcogen) has four neighboring atoms of the chalcogen (metal), from which follows that two bonds Me-X are involved by three electrons of the chalcogen atom and one electron of the metal atom (two electrons on each bond).

Boundary conditions of clusters were formed on base of the following considerations. Two boundary of chalcogen atoms are belonged three electrons by two

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bonds. That means, there are five electrons in two bonds that are not compensated. For compensation of these electrons in the cluster we add carbon atoms (C), which take four electrons from chalcogen and one uncompensated electron take from hydrogen atom (H). That means, there are five uncompensated electrons on two chalcogen atoms, which are compensated by five electrons of carbon and hydrogen atoms.

The cluster A constructed with one metal atom (Me = Zn, Cd) and four chalcogen atoms (X = S, Se, Te), which provides playback of tetrahedral coordination of the central atom in a real crystal, and the saturation of dangling bonds realized by two carbon atoms C and two atoms of hydrogen H, which corresponds to chemical formula $\text{MeC}_2\text{H}_2\text{X}_4$ (Fig. 1a). Except for three structures of the previous cluster, the model of the “large” cluster B (Fig. 1b) includes Me and X atoms, that provides playback of tetrahedral coordination of the central atom and the nearest neighbors, and corresponds to the formula $\text{Me}_4\text{C}_6\text{H}_6\text{X}_{13}$ (Fig. 1b) [4, 5].

The saving of the geometrical parameters after optimization (finding minimum potential energy) within 1 % error defines the rationality of this choice. The application of the presented cluster models allows the calculation of the thermodynamic properties with sufficient accuracy even by using small clusters.

2.2 Calculation Methods

By using the rigid molecule approximation the enthalpy ΔH of the crystals is defined as follows:

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

where H_{elec} is the electronic component of enthalpy, H_{vib} is the vibrational component of enthalpy, H_{vib}^0 is the enthalpy of zero point vibrations, H_{rot} is the rotational component of enthalpy, H_{trans} is the translational component of enthalpy, R is the universal gas constant, and T is the temperature. Similarly, the energy ΔE was calculated.

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

$$\Delta S = S_{\text{trans}} + S_{\text{rot}} + S_{\text{vib}} + S_{\text{elec}} - nR[\ln(nN_0) - 1], \quad (2)$$

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

After calculating the contributions of zero point energy and the entropy of certain members of the molecules of reagents A (Me) and B (X), we calculated the Gibbs free energy of the crystal at the given temperature T :

$$\Delta G = H_A - H_B + \frac{1}{2} \sum_{i \in A} hv_i - \frac{1}{2} \sum_{j \in B} hv_j - T(S_{\text{vibr}}^A - S_{\text{vibr}}^B + S_{\text{rot}}^A - S_{\text{rot}}^B + S_{\text{trans}}^A - S_{\text{trans}}^B). \quad (3)$$

For calculations of ΔE , ΔH , ΔS , and ΔG we used the following method taking into account the initial conditions, which is illustrated by the energy ΔE . At first we calculated the energy ΔE_A of cluster A (Fig. 1a) according [4]:

$$\Delta E_A = E - \sum E_{\text{el}} + \sum E_{\text{at}}, \quad (4)$$

where E is the total energy of system, E_{el} is the electronic energy of the atoms that formed system (in atomic state), and E_{at} is the atomization energy of atoms. Total and electronic energies of system were taken from the results of the quantum-chemical calculation, and all other values were taken from the reference materials [14].

The formation energy ΔE_B of cluster B (Fig. 1b) was calculated similarly. So, from the formation energy of cluster B subtracted the triple value of the formation energy of cluster A. That means, from the formation energy of the cluster consisting of a sphalerite crystal fragment and three ligands subtracted the formation energy of three ligands. This value can be related to a real crystal [6]:

$$\Delta E = \Delta E_B - 3 \cdot \Delta E_A. \quad (5)$$

Based on the calculated vibrational spectrum, the calculation of the thermodynamic properties of CdTe crystals at different temperatures has been spent (Figs. 2-4).

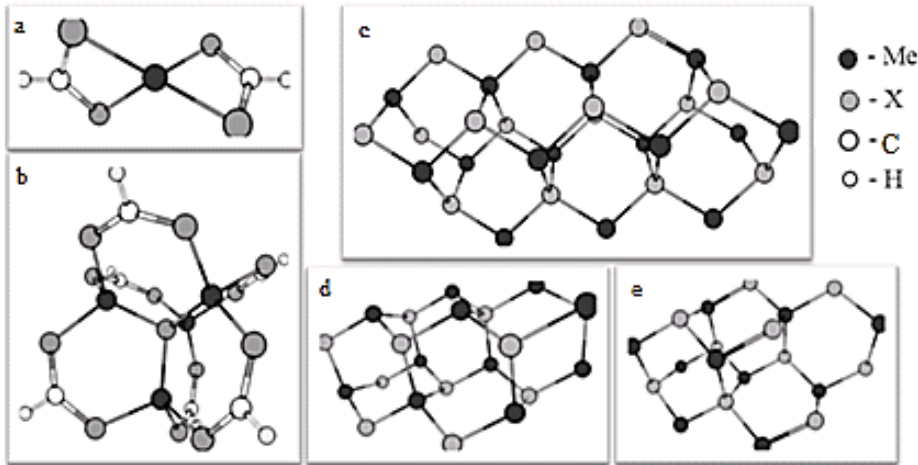


Fig. 1 – Cluster models of sphalerite (a, b) and wurtzite (c, d, e) phases of MeX crystals (Me-Zn, Cd; X = S, Se, Te): a – A ($\text{MeC}_2\text{H}_2\text{X}_4$), b – B ($\text{Me}_4\text{C}_6\text{H}_6\text{X}_{13}$), c – C ($\text{Me}_{15}\text{X}_{15}$), d – D ($\text{Me}_{11}\text{X}_{11}$), e – E ($\text{Me}_{10}\text{X}_{10}$)

2.3 Details of the Calculations

The first step for the quantum-chemical calculation of the cluster properties was the determination of the lowest energy configuration. All calculations started with SCF convergence and geometry optimization; after obtaining a stable minimum, the frequencies were calculated. The calculations were carried out using density functional theory, on the basis of Stevens-Basch-Krauss-Jasien-Cundari (SBKJC) [12] parameterization. In this basic set only the valence electrons which are directly involved in chemical bonding are considered. DFT calculations were performed by using Becke's three parameter hybrid method [8] with Lee, Yang, and Parr (B3LYP) gradient corrected correlation functional [9] using the FireFly program packages [7]. The visualization of the spatial structures was carried out using Chemcraft. The adequacy of the proposed calculation method is confirmed by number of papers on this subject and convergence of calculated data with experimental results [5-6, 10-11].

3. RESULTS AND DISCUSSION

Obtained from *ab initio* method results for $\Delta E(T)$, $\Delta H(T)$, $\Delta G(T)$ in the temperature range $T = (100-1000)$ K for ZnX and $T = (50-700)$ K for CdX are approximated by linear functions of the form (6) (Table 1):

$$\Delta E(T)[\Delta H(T), \Delta G(T)] = a_i T + b_i, \quad (6)$$

and for ΔS :

$$\Delta S(T) = a_i \ln(T) - b_i. \quad (7)$$

Here, a_i and b_i are the constant coefficients that depend on the chemical composition of the MeX compound.

It should be noted that all defined thermodynamic parameters are increased with the temperature. However, at constant temperature, their absolute values are reduced in line MeS – MeSe – MeTe (Me = Zn, Cd), which logically explained by a change in lattice energy values and contribution of ionicity in the bond of the present line. The thermodynamic parameters of stoichiometric crystals can serve as references points for the synthesis of real non-stoichiometric crystals and for their operation.

Table 1 – The approximation coefficients (a_i, b_i) of the temperature dependences of thermodynamic parameters $\Delta E(T)[\Delta H(T), \Delta G(T)] = a_i T + b_i$ and $\Delta S(T) = a_i \ln(T) - b_i$ in zinc ($T = (100-1000)$ K) and cadmium ($T = (50-700)$ K) chalcogenide crystals ZnX, CdX (X = S, Se, Te)

| Thermodynamic parameter | ZnS | | ZnSe | | ZnTe | |
|--------------------------------|--------|---------|--------|--------|--------|--------|
| | a_i | b_i | a_i | b_i | a_i | b_i |
| Energy ΔE^* | 0.0633 | 197.79 | 0.0632 | 166.55 | 0.0636 | 115.35 |
| Entalphy ΔH^* | 0.0429 | 199.83 | 0.0441 | 168.12 | 0.0459 | 116.41 |
| Gibbs free energy ΔG^* | 0.3803 | 214.15 | 0.3744 | 185.32 | 0.3597 | 133.97 |
| Entropy ΔS^{**} | 44.525 | 170.39 | 43.033 | 166.66 | 40.098 | 165.53 |
| | CdS | | CdSe | | CdTe | |
| Energy ΔE^* | 0.1514 | 124.24 | 0.0566 | 91.556 | 0.0209 | 84.275 |
| Entalphy ΔH^* | 0.1378 | 114.46 | 0.0529 | 90.343 | 0.0147 | 84.045 |
| Gibbs free energy ΔG^* | 0.3116 | 132.22 | 0.2492 | 98.917 | 0.1334 | 84.327 |
| Entropy ΔS^{**} | 38.761 | 111.271 | 34.657 | 104.96 | 26.696 | 89.675 |

* $[\Delta E]$, $[\Delta H]$, $[\Delta G]$, $[b_i] = \text{kJ/mol}$, $[a_i] = \text{kJ}/(\text{mol} \cdot \text{K})$;

** $[\Delta S]$, $[b_i] = \text{J}/(\text{mol} \cdot \text{K})$, $[a_i] = \text{J}/(\text{mol} \cdot \text{K}^2)$.

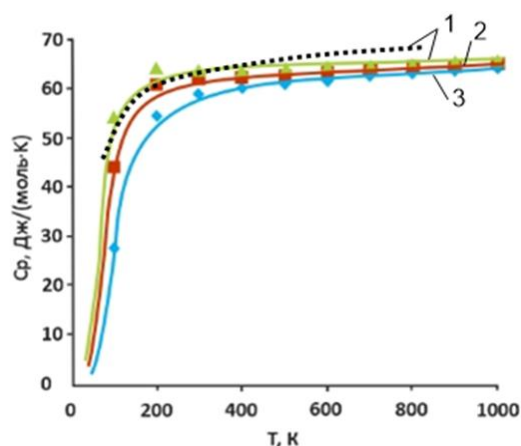


Fig. 2 – Temperature dependence of isobaric molar heat capacity C_p of zinc chalcogenides crystals (1 – ZnTe, 2 – ZnSe, 3 – ZnS): points are the first principle calculations, lines are the approximation of analytic functions (3), point curve is the experiment for ZnTe [13]

At low temperatures, the variance between the experimental results [13] and calculated approximation curve for C_p is less than 2 % (Fig. 2). In the sufficiently high temperatures, the experimental values of isochoric heat capacity slightly inflated relative to the theoretically calculated values that, for our opinion, logically explained by an anharmonicity oscillations of real crystal.

It should be noted that the results obtained on the basis of selected models for *ab initio* calculations are in good agreement in a wide temperature range as with the Debye and Einstein theory of heat capacity of solids and with the experimental data.

There are quite contradictory data about the polymorphism of zinc chalcogenides in the references. According to [14], the polymorphic transition "sphalerite-wurtzite" for ZnS occurs at $T_T = (1250-1450)$ K, and for ZnSe at $(1420-1713)$ K [15-16]. We were unable to find this information for ZnTe. Therefore, the evaluation of the characteristics of the polymorphic phase transition for zinc chalcogenides remains relevant.

Table 2 – Coefficients a_i , b_i , c_i of the temperature dependences approximation $C = a_i + b_i \cdot 10^{-3}T - c_i \cdot 10^5 T^{-2}$ of isochoric C_V and isobaric C_P heat capacities in ZnX ($T = (100-1000)$ K), CdX ($T = (50-700)$ K) (X = S, Se, Te) crystals

| Crystals | $C_V, \text{J}/(\text{mol}\cdot\text{K})$ | | | $C_P, \text{J}/(\text{mol}\cdot\text{K})$ | | |
|----------|---|---------|---------|---|---------|---------|
| | a_i^* | b_i^* | c_i^* | a_i^* | b_i^* | c_i^* |
| ZnS | 42.608 | 5.393 | 1.719 | 56.347 | 0.829 | 3.356 |
| ZnSe | 44.131 | 4.182 | 3.711 | 58.367 | 0.817 | 4.354 |
| ZnTe | 48.0859 | 0.14 | 1.033 | 60.760 | 0.418 | 3.706 |
| CdS | 24.0004 | 33.3837 | 0.0259 | 29.8814 | 36.450 | 0.0321 |
| CdSe | 37.888 | 23.470 | 0.240 | 47.100 | 20.998 | 0.036 |
| CdTe | 41.608 | 21.009 | 0.036 | 54.334 | 23.246 | 0.712 |

* $[a_i] = \text{J}/(\text{mol}\cdot\text{K})$; $[b_i] = (\text{J}/\text{mol}\cdot\text{K}^2)$; $[c_i] = (\text{J}\cdot\text{K}/\text{mol})$.

In order to calculate the "sphalerite-wurtzite" polymorphic phase transition temperature for ZnX crystals we also developed models for wurtzite structure. This structure was studied by using 3 models: C, D, and E. Cluster C (general formula $\text{Zn}_{15}\text{X}_{15}$, Fig. 1c) was the base for the calculation of the spatial and electronic structure and the thermochemical quantities. This model consists of 30 atoms and contains 2 pairs of 4-coordinated, 8 pairs of 3-coordinated, and 5 pairs of 2-coordinated atoms. Cluster D (the general formula $\text{Zn}_{11}\text{X}_{11}$, Fig. 1d) consists of 22 atoms. It contains 1 pair of 4-coordinated, 6 pairs of 3-coordinated, and 4 pairs of 2-coordinated atoms. Cluster E of wurtzite modification (with the general formula $\text{Zn}_{10}\text{X}_{10}$, Fig. 1e) consists of 20 atoms. It contains 1 pair of 4-coordinated, 4 pairs of 3-coordinated, and 5 pairs of 2-coordinated atoms. The clusters presented in Fig. 1, c, d, e are more stable and better reflect the structural properties of II-VI crystals in the hexagonal phase than in case of similar clusters with the boundary atoms [4].

For these cases, the Gibbs free energy will be defined as:

$$\begin{cases} 2\Delta G_4^* + 8\Delta G_3^* + 5\Delta G_2^* = \Delta G_C, \\ \Delta G_4^* + 6\Delta G_3^* + 4\Delta G_2^* = \Delta G_D, \\ \Delta G_4^* + 4\Delta G_3^* + 5\Delta G_2^* = \Delta G_E, \end{cases} \quad (8)$$

where the coefficients before ΔG_i^* correspond to the number of pairs of bonds with the coordination number equal to the index $i = 2, 3, 4$ at ΔG_i^* . ΔG_C , ΔG_D and ΔG_E are the Gibbs free energy of C, D, and E clusters respectively, which have been obtained from the computer calculations. Then ΔG_4^* is the required value for the Gibbs free energy of the crystal at the given temperature.

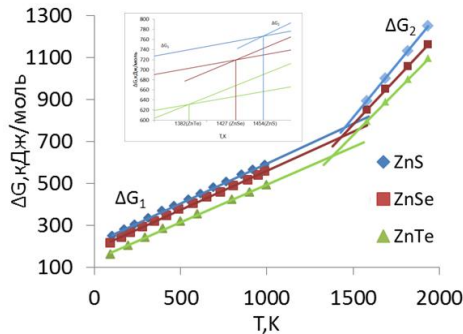


Fig. 3 – Temperature dependence of the Gibbs free energy of sphalerite ΔG_1 and wurtzite ΔG_2^i phases of ZnS, ZnSe, ZnTe crystals and the "sphalerite-wurtzite" phase transition temperatures T_T

The unknown integrated value of Gibbs free energy in the wurtzite phase will be equal to:

$$\Delta G_4^* = \frac{7\Delta G_C - 10\Delta G_D + \Delta G_E}{5}, \quad (9)$$

In the solid-solid transition of matter the Gibbs free energy must be the same value (Fig. 3). In our case, the point of intersection of the dependencies $\Delta G_1(T)$ and $\Delta G_2(T)$ ($\Delta G_1(T) = \Delta G_2(T)$) will be the temperature of the phase transition from sphalerite to wurtzite phases. According to our data, for ZnS $T_T = 1454$ K; for ZnSe $T_T = 1427$ K; for ZnTe $T_T = 1382$ K.

We can see that the phase transition temperature increases as we move from zinc telluride to selenide and to sulfide. This phenomenon was explained by the increase of the binding energy in ZnS-ZnSe-ZnTe line. Note that according to [15-16] the transition temperature of ZnSe is higher than the phase transition temperature for ZnS, which in our opinion is less regular. The obtained results of calculated "sphalerite-wurtzite" polymorphic phase transition temperatures for ZnS, ZnSe, ZnTe crystals are in good agreement with the data of paper [6].

4. CONCLUSION

Spent in the paper theoretical calculations of the important thermodynamic parameters of II-VI crystals allowed both to obtain new results and to clarify the known laws and substantiate their physical and chemical nature:

1. Based on the crystal and electronic structures of ideal stoichiometric zinc and cadmium chalcogenides ZnX, CdX (X = S, Se, Te) and paying attention to their physical and chemical properties, the cluster models for calculating the thermodynamic parameters for sphalerite and wurtzite have been proposed.

2. Using the first principles' calculations we defined: energy ΔE , enthalpy ΔH , Gibbs free energy ΔG , entropy ΔS for sphalerite phases of ideal stoichiometric crystals ZnS, ZnSe, ZnTe and CdS, CdSe, CdTe for a wide temperature range: (100-1000)K for ZnX and (50-700) K for CdX. These results can be used to predict properties of II-VI crystals during annealing.

3. The calculation of isochoric C_V and isobaric C_P molar heat capacities for stoichiometric crystals of zinc and cadmium chalcogenides and their temperature dependences approximated by the analytic functions $c = a + b \cdot 10^{-3} \cdot T - c \cdot 10^5 \cdot T^{-2}$, where a_i, b_i, c_i are the coefficients that depend on the structure and type of

materials. A correlation between the values of "a" and ion replacement in cationic and anionic sublattices has been established.

4. For stoichiometric crystals of zinc chalcogenides provided the equality of Gibbs free energy of sphalerite $\Delta G_1(T)$ and wurtzite $\Delta G_2(T)$ phases have been defined transition temperature of "sphalerite-wurtzite" that are falling in the line $\text{ZnS} \rightarrow \text{ZnSe} \rightarrow \text{ZnTe}$ and equal to

1454 K, 1427 K, 1382 K, respectively.

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Моделювання структури, термодинамічні властивості та температури фазових переходів кристалів II-VI

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У роботі запропоновано моделі кластерів поліморфних модифікацій – кубічного сфалериту і гексагонального вюрцититу для стехіометричних кристалів II-VI (ZnX , CdX ; $X = \text{S}$, Se , Te). Із використанням *ab initio* розрахунків обчислено величини термодинамічних параметрів за нормальних умов, визначено аналітичні вирази температурних залежностей енергії ΔE та ентальпії ΔH , вільної енергії Гіббса ΔG , ентропії ΔS для сфалеритних фаз стехіометричних кристалів цинк і кадмій халькогенідів. Розраховано температурні залежності теплоємності при сталому тиску C_P і при сталому об'ємі C_V , визначено температури фазового переходу "сфалерит-вюрцит" для кристалів ZnTe , ZnSe , ZnS .

Ключові слова: Квантово-хімічні розрахунки, Кластерні моделі, Термодинамічні параметри, Халькогенідні кристали.

Моделирование структуры, термодинамические свойства и температуры фазовых переходов кристаллов II-VI

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На основе кристаллографических параметров и электронного строения идеальных стехиометрических кристаллов цинк и кадмий халькогенидов ZnX , CdX ($X = \text{S}$, Se , Te) разработаны модели кластеров для сфалеритной и вюрцитной фаз, с использованием которых вычислены энергия ΔE , энтальпия ΔH , свободная энергия Гиббса ΔG и энтропия ΔS кубических идеальных стехиометрических кристаллов ZnS , ZnSe , ZnTe и CdS , CdSe , CdTe . Осуществлен расчет и сравнение с экспериментом изохорной C_V и изобарной C_P молярных теплоемкостей стехиометрических кристаллов цинк и кадмий халькогенидов. Из полученных температурных зависимостей свободная энергия Гиббса определены температуры полиморфных фазовых переходов «сфалерит-вюрцит».

Ключевые слова: Квантово-химические расчеты, Кластерные модели, Термодинамические параметры, Халькогенидные кристаллы.

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