



Review

Method of the correlative optimization of heat capacities of isostructural compounds

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ARTICLE INFO

Article history:

Received 23 August 2012

Received in revised form 14 October 2012

Accepted 17 October 2012

Available online 29 October 2012

Keywords:

Semiconductors

Heat capacity

Thermodynamic properties

Computer simulation

ABSTRACT

A semi-empirical approach to the critical analysis of thermodynamic data is proposed and applied in this work. As an example, sets of numerous experimental and calculated heat capacity values of 16 isostructural $A^{III}B^V$ compounds were taken from the literature. A critical analysis of heat capacities of 16 $A^{III}B^V$ compounds was then made based on the correlative optimization method. As a result, a set of mutually agreed equations $C_p^c = a + b \cdot 10^{-3} - c \cdot 10^5 \cdot T^{-2}$ was proposed to describe the heat capacities of these phases. Two continuums of relations $C_p(T)$ vs. logarithm of the sum of atomic numbers of elements A and B were obtained for the $A^{III}B^V$ phases, of both sphalerite and wurtzite types, in the temperature range from 260 to 1500 K. Based on the proposed equations, heat capacity values were predicted for the previously unstudied (or poorly studied) phases TiN and AlP within the temperature ranges from 260 to 1018 K from 260 to 1500 K, respectively. The proposed correlative method of thermodynamic functions can be applied to other different groups of isostructural organic and inorganic compounds.

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1. Introduction

Semiconductors based on the $A^{III}B^V$ phases have a wide-ranging spectrum of attractive physical properties. They are widely used in the domains of linear and nonlinear optics, solar cells, light-emitting diodes, laser diodes, integral optical devices, etc. [1]. The detailed and accurate knowledge of thermodynamic values of various $A^{III}B^V$ phases permits to optimize the heat balance during the growth of their single crystals or epitaxial structures from gas phase, thus advancing the technology and devices based on such materials.

A new approach of mutual coherence of the thermodynamic data for isostructural phases has been recently applied to $A^{III}B^V$ phases with the sphalerite and wurtzite structures [2]. Examined correlations have been used to obtain the optimized standard thermodynamic functions based on reduced enthalpies $\Delta_f H_{298}^0/T_m$, the reduced Gibbs energies of formation $\Delta_f G_{298}^0/T_m$ and the sum of atomic numbers of elements $Z_i = (Z_A + Z_B)$ of 16 $A^{III}B^V$ phases. Besides, the correlation between standard entropies and the sums of atomic numbers have been demonstrated [2]. The calculation of the thermodynamic functions of individual compounds at high temperatures is not possible without knowing their heats capacities. At present, numerous reference data available from different sources are to some extent unreliable, as their origin is often not given or explained in detail to the reader and the criteria of their selection are often not clear. In early work [3], Gorbov made a deep

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and comprehensive analysis of the literature on the thermodynamic characteristics of $A^{III}B^V$ phases (except for nitrides) up to 1973. However, since then much new information on heat capacities of $A^{III}B^V$ compounds has been published [4–32] which was not covered by Gorbov's work [3]. In a recent paper, Pashinkin and coauthors [4] analyzed the high-temperature heat capacities of phosphides, arsenides and antimonides of gallium and indium, and re-measured the specific heat of indium phosphide from 298 K to 800 K. Pashinkin and coworkers [4] have analyzed high-temperature heat capacities of Ga and In phosphides, arsenides and antimonides, both from the literature [7,8] and obtained in their studies [4,5,30], and re-measured the specific heat capacity of indium phosphide between 298 and 800 K. The compounds of aluminum and boron, as well as of IIIB subgroup nitrides, were not considered in [4].

In the present work, we carried out a critical analysis of the heat capacities of $A^{III}B^V$ phases of both sphalerite and wurtzite types. We found that the low-temperature (below 298 K) heat capacities of such isostructural phases with the same sum of atomic numbers of constituent elements are not different from each other within the accuracy of experimental measurement. This approach was extended from room temperature to melting points of the studied phases. Numerical data on heat capacities for $A^{III}B^V$ phases available in the literature have been analyzed with the assumption that the properties of the phases should also be similar at high temperatures, and the phases have no phase transformations in solid state. As a result, a set of linear isotherms of heat capacities vs. the sum of atomic numbers of the constituents A and B was obtained. In addition, the data selection criteria proposed in the present study allowed us to calculate and present the values of heat capacities through equations $C_p^o = a + b \cdot 10^{-3} - c \cdot 10^5 \cdot T^{-2}$ for all the phases $A^{III}B^V$ except for hBN. As for hexagonal boron nitride a polynomial $C_p^o = a + b \cdot 10^{-3} - c \cdot 10^5 \cdot T^{-2} + d \cdot 10^3 \cdot T^{-1}$ was used. The equation for hexagonal BN was obtained by the least-squares method. We used Gavrichiev's and Landolt-Bernstein's data with equal weights. All points are shown in Fig. 1. Similarly, all the points have been used in other figures, except for cases mentioned otherwise. The values of errors for heat capacities were taken on the basis of optimized values of isotherms C_p^o ($\ln Z_i$). Obtaining

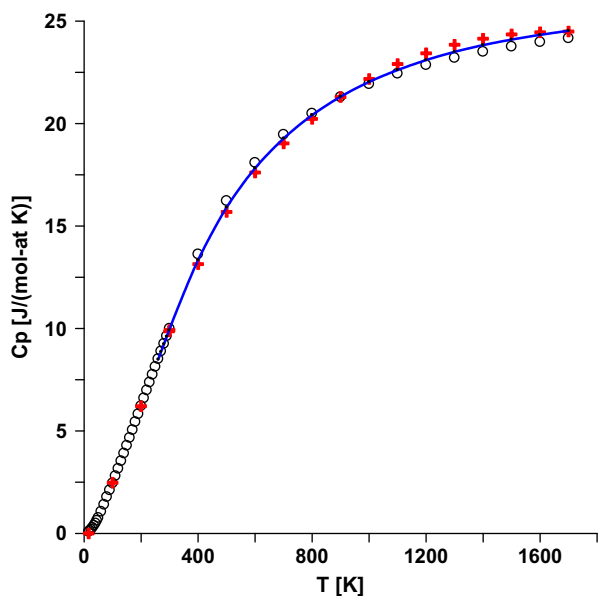


Fig. 1. Heat capacity of hBN vs. temperature. ○ denotes data from Refs. [9,10], ● denotes data from Ref. [6], — denotes optimized values.

and accumulating of missing thermochemical values remains one of the major problems of modern thermodynamics, and therefore, the development of thermodynamic computational and correlative methods have high importance.

2. Literature results and their discussion

In general, the thermochemical experiment involves two separate and independent aspects, each being equally important. First of them is the apparatus, or calorimeter, which is designed to measure the energy received by the sample in study as accurately as possible. Here, potential problems are solved by using an optimum device design and applying precise measuring tools [35]. The second aspect of thermochemical experiments can be conventionally referred to as “chemical” as it is all about describing accurately the initial and final states of the studied system, so that the required accuracy level is satisfied. This implies that any heats of secondary processes (which are always present in the calorimetric experiment) should be considered as carefully as possible, and therefore processes such as oxidation, evaporation, decomposition, as well as any chemical interaction between the studied sample and the container, are to be maximally limited. In this work, the critical analysis of heat capacities for $A^{III}B^V$ phases was carried out for 16 compounds, which totaled at more than 1200 points. The analyzed sets of values are presented in Figs. 1–8, given the assumption that all the phases with the same sum of atomic numbers of elements A and B should be similar both at low and high temperatures. Lichter and Sommelet were first to point at the similarity of heat capacities for $A^{III}B^V$ phases [7]. Studying two groups of phases with similar molecular masses (first group: AlSb, GaAs and InP; and second group: GaSb and InAs), they noticed similar temperature dependencies of heat capacities vs. molecular masses of $A^{III}B^V$ within the groups (at $T > 298$ K).

We have developed this rule and established that the experimental heat capacities of phases like BP and AlN ($Z_i = 20$), BAs and GaN ($Z_i = 38$), AlAs and GaP ($Z_i = 46$), AlSb, GaAs and InP ($Z_i = 64$), GaSb and InAs ($Z_i = 82$), i.e. having same sums of atomic numbers of elements (Z_i), are equal within all temperature ranges where the solid phases exist. Molecular masses of $A^{III}B^V$

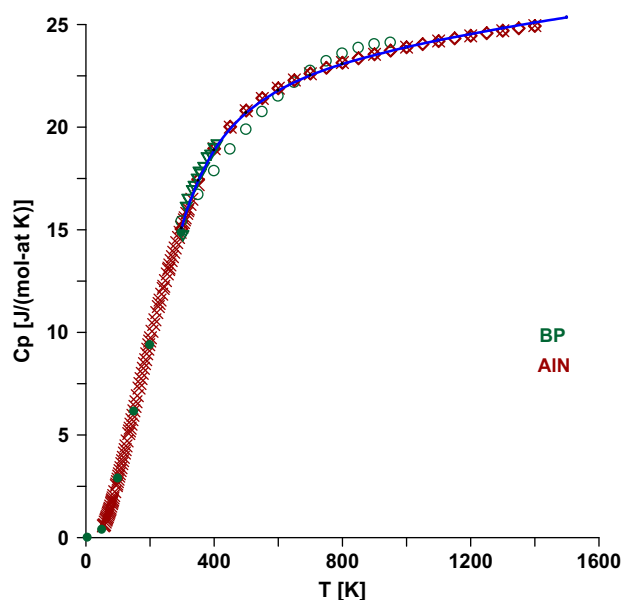


Fig. 2. Heat capacity of BP and AlN ($Z_i = 20$) vs. temperature. BP: ● – [11], ○ – [12], ▽ – [13]; AlN: × – [11], ◇ – [14]; — optimized values. The experimental heat capacities of BP from Refs. [11,13] are only used in the ranges 5–298 and 302.3–357.2 K, respectively.

compounds are related to the sum of atomic numbers of their constituent elements, (Z_i). In the present study, we show that all isotherms of the heat capacities have strict linear correlations vs. the logarithm of the sum of atomic numbers of elements A and B for isostructural $A^{III}B^V$ phases of both the sphalerite and wurtzite types. Figs. 1, 2 and 5–7 show that low-temperature heat capacities coincide within the experimental error. Therefore, one can assume that the behavior of specific heat capacities of isostructural $A^{III}B^V$ phases with the same atomic numbers of constituent components will also be similar at temperatures above room temperature. As seen in Fig. 3, one of the biggest discrepancies in the previously reported data on heat capacities (± 2 J/(mol-at-K)) is observed above 300 K for GaN and BAs compounds (both having $Z_i = 38$). The variance of the data for the same phases in the low-temperature region (see Fig. 3) is ± 1 J/(mol-at-K). The observed discrepancies might be caused by the presence of other crystalline admixtures in the BAs sample. For example, Gavrichev and coworkers have reported on four different crystalline modifications of boron nitride [9,10].

At high temperatures, one faces problems of a different nature, i.e. those related to sample's volatility, decomposition, interactions with the container, and others that are often very difficult to account for. In particular, it is necessary to take into consideration the significant vapor pressure of the group five elements (N, P, As, Sb) and their compounds with those of group three (B, Al, Ga, In), especially at high temperatures. Among the numerous $A^{III}B^V$ phases analyzed in this study, the most contradictory thermodynamic data were reported for nitrides, phosphides and arsenides, which is believed to be directly related to the volatility issue.

Phosphorus, arsenic and their compounds with the elements of subgroup IIIB are known to have a high vapor pressure. The effect of decomposition and evaporation of phosphides and arsenides is also considerable, especially at elevated temperatures. Fig. 6 (curve b) shows the vapor pressure of InP as a function of temperature. In addition, some compounds, such as AlP and AlAs, are readily hydrolyzed in air. It is also necessary to take into account the aggressive elements, such as arsenic and phosphorus, which easily interact with almost all elements, especially at high temperatures.

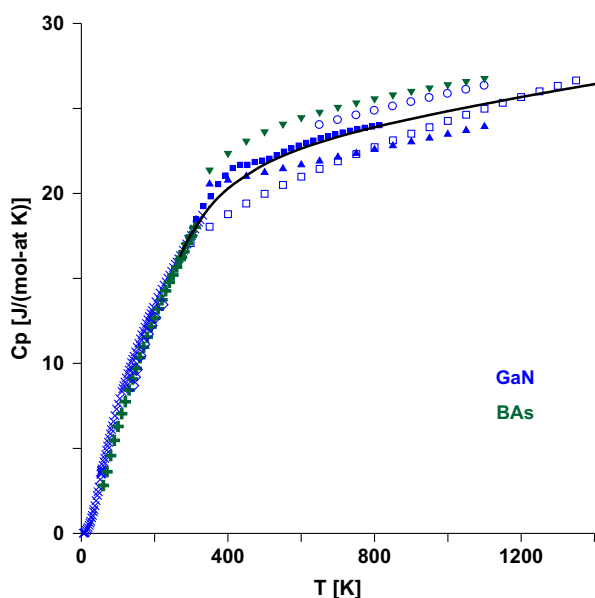


Fig. 3. Heat capacity of BAs and GaN ($Z_i = 38$) vs. temperature. GaN: \times – [15], \circ – [16], \diamond – [17], \blacktriangle – [6], \square – [18], \blacksquare – [19]; BAs: \blacktriangledown – [6], $+$ – [20]; – optimized values. The experimental heat capacities from Ref. [17] are only used in the range 140–220 K.

The nitrides of group IIIA elements are known to begin decomposing and losing nitrogen at temperatures well below their melting points, and therefore the liquidus curve in their T - x phase diagrams deviates from the maximum melting point toward a nonvolatile component [18]. To maintain equilibrium in such a nitrogen system, the melting point of the nitride should be determined at high nitrogen pressures from 6 to 10 GPa. As an example, the Ga-N system was investigated and described by Unlande et al. [18], and results are presented in Fig. 10.

The decomposition of InN during measurements was clearly manifested in [20], where, unlike the other works, the heat capacity of InN was reported to be almost constant in the entire temperature range, as seen in Fig. 4 (solid triangles). While at room temperature, the data in [20] are consistent with those from other works (Fig. 4), the decomposition of InN above from 350 to 400 K was very likely the reason for the ambiguous results observed in Fig. 4 (solid triangles). At the same time, the data obtained by the same group of authors for GaN (presented in Fig. 3) [19] are consistent with the optimized values of the specific heat capacity of this compound, which also implies some experimental errors (or decomposition) in the work [20].

The literature data available on heat capacity of AlP are seen in Fig. 9 not to be well consistent. There is a considerable difference between the data in [6,16,26,31]. The results in [31] can only be regarded as estimates. As stated above, this compound is easily hydrolyzed in air and obtaining reliable experimental data is very difficult. The difference between the accepted values $C_p^o(T)$ in handbook [6] and experimental values in works [16,26] reaches 4 J/(mol-at K). This exceeds even the largest difference observed for the compounds BAs and GaN with ($Z_i = 38$) observed from room temperature to 1400 K (Fig. 3) and could probably originate from experimental errors during measurements or different purity of the analyzed samples. The predicted dependence of $C_p^o(T)$ for AlP (thick line in Fig. 9) will be explained in greater detail below.

Theoretical calculation of temperature dependencies of heat capacities for GaN and InN was made in work [32]. The authors [32] used the properties of AlN as a model. The comparison of

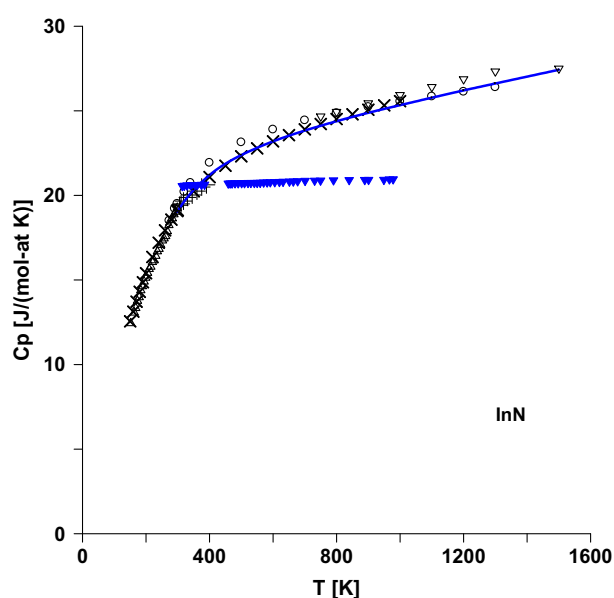


Fig. 4. Heat capacity of InN ($Z_i = 56$) vs. temperature. $+$ – [22] (experimental), \times – [22] (calculated), \circ – [23], ∇ – [24], \blacktriangledown – [20], – optimized values. The experimental heat capacities from Ref. [20] were not used in this study since the errors of the results exceed the confidence interval accepted for the compounds.

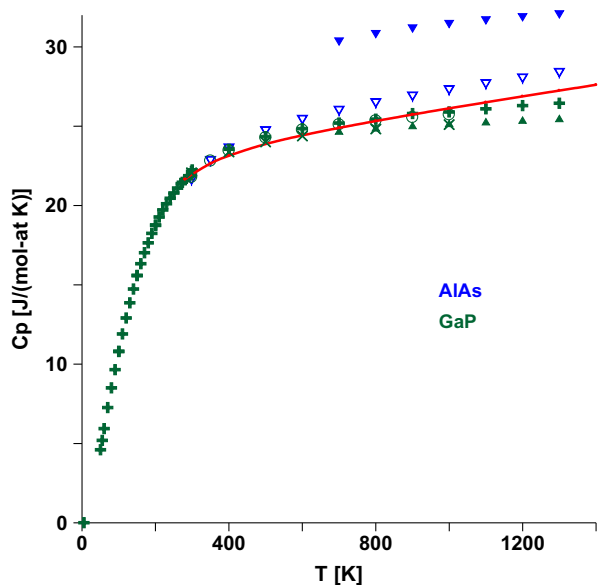


Fig. 5. Heat capacity of AlAs and GaP ($Z_1 = 46$) vs. temperature. AlAs: ∇ – [6], \blacktriangledown – [16]; GaP: \times – [5], \blacktriangle – [16], $+$ – [21], \circ – [27]; – optimized values. The experimental heat capacities of GaP from Ref. [16] were not used in this study since the errors of the results exceed the confidence interval accepted for the compounds. For the same reason, the data from Ref. [5] were only used in the range 298–800 K.

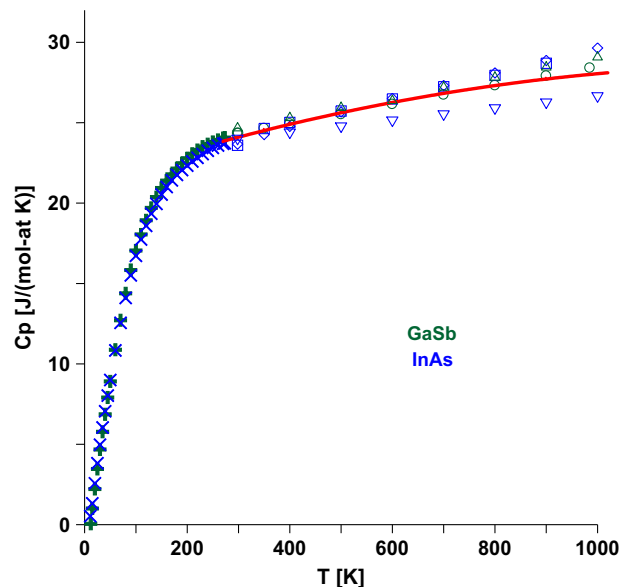


Fig. 7. Heat capacity of GaSb and InAs ($Z_1 = 82$) vs. temperature. GaSb: \triangle – [6], \circ – [7], $+$ – [28]; InAs: ∇ – [6], \square – [7], \times – [28], \diamond – [30]; – optimized values.

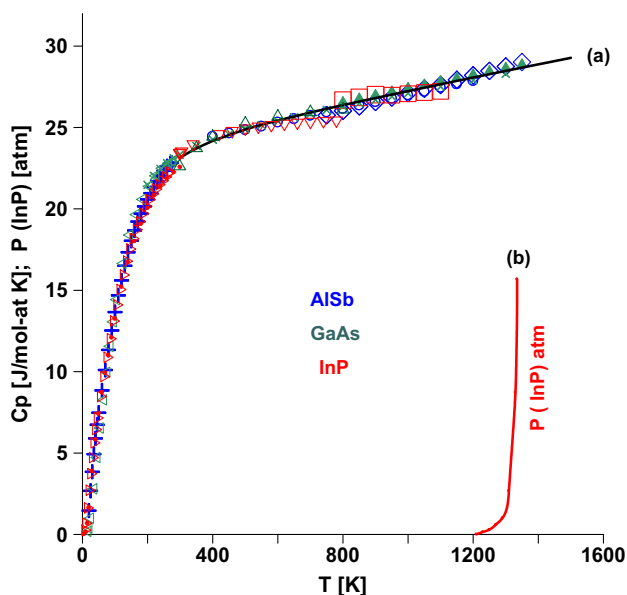


Fig. 6. Heat capacity of AlSb, GaAs and InP ($Z_1 = 64$) vs. temperature. AlSb: \circ – [7], \diamond – [16], $+$ – [28]; InP: \triangle – [4], \square – [16], ∇ – [27], \triangleright – [28], \bullet – [29]; GaAs: \times – [4], ∇ – [16], \triangleleft – [28]; – optimized values. (a) Heat capacities and (b) vapor pressure for InP, in atmospheres.

our results and those of Marmallyuk and co-workers [32], which were obtained via two independent methods, shows good agreement within the range of acceptable experimental errors (Fig. 11). The maximum difference in C_p° values is seen to be ± 0.6 J/(mol-at K) for GaN and 0.8 J/(mol-at K) for InN (at temperatures as high as 1500 K).

If we turn to the Table 1 and calculate the heat capacities ($C_p^\circ(T)$) of $A^{III}B^V$ phases near their maximum temperatures in solid state (point of fusion) we can plot a correlation between the heat capacities and the temperatures of fusion for all compounds (line a) except

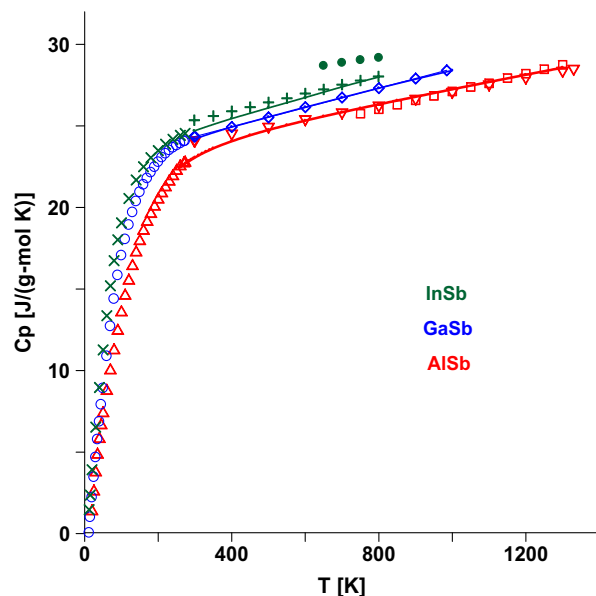


Fig. 8. Comparison of heat capacity of Al, Ga and In antimonides vs. temperature. InSb: $+$ – [7], \times – [28], \bullet – [16]; GaSb: \diamond – [7], \circ – [28]; AlSb: ∇ – [7], \square – [16], \triangle – [28]; – optimized values. The experimental heat capacities of InSb from Ref. [16] were not used in this study since the errors of the results exceed the confidence interval accepted for the compounds.

of boron's compounds and thallium nitride (line b). It is seen that the determination of heat capacities at high temperatures (above 1200 K) with the accuracy of ± 1 J/(mole-at-K) is quite realistic for these compounds (see correlation (a) in Fig. 12). The correlation (a) and (b) in Fig. 12 can be described by Eqs. (1) and (2) given below:

$$C_p = 27.28 + 8.50 \cdot 10^{-4} \cdot T_m; r = 0.77, 2S_0 = \pm 1 \text{ J/(mol-at K)} \quad (1)$$

$$C_p = 26.13 - 3.17 \cdot 10^{-4} \cdot T_m; r = 0.95, 2S_0 = \pm 0.25 \text{ J/(mol-at K)} \quad (2)$$

The concept of linear dependence of the heat capacity vs. the sum of atomic numbers follows from the previous deduction as result of optimization and permits to order the experimental and

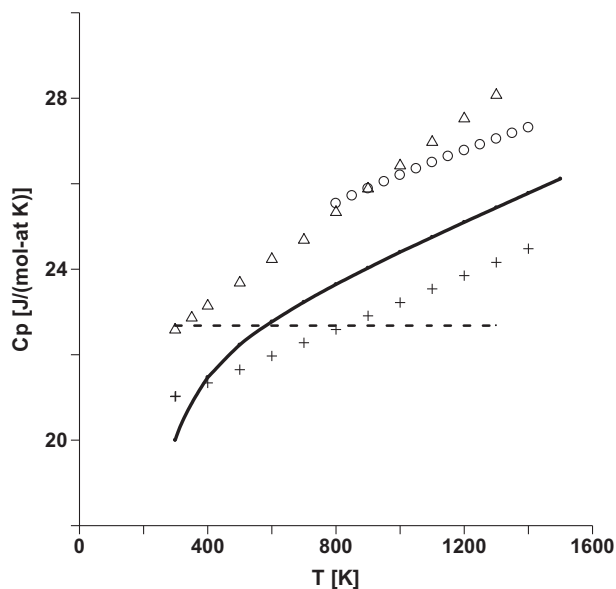


Fig. 9. Heat capacity of AlP vs. temperature (298–1500 K): + – [6], o – [16], Δ – [26], --- [31]; – our prediction.

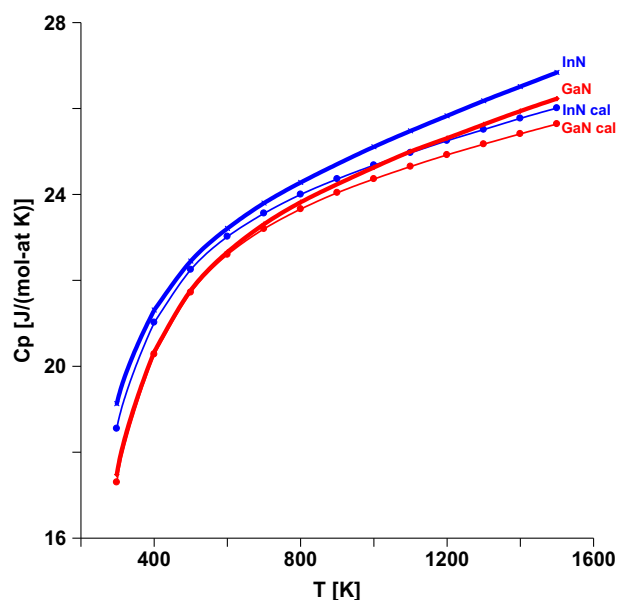


Fig. 11. Comparison of $C_p(T)$ for gallium and indium nitrides [31] (thin lines with points) and our results (thick lines) at 298–1500 K.

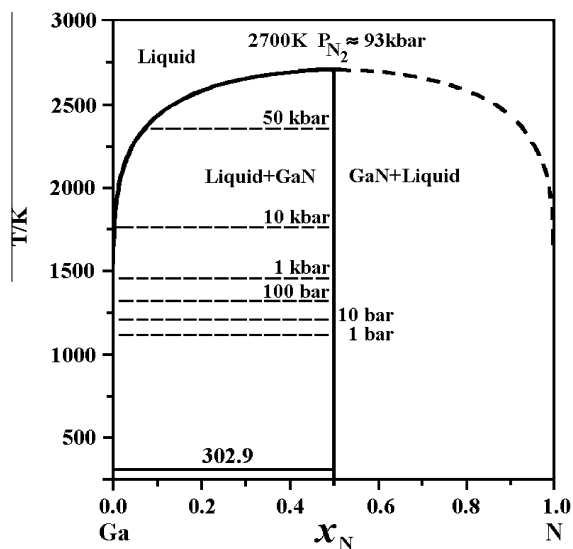


Fig. 10. Calculated phase diagram of the Ga–N system [18].

calculated values. The slope of the isotherms changes from higher to lower values with increasing temperature. (Figs. 13a and 14a). The term ‘mutual agreement of heat capacity’ was adopted because we used all the experimental and theoretical data available in the literature, and the results were mutually consistent, without conflicting each other, in contrast to the original data set. Examining all the values $C_p^o(T)$ for the 16 $A^{III}B^V$ phases (presented in Table 1) as a function of the sum of atomic numbers or their constituents ($Z_i = Z_A + Z_B$), two continuums of linear relations (correspondingly for the sphalerite and wurtzite types) can be obtained for each temperature. These relations are presented in Fig. 13 (sphalerite phases) and Fig. 14 (wurtzite phases) for some temperatures from 298 K to 1500 K. The equations describing heat capacities and previously presented as optimized data in Figs. 1–8 were obtained by the least-squares method and are given in Table 1. The equations for $C_p^o(T)$ of the insufficiently studied phase AlP and unstudied phase TiN were obtained by the linear extrapolation of relations

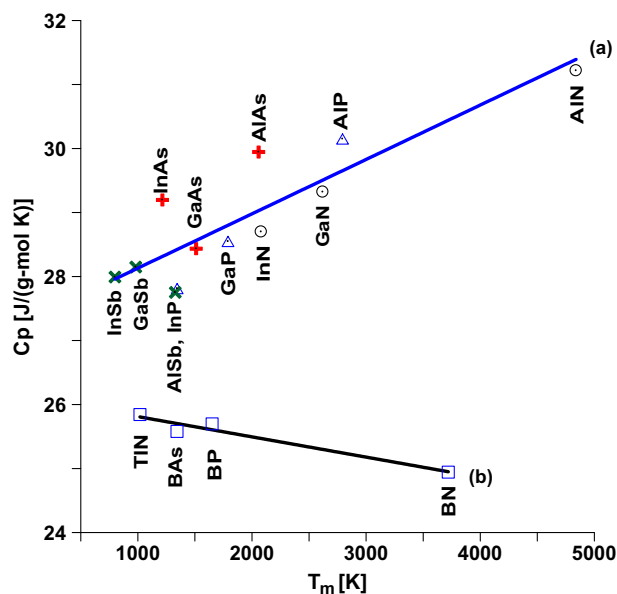


Fig. 12. Correlation between heat capacities (C_p) of $A^{III}B^V$ phases in solid state near their temperature of fusion.

$C_p^o(Z_i)$ for the series of arbitrary temperatures (see Figs. 13 and 14) and are also presented in Table 1. The equation for $C_p^o(T)$ of AlP was calculated independently from literature data reported elsewhere [6,16,31].

The maximum discrepancy of the relations $C_p^o(T)$ vs. the logarithm of the sum of atomic numbers of constituent elements of phases $A^{III}B^V$ is seen in Figs. 13 and 14 to be smaller than ± 0.3 J/mol-at-K, provided that all the crystal phases are well ordered and there are no phase transformations within all temperature regions of their existence in solid state. We took the discrepancy for all equations $C_p^o(T)$ in Table 1 equal to ± 0.3 J/(mol-at-K). The values $C_p^o(T)$ between 1200 and 1600 K are accepted with the accuracy of ± 0.3 – 0.5 J/(mol-at-K), while above 1700 K the discrepancy reaches ± 0.6 – 1.0 J/(mol-at-K). It is recommended to use the greatest errors

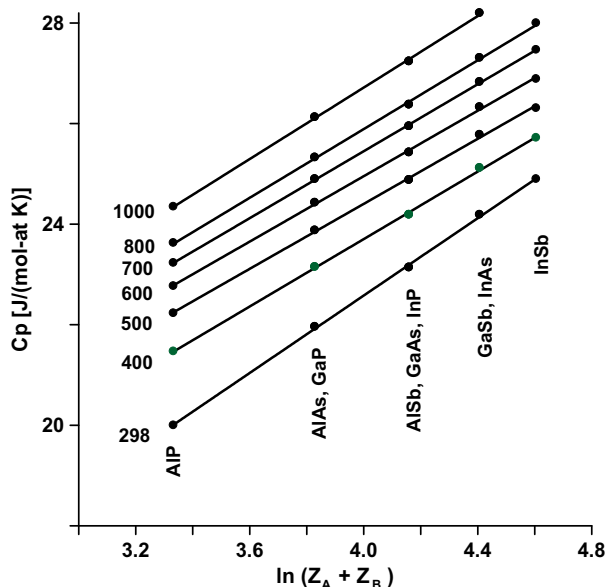


Fig. 13a. $C_p(T)$ vs. logarithm of the sum of atomic numbers of elements for $A^{III}B^V$ phases of the sphalerite type at 298–1000 K.

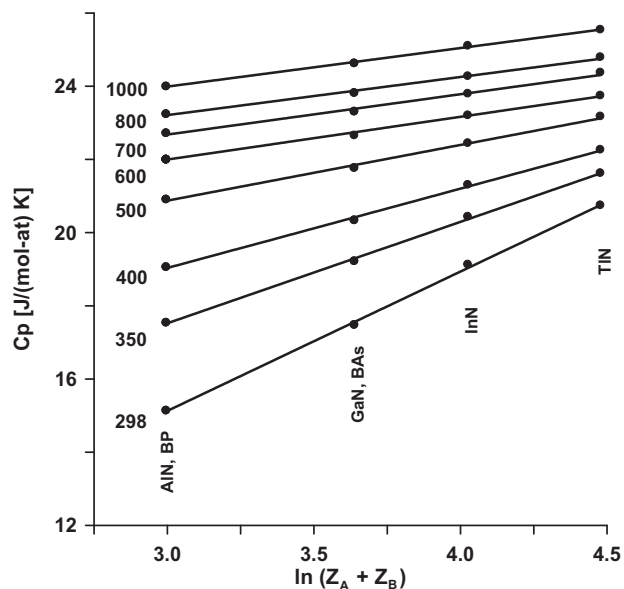


Fig. 14a. $C_p(T)$ vs. logarithm of the sum of atomic numbers of elements for $A^{III}B^V$ phases of the wurtzite type at 298–1000 K.

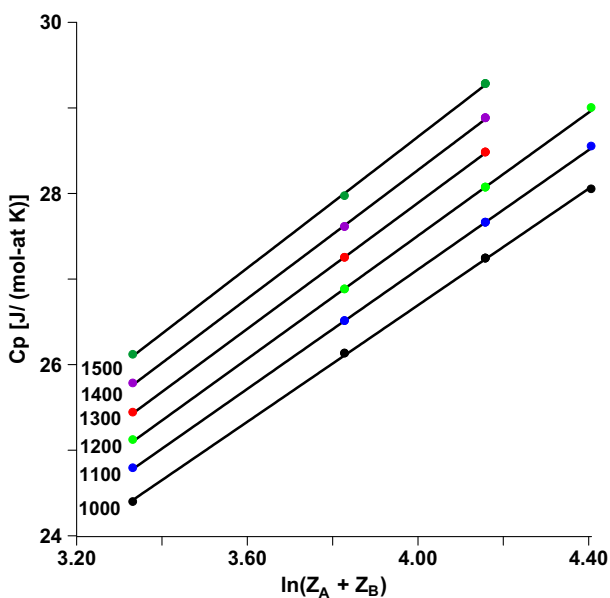


Fig. 13b. $C_p(T)$ vs. logarithm of the sum of atomic numbers of elements for $A^{III}B^V$ phases of the sphalerite type at 1000–1500 K.

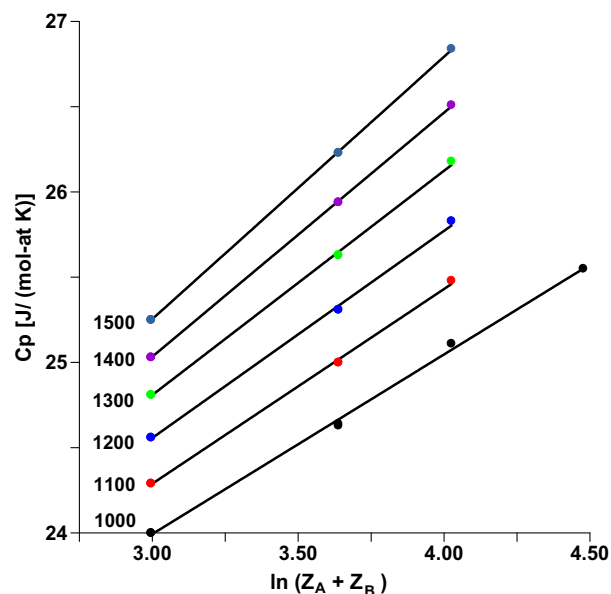


Fig. 14b. $C_p(T)$ vs. logarithm of the sum of atomic numbers of elements for $A^{III}B^V$ phases of the wurtzite type at 1000–1500 K.

of $C_p^0(T)$ for gallium and aluminum arsenides and aluminum phosphide (see Fig. 12, correlation (a)).

As mentioned earlier, the measurements of the heat capacities of arsenides and phosphides pose numerous experimental problems at high temperatures above 1200 K, when the vapor pressures of these compounds are as high as several atmospheres and it is necessary to take into consideration the high chemical activity of As and P (as active and highly reactive elements).

Based on the above results, it is now possible to calculate all thermodynamic values of all the phases listed in Table 1 at high temperatures using the optimized values $\Delta_f H_{298}^0$, S_{298}^0 , $\Delta_f S_{298}^0$, and $\Delta_f C_{298}^0$ taken from work [2] and the well-known general thermodynamic relations previously given in [8]:

$$\Delta_f G_T = \Delta_f H_{298}^0 + \int_{298}^T \Delta C_p dT - T \Delta S_{298}^0 - T \int_{298}^T (\Delta C_p / T) dT \quad (3)$$

The equation VII in Table 1 was obtained based on the recent data of Pashinkin et al. for InP [4]. The new numerical values of the heat capacities of AlSb, GaAs, and InP (Table 1) are very close to those accepted in Ref. [2] which were described for the temperature range 260–1500 K by: $C_p^0(T) = 23.09 + 4.275 \cdot 10^{-3} \cdot T - 1.173 \cdot 10^{-5} \cdot T^2$. J/(mol-at K) without the Ref. [4]. The calculation of Gibbs energies at high temperatures using the previously reported results $\Delta_f G_{298}^0(\text{InP}) = -29.55 \pm 0.8 \text{ kJ/mol-at}$ and $\Delta_f G_{298}^0(\text{InSb}) = -13.02 \pm 0.3 \text{ kJ/mol-at}$ (both from Ref. [2]) and the proposed equations (VII) and (X) (Table 1) gives the values of $\Delta_f G_T^0$ within experimental errors for all experimental ranges 657–766 K [33] and 498–600 K [34]. The calculation was performed according to the standard procedure described in [8].

Table 1
Heat capacities of A^{III}B^V phases.

No.	Phase and its melting point (T_m , K [2])	$Z_A + Z_B$	$C_p^0 = a + b \cdot 10^{-3} - c \cdot 10^5 \cdot T^{-2} + d \cdot 10^3 \cdot T^{-1}$; in J/(mol-at K)				Temperature range, K
			a	b	c	d	
I	BN _{hex} (3720)	12	31.55	−1.093	−8.785	−9.300	260–1500
II	BP (1650); AlN (4840)	20	23.08	1.688	7.500		260–1500
III	AlP (2793)	28	21.34	3.239	1.838		260–1500
IV	BAs (1343); GaN (2620)	38	22.53	2.621	5.181		260–1500
V	AlAs (2058); GaP (1790)	46	22.79	3.505	1.665		260–1500
VI	InN (2080)	56	22.42	3.060	3.738		260–1500
VII	AlSb (1328); GaAs (1511); InP (1344)	64	23.43	3.941	1.303		260– T_m
VIII	GaSb (981); InAs (1215)	82	24.00	4.332	0.976		260– T_m
IX	TlN (1018)	88	22.49	3.331	2.473		260– T_m
X	InSb (799)	100	23.44	5.774	0.394		260– T_m

3. Conclusions

Critical analysis of the heat capacities of 16 A^{III}B^V compounds was made by using the method of correlative optimization. Two continuums of relations for both sphalerite and wurtzite forms of the compounds were obtained for each temperature within the temperature range from 298 to 1500 K. The values of heat capacity of thallium nitride between 298 and 1018 K and aluminum phosphide between 298 to 1500 K were predicted. The present results can be used for thermodynamic calculations of quasi-binary and quasi-ternary solid solutions based on the A^{III}B^V compounds, as well as for thermodynamic databases. The knowledge of obtained high temperature thermodynamic values also permits to optimize the heat balance of single-crystal growth and epitaxial structure growth from gas phases, which is of demand in the field of optoelectronic material technology. The proposed correlative method of thermodynamic functions can also be applied to other different groups of isostructural organic [35,36] and inorganic compounds [2,37].

Acknowledgements

This work was financially supported by the Russian Foundation for Fundamental Research (RFFI, project 11-08-01154). We would also like to thank Prof. J.P. Bros (Provence University, France) for helpful discussions.

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