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Original scientific paper

CLARIFICATION OF THE DESCRIPTION OF THE HIGH-TEMPERATURE HEAT CAPACITY OF PHASES WITH WURTZITE AND SPHALERITE STRUCTURES

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Abstract

The description of the experimental data $C_p(T)$ of substances in the solid state was carried out separately for phases with wurtzite (hexagonal) and sphalerite (cubic) structures. The fitting parameters of the multiparameter function (X), where X = {T_o, a, b, A_1, A_2, Θ_1, Θ_2} are different for different structures. The X parameters, in turn, are a function of the atomic number of the fourth group element or half the sum of the atomic numbers of the $A^{III}B^{V}$ or $A^{II}B^{VI}$ binary phases, while the element germanium has a specific point for the X parameters vs. atomic number. In this case, either a breakpoint or an inflection point attributable to germanium is observed for parameter dependencies on Ln(N). The high-temperature coefficient b occupies a special position which, which, within the limits of experimental errors, has the same values for both structural types. The coefficient b has no effect on the low-temperature region of $C_p(T)$.

***Keywords**: optimization, heat capacity, wurtzite, sphalerite*

1. INTRODUCTION, MODEL and RESULTS

Analysis of the coefficients of the multiparameter function [1, 2] carried out for the Debye-Maier-Kelley model $\sigma^2(T_0, X) = \sum_{i=1}^{n}\left(C_p(X) - C_p^{(exp)}(T_i)\right)^2 / n$ (1)

where the independent adjustable parameters (*X*) of the function (1) is

$$X=\{T_0,a,b,A_1, A_2,\Theta_1,\Theta_2\} \text{ with } A_1,A_2\geq 0 \text{ and } A_2 = 1 - A_1$$

Equation 1 is suitable for describing both the heat capacity of phases with the sphalerite and wurtzite structures. At the same time, the coefficient (b), responsible for describing the heat capacity $C_p(T)$ of the high-temperature region for both types of structures, showed that these coefficients do not differ from each other within the limits of experimental errors.

Tables 1 and 2 show the coefficients of the multiparameter function (1). These coefficients' dependence on the natural logarithm of N (Ln(N)) is shown for each coefficient in both types of structures. In this paper, Fig. 1 shows the new values of the coefficients (b). For each value of Ln(N), the coefficient (b) for both types of phases lies within the experimental errors. The other coefficients mentioned remained unchanged. As an illustration, Fig. 2-4 shows the heat capacity graphs $C_p(T)$ for AlN, Si (AlP) and TlN.

Table 1. Coefficients of the multiparameter function (1) sphalerite structure

Phase	Ln(N)	a ±0.003	$b \cdot 10^{-3}$ ±0.1	T_0 ±1	Θ_1 ±1	Θ_2 ±1	A_1 ±0.001	C_{p298} J/mol-at K (±0.02)
Diamond	1.79176	24.943	0.222	1350	1850	1944	0.479	5.89
AlN	2.30259	24.455	1.702	1031	500	1075	0.389	17.38
Si,AlP	2.63906	24.211	2.346	825	341	847	0.361	19.96
GaN	2.94444	24.042	2.792	629	253	695	0.351	21.53
GaP, AlAs	3.13549	23.959	3.021	513	216	617	0.348	22.22
InN	3.33220	23.894	3.226	395	190	537	0.347	22.93
Ge, GaAs	3.46574	23.860	3.34	320	185	483	0.347	23.28
InAs, GaSb	3.71357	24.398	3.261	251	145	384	0.351	24.19
TlN	3.78419	24.570	3.206	232	134	356	0.355	24.45
HgS	3.87120	24.808	3.126	210	121	323	0.360	24.79
Sn	3.91202	24.938	3.084	200	115	307	0.363	24.95
HgSe	4.04305	25.393	2.930	167	96	257	0.374	25.52
NhN	4.09434	25.604	2.860	154	88	237	0.379	25.77
HgTe	4.18965	26.049	2.709	131	75	201	0.390	26.27
Pb	4.40672	27.353	2.201	80	45	121	0.418	27.70
Fl	4.74620	30.37	0.508	3	0.4	0.5	0.475	30.52

Table 2. Coefficients of the multiparameter function (1) wurtzite structure

Phase	Ln(N)	a ±0.003	$b \cdot 10^{-3}$ ±0.1	T_0 ±1	Θ_1 ±1	Θ_2 ±1	A_1 ±0.001	C_{p298} J/mol-at K (±0.02)
BN	1.79176	24.33	0.222	1137	1400	1730	0.400	8.31
AlN	2.30259	22.75	1.702	920	650	1235	0.364	15.07
Si	2.63906	22.54	2.346	777	550	1181	0.373	16.10
GaN	2.94444	22.37	2.792	648	458	1105	0.403	17.38
InN	3.33220	22.18	3.226	480	340	987	0.461	19.15
Ge,	3.46574	22.14	3.34	426	300	940	0.490	19.79
TlN	3.78419	22.45	3.206	324	219	759	0.549	21.47
Sn	3.91202	22.78	3.084	284	188	675	0.577	22.19
NhN	4.09434	23.55	2.860	226	149	551	0.616	23.27
Pb	4.40672	25.95	2.201	127	89	316	0.683	25.92
Fl	4.74620	30.37	0.508	20	43	44	0.75	30.47

The smoothed values of the coefficients b are the same for each of the values of Ln(N) in Tables 1 and 2, regardless of the type of crystal lattice, and are presented in Fig. 1. The values of other coefficients of the multiparameter function (1) vs. Ln(N) can be easily plotted graphically using the data in Tables 1 and 2.

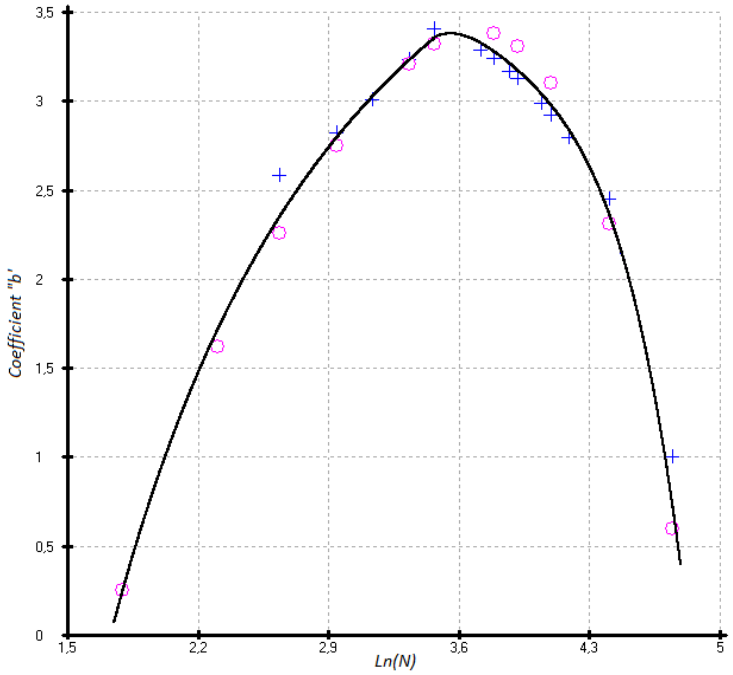

Figure 1. Joint description of coefficients 'b' vs. Ln(N) of the Maier-Kelley equation with wurtzite (o) and sphalerite (+) structures. The maximum of the curve occurs at of Ln(N) of Ge

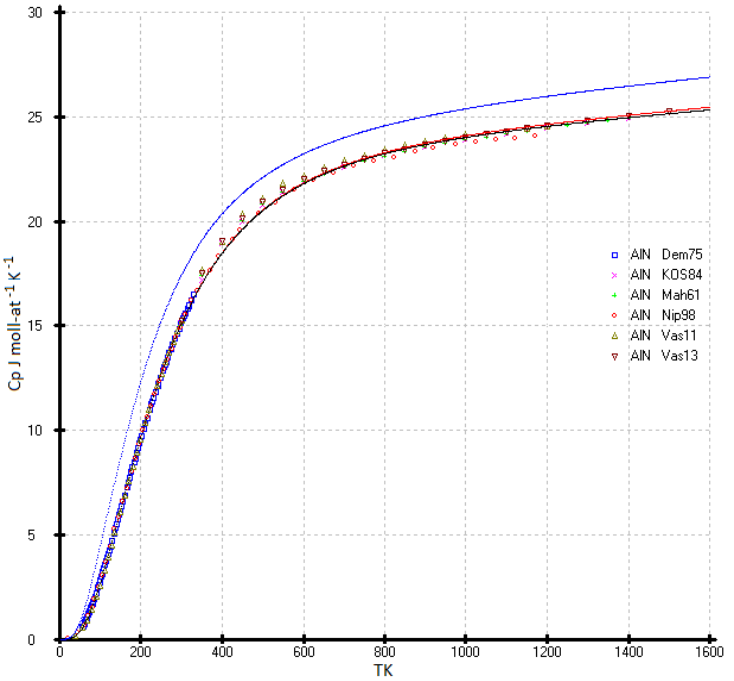

Figure 2. C_p(T)AlN_w [2] black curve, AlN_w [this work] red curve, AlN_{sph} [1] blue curve

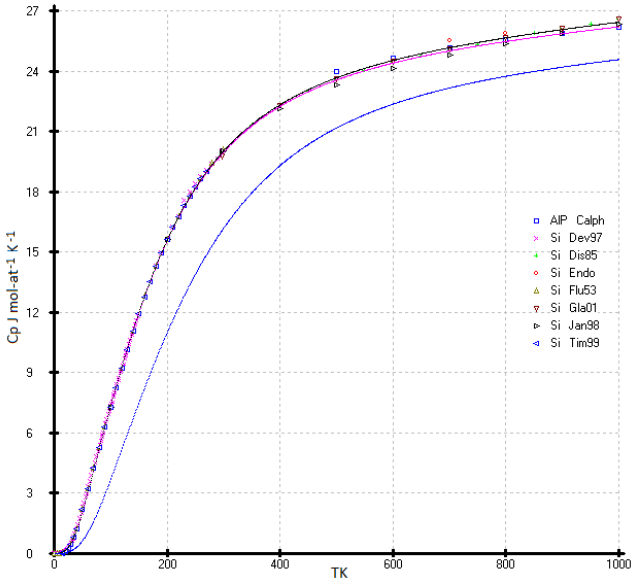

Figure 3. $C_p(T)Si_w$ [2] blue curve, Si_{sph} [this work] red curve, Si_{sph} [1] black curve

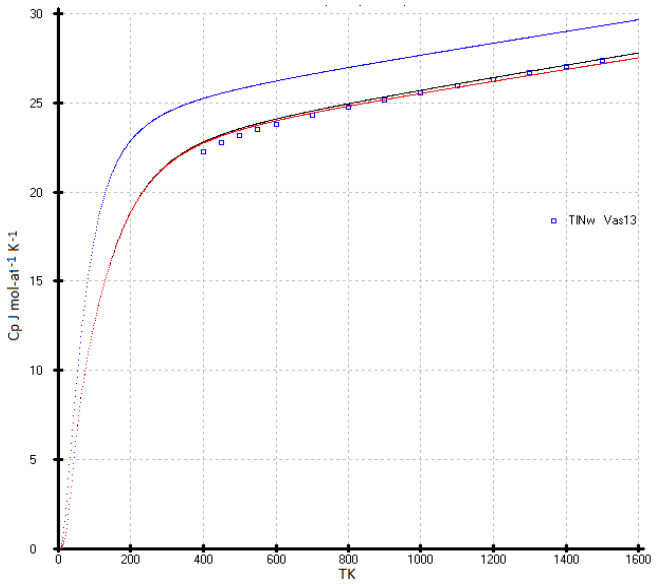

Figure 4. $C_p(T)TlN_w$ [2] black curve, TlN_w [this work] red curve, TlN_{sph} [1] blue curve

The values of heat capacity $C_p(T)$ can be reconstructed based on Tables 1 and 2 and the MATLAB program.

The necessary literature references on the heat capacity of phases with sphalerite and wurtzite structure can be taken from [1-3].

2. CONCLUSION

The data obtained on the heat capacity of phases with the wurtzite and sphalerite structures can be used as reliable reference data.

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