

Thermodynamic Calculation of Melting Heat

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Abstract

In the present paper, the method for approximate calculation of phase space volumes proposed in Ref. [1] is extended. Expressions for the melting heat of materials with f.c.c., b.c.c. and h.c.p. lattices are derived. Experimental results are compared to numerical calculations for a number of elements.

Keywords: Thermodynamic; Heat; First-order phase transitions

Calculation of a Phase Volume for Solids

A principally new approach to the calculation of the heat of first-order phase transitions was proposed in Ref. [1]. It is based on an approximate calculation of the phase volumes of a system in different phases: solid, liquid or gaseous and calculation of the change of entropy given as a logarithmic ratio of the volumes of old and new phases $\Delta S = k_B \ln \frac{V_{phL}}{V_{phG}}$. The volumes of phase space for liquid and gaseous phases are also calculated therein:

$$V_{phL} = \frac{(3\pi mRT)^{3N/2}}{(3N/2)!} V_L^N \quad (1)$$

$$V_{phG} = \frac{(3\pi mRT)^{3N/2}}{(3N/2)!} V_G^N \quad (2)$$

Where V_L and V_G are the volumes of liquid and gas, respectively. The expression for the evaporation heat is obtained in Ref. [1] in terms of other thermodynamic parameters of the process. A good agreement of numerical results and experimental data suggests that the method is versatile and can be used for calculating the transition heat of other first-order phase transitions. As it was shown in Ref. [1], the calculation should take into account the work performed against external forces during a phase transition with employment of the free volume. The expression for the phase volume of liquid was obtained in Ref. [1], whereas the calculation of a melting heat requires the phase space volume of solid state. The following model is used to find this volume. Every atom (molecule, ion) of a solid is assumed to vibrate near the equilibrium state, and its energy in a self-consisted periodic field is $e_n(\vec{r}, \vec{p})$.

Quadratic expansion of energy into powers of \vec{p} gives:

$$e_n(\vec{r}, \vec{p}) = e_n(\vec{r}) + \sum_{i,j} \frac{\partial^2 e_n}{\partial p_i \partial p_j} p_i p_j$$

$e_n(\vec{r})$ can be interpreted as an effective potential energy $U_n(\vec{r})$, $\left. \frac{\partial e_n}{\partial p_i} \right|_{p_i=0} = 0$.

By diagonalizing the quadratic form according to the standard technique, we obtain:

$$\frac{p_x^2}{2m_{xx}} + \frac{p_y^2}{2m_{yy}} + \frac{p_z^2}{2m_{zz}} = e_n - U_n(\vec{r}) \quad (3)$$

Where m_{xx} , m_{yy} , m_{zz} are components of the effective mass tensor. $1/m_{ij} = \partial^2 e_n / \partial p_i \partial p_j |_{0,0}$. This approach is utilized in solid state physics, for example, in Ref. [2]. Equation (3) is the elliptic equation with the axes $(2m_{xx}(e_n - U_n(\vec{r})))^{1/2}, (2m_{yy}(e_n - U_n(\vec{r})))^{1/2}, (2m_{zz}(e_n - U_n(\vec{r})))^{1/2}$, the corresponding volume of the ellipsoid is

$$\frac{4\pi}{3} (8m_{xx}m_{yy}m_{zz})^{1/2} (e_n - U_n(\vec{r}))^{3/2}$$

Integration over \vec{p} in the phase space gives:

$$V_{ph} = \int \int \prod_{3N} \frac{4\pi}{3} (8m_{xx}m_{yy}m_{zz})^{1/2} (e_n - U_n(\vec{r}))^{3/2} d^3\vec{r}$$

It was assumed in Ref. [1] that near a point of first-order phase-transition, the majority of atoms are in the state with the average kinetic energy. This assumption is proved by a good agreement between numerical results and experimental data on evaporation heat. Consequently, according to the equipartition theorem for kinetic energy [3], one can substitute $3KT/2$ for $(e_n - U_n(\vec{r}))$. Thus, the approximate volume of phase space for solid is given by:

$$V_{phS} = \left(\frac{4\pi}{3} (8m_{xx}m_{yy}m_{zz} (3kT/2)^3)^{1/2} V_S \right)^N = \left(\frac{4\pi}{3} (m_{xx}m_{yy}m_{zz} (3kT)^3)^{1/2} V_S \right)^N \quad (3)$$

Calculation of the Melting Heat

The volume of phase space for solid is given by (3). In the first part of the present work [1] it was shown that the employment of the free volume (for unit mole, the free volume is $V_f = V - N_A V_a$, where V is the geometrical volume, N_A is the Avogadro constant, and V_a is the volume of atom (molecule, ion)) gives a substantially better agreement between numerical and experimental results. The phase space volume for solid state is expressed as:

$$V_{phS} = \left(\frac{4\pi}{3} \pi (m_{xx}m_{yy}m_{zz} (3kT)^3)^{1/2} V_{sf} \right)^N \quad (4)$$

and the phase space volume for liquid state is, respectively, (1):

$$V_{phL} = \frac{(3\pi mRT)^{3N/2}}{(3N/2)!} V_{lf}^N$$

Correspondingly, the logarithm of the ratio V_{phL} / V_{phS} is equal to:

$$\ln \left(\frac{(3\pi mRT)^{3N/2} V_{lf}^N}{(3N/2)!} \right) - \ln \left(\frac{4\pi \pi (m_{xx}m_{yy}m_{zz} (3kT)^3)^{1/2} V_{sf}^N}{3} \right)$$

By using the Stirling formula $\ln((3N/2)!) = 3N(\ln(3N/2)) - 2 - 3N/2$ and taking into account $R = kNA$, we obtain:

$$\Delta S = \frac{R}{2} \left(\ln \frac{\pi e^3}{6} + \ln \frac{m^3}{m_{xx}m_{yy}m_{zz}} \right) + R \ln \frac{V_{lf}}{V_{sf}}$$

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Thus, the expression for the melting heat has the form:

$$\lambda = \frac{RT}{2} \left(\ln \frac{\pi e^3}{6} + \ln \frac{m^3}{m_{xx} m_{yy} m_{zz}} \right) + RT \ln \left(1 + \frac{\Delta V}{V_{sf}} \right) + P\Delta V \quad (5)$$

Under normal pressure, the term $P\Delta V$ is on the order of $10^{5*}10^{-6} \sim 10^{-1}$, and the value of the first term is $\sim 10^4$, hence, up to pressures of $\sim 10^{10}$ Pa the term $P\Delta V$ can be neglected. $V_{lf} = V_{sf} + \Delta V$. Finally, the expression for the melting heat at pressures below 10^{10} Pa has the form:

$$\lambda = \frac{RT}{2} \left(\ln \frac{\pi e^3}{6} + \ln \frac{m^3}{m_{xx} m_{yy} m_{zz}} \right) + RT \ln \left(1 + \frac{\Delta V}{V_{sf}} \right) \quad (6)$$

Let us term the dimensionless expression

$$S_0 = \frac{1}{2} \left(\ln \left(\frac{\pi e^3}{6} \right) + \ln \left(\frac{m^3}{m_{xx} m_{yy} m_{zz}} \right) \right) \quad (7)$$

the structural melting constant. Its first term is determined by a substantial difference between liquid and solid states, and the second one makes allowance for the corrections related to symmetry and forces of interaction between atoms for a particular crystal. Note that the expression $\ln \left(\frac{m^3}{m_{xx} m_{yy} m_{zz}} \right)$ is sensitive to the values of effective masses. Let the effective masses be slightly greater than m , then $m_{xx} = m(1+0.0n)$, $m_{yy} = m(1+0.0n)$, $m_{zz} = m(1+0.0n)$, where n is $\sim 3-7$ and we have $\ln \left(\frac{m^3}{(1.0n)^3 m^3} \right) = 3 \ln \left(1 - \frac{n}{100} \right) = -\frac{3n}{100}$, $\ln \left(\frac{\pi e^3}{6} \right) = 2.353$. Taking effective masses into account may reduce the value of the structural melting constant by 10-15% since the effective mass is, as a rule, greater than the mass of a free particle.

Calculation of effective masses is beyond the scope of the present work because it is a hard computational task for a particular material. The effective masses can be found from the analysis of phonon spectra as well, but this is the subject to a separate work. The present work considers only geometric factors in the expressions for effective masses for three different types of lattice: the face-centered lattice (f.c.c.), body-centered lattice (b.c.c.), and hexagonal close-packed lattice (h.c.p.). In calculations of metal ion volumes, the ion radii are used, and in calculations of the volumes of atoms Ne, Ar, Kr, and Xe the corresponding van der Waals radii are used [4,5].

The expression for the melting heat (6) has the form:

$$\lambda = \frac{RT}{2} \left(\ln \frac{\pi e^3}{6} + \ln \frac{m^3}{m_{xx} m_{yy} m_{zz}} \right) + RT \ln \left(1 + \frac{\Delta V}{V_s} \right)$$

Since, according to the Clapeyron-Clausius equation

$$\frac{dT}{dP} = \frac{\Delta V}{\Delta S} \text{ and } \Delta S = \frac{\lambda}{T} \text{ we have } \Delta V = \frac{\lambda}{T} \frac{dT}{dP}$$

By substituting this result into (6) we obtain the equation for calculating λ :

$$\lambda = RTS_0 + \ln \left(1 + \frac{\lambda}{TV_{sf}} \frac{dT}{dP} \right), \quad (8)$$

Where dT/dP is the initial slope of the melting curve [6]. The obtained equation is simply solved numerically by the iterative method and provides the value of the melting heat. The results of calculations by formula (6) and the solutions of equation (8) are given in Tables 1-3. Experimental data for the calculations are taken from Ref. [4,5]. In Tables 1-3 the number of polymorphic phase transitions before melting is marked with asterisks *. Spaces in the tables mean that there is no available data on the jumps of volume in melting.

Melting heat for the f.c.c. lattice

To the f.c.c. lattice in the \bar{p} -space, in which the expansion was performed, corresponds the b.c.c. lattice. In view of the symmetry of b.c.c. lattice, we take: m_{xx}, m_{yy}, m_{zz} . Then, the melting heat for the f.c.c. lattice takes the form:

$$\lambda = \frac{1}{2} RT \ln \left(\frac{\pi e^3}{6} \right) + RT \ln \left(1 + \frac{\Delta V}{V_{sf}} \right) \quad (9)$$

The structural melting constant for the f.c.c. lattice is $S_0 = 1.1765$.

For low-melting elements with weak interaction between atoms the effective masses are approximately equal to atomic masses, whereas for hard-melting materials the difference can be substantial. Results of calculations of the melting heat for f.c.c. lattices by formula (9) and solutions of equation (8) are given in Table 1.

T is the melting temperature in K, λ_{ex} [J/mol] is the experimental value of the melting heat, $V_s^* 10^5$ [m³/mol] is the molar volume of the solid state, $\Delta V^* 10^5$ [m³/mol] is the volume jump in melting, $r^* 10^{10}$ [m] is the radius of atom (ion), $V_{sf}^* 10^5$ [m³/mol] is the free volume, $(dT/dP)^* 10^8$ [K/Pa] is the initial slope of the melting curve, λ_{T1} [J/mol] is the molar melting heat calculated by formula (9), λ_{T2} [J/mol] is the molar melting heat obtained by solving equation (8), δ_1 and δ_2 [%] are inaccuracies of λ_{T1} and λ_{T2} , respectively.

El-t	T	λ_{ex}	V_s	ΔV	r_a	V_{sf}	λ_{T1}	δ_1	dT/dP	λ_{T2}	δ_2
Ne	24,48	324	1,397	0,22	1,60	0,365	335,4	-3,5	13,16	317	2,0
Ar	83,87	1210	2,412	0,35	1,91	0,656	1118	7,6	24,89	1102	8,9
Kr	116,6	1640	2,968	0,45	1,98	1,012	1497	8,7	30,13	1444	11,9
Xe	161,3	2290	3,709	0,56	2,18	1,098	2129	7,0	38,9	2082	9,1
Pb	600,7	4770	1,826	0,07	1,32	1,246	6146	-28,8	7,73	6182	-30,0
Al	933,5	10670	1,000	0,07	0,57	0,953	9676	9,3	6,41	9648	9,6
Ar	1235	11300	1,027	0,06	0,89	0,849	12775	-13,1	4,9	12664	-12,1
Au	1338	12700	1,019	0,05	0,91	0,829	13732	-8,1	6,2	13914	-9,6
Cu	1357	13000	0,709	0,04	0,72	0,615	13978	-7,5	4,69	14129	-8,7
Ac	1370	14200	2,260	...	1,18	1,846	19,4	14603	-2,8
Ni	1726	17600	0,659	0,05	0,78	0,539	18146	-3,1	3,7	17858	-1,5
Pd	1825	17200	0,885	...	0,64	0,819	6,4	19030	-10,6
Pt	2045	19700	0,910	0,06	0,70	0,824	21188	-7,6	6,2	21275	-8,0
Rh	2239	22600	0,829	...	0,86	0,669	5,9	23540	-4,2
Ir	2683	26400	0,857	...	0,89	0,679	6,2	28280	-7,1

Table 1: Calculation results of melting heat for f.c.c. lattices.

El-t	T	λ_{ex}	V_s	ΔV	r_a	V_{sf}	λ_{T1}	δ_1	dT/dP	λ_{T2}	δ_2
Cs	301,5	2090	7,096	0,169	1,65	5,964	2150	-2,8	25,9	2156	-3,2
Rb	312,2	2200	5,579	0,193	1,49	4,745	2257	-2,6	21,1	2234	-1,6
K	336,8	2400	4,536	0,117	1,33	3,943	2405	-0,2	17,7	2411	-0,5
Na	371	2640	2,368	0,064	0,98	2,131	2650	-0,4	8,77	2648	-0,3
Li	453,7	3130	1,300	0,032	0,78	1,180	3230	-3,2	3,41	3205	-2,4
Pb	600,7	4770	1,826	0,070	1,32	1,246	4416	7,4	7,73	4363	8,5
Ba	983	7530	3,821	0,030	1,43	3,084	6859	8,9	4,3	6990	8,7
Sr**	1042	8000	3,450	0,177	1,27	2,934	7694	3,8	16,5	7531	5,9
Eu	1095	9200	2,898	0,140	1,12	2,544	8040	12,6	12,8	7875	14,4
Yb*	1097	7700	2,484	0,100	1,07	2,175	7976	-3,6	17,0	8075	-4,9
La**	1194	10040	2,260	0,012	1,14	1,887	8298	17,3	2,5	8325	17,1
Pr*	1204	8200	2,080	...	1,06	1,780	2,2	8389	-2,3
Nd*	1294	10680	2,059	0,019	0,99	1,814	9037	15,4	2,6	9031	15,4
Sm*	1350	10900	2,000	0,072	1,20	1,564	9816	9,9	6,0	9612	11,8
U**	1405	9200	1,256	0,029	0,97	1,026	10016	-8,9	2,8	9920	-7,8
Mn***	1517	12070	0,738	0,042	0,91	0,548	11392	5,6	3,3	11000	8,8
Be*	1551	13000	0,488	0,056	0,35	0,477	12128	6,7	5,0	11675	10,2
Gd*	1586	10200	1,990	0,041	0,97	1,760	11243	-10,2	5,7	11237	-10,2
Tb*	1629	10800	1,931	0,061	0,89	1,753	11699	-8,3	7,4	11636	-7,7
Dy*	1685	10900	1,900	0,093	0,89	1,722	12358	-13,4	12,0	12316	-13,0
Ho*	1747	14160	1,875	0,140	0,95	1,659	13226	6,6	14,3	12947	8,5
Y*	1795	11390	1,989	...	1,06	1,689	16,5	13432	-17,9
Er*	1802	17200	1,844	0,166	0,93	1,641	13872	19,3	15,0	13413	22,0
Fe**	1808	13800	0,709	0,030	0,83	0,565	13248	4,0	3,0	13033	5,5
Sc*	1814	15900	1,504	...	0,83	1,360	15,1	13726	13,7
Ti*	1933	15000	1,055	...	0,90	0,871	15,4	15454	-3,0
Th*	2023	15600	1,980	...	1,11	1,635	18,6	15342	1,6
Cr	2110	21000	0,723	...	0,84	0,574	15,9	18336	12,7
Zr*	2125	20000	1,402	...	1,09	1,076	16,3	16635	16,8
V	2160	23100	0,834	...	0,88	0,662	15,7	18158	21,4
Hf*	2503	20935	1,341	...	0,84	1,192	17,3	19489	6,9
Nb	2741	27200	1,084	...	0,77	0,969	16,2	21739	20,1
Mo	2890	27600	0,939	0,010	0,92	0,743	20254	26,6	0,96	20146	27,0
Ta	3269	31400	1,087	0,056	0,77	0,972	24069	23,3	5,4	23613	24,8
W	3680	35200	0,953	0,125	0,77	0,838	29634	15,8	7,8	27430	22,1

Table 2: Calculation results of melting heat for b.c.c. lattices.

El-t	T	λ_{ex}	V_s	ΔV	r_a	V_{sf}	λ_{T1}	δ_1	dT/dP	λ_{T2}	δ_2
Cd	594,1	6110	1,300	0,04	1,14	0,927	5516	9,7	5,3	5565	8,9
Zn	692,7	6670	0,917	0,04	0,83	0,773	6479	2,9	4,8	6516	2,3
Mg	992	9040	1,398	0,04	0,78	1,278	9116	-0,8	7,5	9303	-2,9
Ca**	1112	9330	2,586	0,13	1,06	2,286	10445	-11,9	14,9	10485	-12,4
Pm	1441	12600	2,010	...	1,06	1,710	31,3	14956	-18,7
Co*	1768	15200	0,662	0,01	0,82	0,523	15014	1,2	3,5	15578	-2,5
Tm	1818	18400	1,812	0,13	0,87	1,646	17389	5,5	12,0	17251	6,2
Lu	1936	19200	1,778	0,06	0,85	1,623	17879	6,9	15,9	18753	2,3
Tc	2445	23810	0,860	...	0,95	0,644	5,5	23441	1,5
Ru	2583	23700	0,814	...	0,77	0,699	6,1	24802	-4,6
Os	3327	29300	0,843	...	0,89	0,665	6,5	32220	-10,0
Re	3453	33100	0,886	0,03	0,72	0,792	31913	3,6	3,2	31898	3,6

Table 3: Calculation results of melting heat for h.c.p. lattices.

Experimental values of the melting heat and the line of a simple regression are shown in Figure 1. The slope of the regression line is 1.1670, which well coincides (with a good accuracy of ~ 0.85%) with the structural melting constant of the f.c.c. lattice $S_0=1.1765$.

Melting heat for the b.c.c. lattice

To the b.c.c. lattice in the \bar{p} -space corresponds the f.c.c. lattice. Hence, taking into account geometrical factors we take

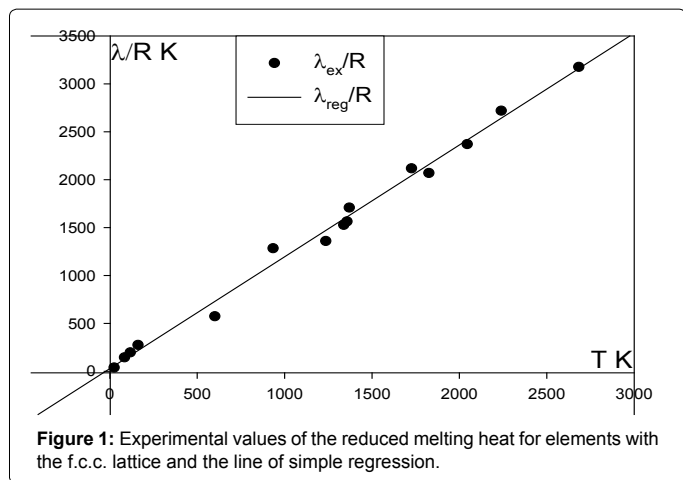


Figure 1: Experimental values of the reduced melting heat for elements with the f.c.c. lattice and the line of simple regression.

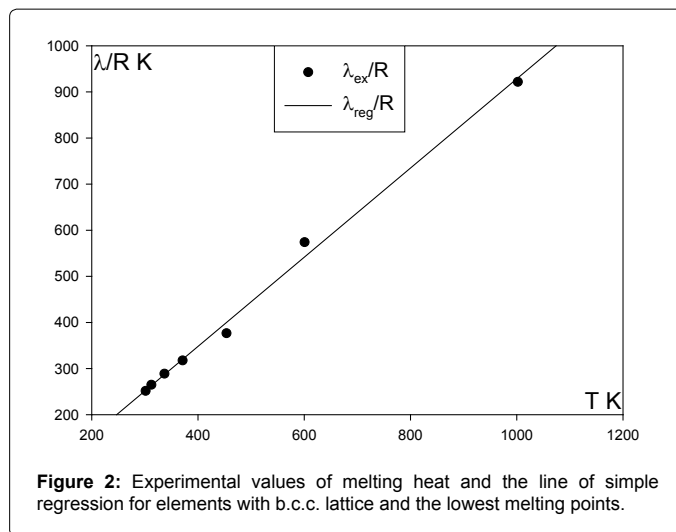


Figure 2: Experimental values of melting heat and the line of simple regression for elements with b.c.c. lattice and the lowest melting points.

$m_{xx} = m_{yy} = m, m_{zz} = m\sqrt{2}$. Then the expression for the melting heat in the case of b.c.c. lattice takes the form

$$\lambda = \frac{1}{2}RT \left(\ln\left(\frac{\pi e^3}{6}\right) + \ln\left(\frac{m^3}{\sqrt{2}m^3}\right) \right) + RT \ln\left(1 + \frac{\Delta V}{V_{sf}}\right)$$

or

$$\lambda = \frac{1}{2}RT \ln\left(\frac{\pi e^3}{6\sqrt{2}}\right) + RT \ln\left(1 + \frac{\Delta V}{V_{sf}}\right) \quad (10)$$

The structural melting constant for the b.c.c. lattice is $S_0=1.0032$.

Results of calculations of the melting heat for b.c.c. lattices by formula (10) are given in Table 2 along with the results of solving equation (8).

T is the melting temperature in K, λ_{ex} [J/mol] is the experimental value of the melting heat, $V_s \cdot 10^5$ [m³/mol] is the molar volume of the solid state, $\Delta V \cdot 10^5$ [m³/mol] is the volume jump in melting, $r \cdot 10^{10}$ [m] is the radius of atom (ion), $V_{sf} \cdot 10^5$ [m³/mol] is the free volume, $(dT/dP) \cdot 10^8$ [K/Pa] is the initial slope of melting curve, λ_{T1} [J/mol] is the molar melting heat calculated by formula (10), λ_{T2} [J/mol] is the molar melting heat obtained by solving equation (8), δ_1 and δ_2 [%] are the inaccuracies of λ_{T1} and λ_{T2} , respectively.

Experimental values of the melting heat and the line of simple regression are presented in Figure 2 for the most low-melt elements. First seven metals were chosen with the lowest melting points for which the most relevant experimental data on melting temperature and melting heat are available. The slope of the regression line is 0.967 and matches the structural melting constant of the b.c.c. lattice $S_0=1.0032$ with a good accuracy of ~ 3.6%.

Melting heat for the h.c.p. lattice

h.c.p lattice transforms into itself in the \bar{p} - space. The effective masses are, respectively, $m_{xx} = m_{yy} = m, m_{zz} = 2\frac{a}{c}m$. Thus, the expression for the melting heat for h.c.p. lattice has the form

$$\lambda = \frac{1}{2}RT \left(\ln\left(\frac{\pi e^3}{6}\right) + \ln\left(\frac{c}{2a}\right) \right) + RT \ln\left(1 + \frac{\Delta V}{V_{sf}}\right), \quad (11)$$

where a and c are parameters of the h.c.p. lattice. Since the ratio c/a for the elements does not differ much from the ideal case $\frac{c}{a} = \sqrt{8/3}$, we may replace real values of the ratio a/c in the expression for S_0 with the ideal value and obtain the relationship for the melting heat for the h.c.p. lattice:

$$\lambda = \frac{1}{2}RT \ln\left(\frac{\pi e^3}{3\sqrt{6}}\right) + RT \ln\left(1 + \frac{\Delta V}{V_{sf}}\right) \quad (12)$$

The structural melting constant for the h.c.p. lattice is $S_0=1.075$.

Results of calculations by formula (12) are given in Table 3. The results of solving equation (8) for h.c.p. lattices are also presented in the table.

T is the melting temperature in K, λ_{ex} [J/mol] is the experimental value of the melting heat, $V_s \cdot 10^5$ [m³/mol] is the molar volume of the solid state, $\Delta V \cdot 10^5$ [m³/mol] is the volume jump in melting, $r \cdot 10^{10}$ [m] is the radius of atom (ion), $V_{sf} \cdot 10^5$ [m³/mol] is the free volume, $(dT/dP) \cdot 10^8$ [K/Pa] is the initial slope of the melting curve, λ_{T1} [J/mol] is the molar melting heat calculated by formula (12), λ_{T2} [J/mol] is the molar melting heat obtained by solving equation (8), δ_1 and δ_2 [%] are the inaccuracies of λ_{T1} and λ_{T2} , respectively.

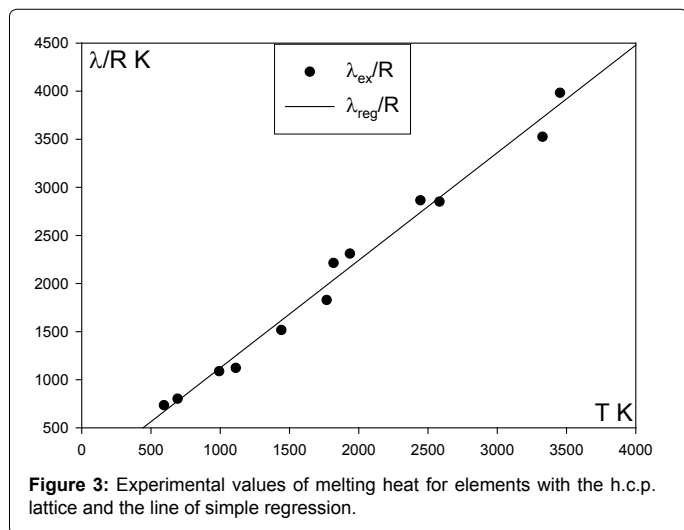
Experimental values of the melting heat are presented in Figure 3 along with the line of a simple regression. The slope of the regression line is 1.1186 and matches the structural melting constant of h.c.p. lattice $S_0=1.0075$ with a good accuracy of ~ 4%.

Analysis and Conclusions

As one can see from Tables 1-3, the proposed model gives a satisfactory description of the melting heat for the elements considered. In Ref. [7], experimental data on temperatures and melting heat values for eight well characterized elements are given. As one can see from Table 4, even for these elements the experimental results noticeably differ.

T_{min} and T_{max} are the minimal and maximal values of experimental melting temperature, λ_{min} and λ_{max} are the lowest and highest values of experimental melting heat. The same trend holds true for the values given in various handbooks. The results only coincide if data are taken from a single source. Consequently, it would not be correct to hope for a good agreement between experimental data and the numerical results calculated by formulae (9-10, 12).

The substantial difference between the experimental value of the melting heat for lead and the corresponding value calculated for the f.c.c. lattice along with the satisfactory agreement with the value of the melting heat calculated for the b.c.c. lattice suggest that a polymorphic transition from the f.c.c. lattice to b.c.c. lattice occurs near the melting point with the phase transition heat equal to $\lambda \approx 1700-1800$ J/mol. The phase transition heat is calculated in the frameworks of the proposed model.



El-t	T _{min}	T _{max}	λ _{min}	λ _{max}	El-t	T _{min}	T _{max}	λ _{min}	λ _{max}
Al	930	933.74	7928.93	11300.9	Nb	2523	2773	26756.9	26849.8
Cu	1356	1357.8	7968.67	13453.3	Mo	2853	2901	20051.5	41254.2
Ni	1721	1744	15984.2	18663.4	Ta	3053	3275	24699.4	32027.8
Ti	1878	2093	15474.3	20923.6	W	3523	3683	33782.4	54971.1

Table 4: Spread of experimental values on temperatures and melting heat.

Thus, one can assert that the molar melting heat at pressures below 10^{10} Pa is given by the expression

$$\lambda = RTS_0 + RT \ln \left(1 + \frac{\Delta V}{V_{sf}} \right)$$

or by a solution of the equation

$$\lambda = RTS_0 + \ln \left(1 + \frac{\lambda}{TV_{sf}} \frac{dT}{dP} \right),$$

Where $S_0=1.1765$ for the f.c.c. lattice, $S_0=1.0032$ for the b.c.c. lattice and $S_0=1.075$ for the h.c.p. lattice. The rest values have been defined earlier.

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