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DEPENDENCE OF LIQUEFACTION HEAT OF METALS ON THEIR MELTING TEMPERATURE

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ABSTRACT

The empirical dependencies of liquefaction heat λ on melting temperature are presented for metals with body-centered (BCC) and face-centered (FCC) crystal lattice. The empirical dependence of λ on T for metals with the hexagonal compact packed (HCP) lattice not undergoing polymorphous (transitions) transformations of $\lambda = 0{,}091 + 2{,}23 \cdot 10^{-3} T \frac{kcal}{mole}$ and undergoing polymorphous transformations $(\alpha \to \beta)\lambda = -1{,}090 + 2{,}47 \cdot 10^{-3} T \frac{kcal}{mole}$ has been determined. The melting entropy has been estimated too.

Keywords: liquefaction heat; melting temperature; hexagonal compact packed; polymorphous transformations; titanium; zirconium.

INTRODUCTION

Many features and parameters, as well as technologies of producing and processing of metals and their alloys depend on their melting temperature T and liquefaction heat λ. Therefore, we have studied [1] the dependencies of liquefaction heat on melting temperature for transition metals taking into account a type of the crystalline lattice because the laws of formation of metallic and covalent bonds are almost identical for each type of crystalline structure.

The dependence of the liquefaction-heat on the melting temperature for refractory metals has been investigated by some researchers [2]. The ratio between the liquefaction temperature and the temperature was 2.27±0.04 and -2.32±0.03 cal/mole K for body-centered cubic (bcc) and face-centered cubic (fcc) metals, respectively in their results.

The empirical dependencies of λ on T has been established for metals with the body-centered cubic (BCC) lattice: $\lambda = -0{,}365 + 2{,}27 \cdot 10^{-3} T$, and with the face-centered cubic (FCC) lattice $\lambda = -0{,}015 + 2{,}40 \cdot 10^{-3} T \frac{kcal}{mole}$ with correlation coefficients 0.999 that are presented in Fig.l. This means that the ratio of liquefaction heat to melting temperature, i.e. the entropy of the metal melting is, proved to be constant for each type of the crystalline lattice and comes to be equal to $\frac{\lambda}{T} = 2{,}27 \pm 0{,}02 \frac{cal}{mole} \cdot K$ for the BCC metals and $\frac{\lambda}{T} = 2{,}32 \pm 0{,}02 \frac{cal}{mole} \cdot K$ for the FCC metals.

More complicated dependence of λ on T has been observed for metals with the hexagonal compact packed (HCP) lattice. Such dependence is connected with changing of structure of the crystalline lattice near the melting point [2], as well as with their activity relative to oxygen and carbon that exist as technological impurities. Therefore, a definite dependence of λ on T has not been observed for transition metals (fig.1).

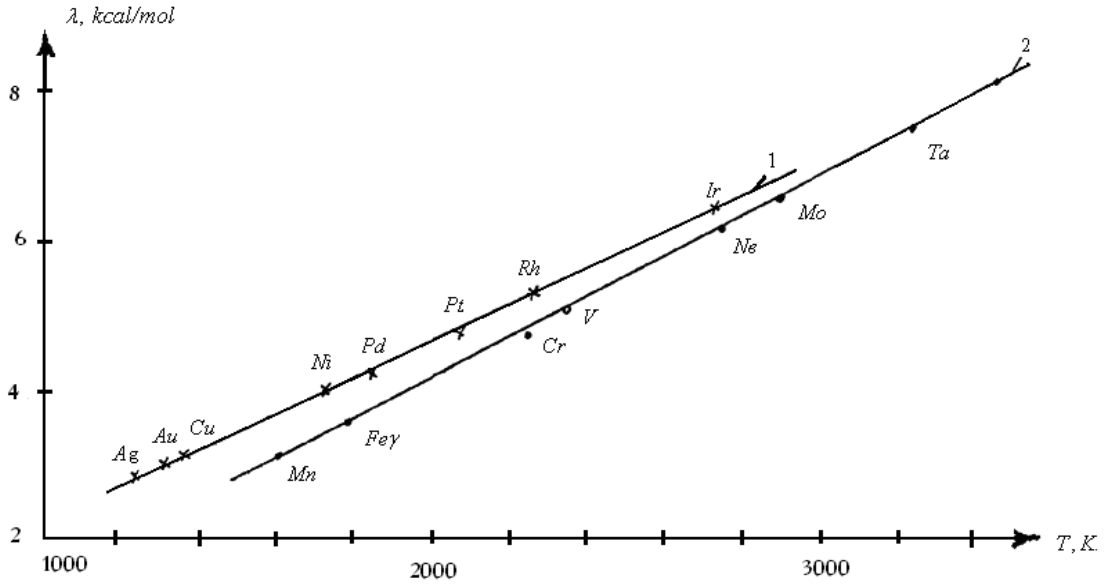

Fig. 1. The dependence of liquefaction heat on melting temperature for metals with FCC lattice (1) and BCC lattice (2).

In connection with this, the dependence of λ on T has been studied for all metals with the HCP lattice for which the values of λ and T are available [3].

These values of λ and T are shown in Fig.2 from which one can see that the dependence of λ on T has a complex character. However, if the fact that the structure of most of these metals before melting differs from their low-temperature structures, i.e. if in the course of heating there were polymorphous transitions are taken into account, then there is some

regularity. For metals with the HCP lattice - Cd, Se, Zn, Te, Ho, Er, Lu, Tm, Tc, Os, Ru and Re - that before melting doesn't not undergo the polymorphous transition $(\alpha \to \beta)$, the dependence of λ on T is sufficiently well described by the empirical formula $\lambda = 0{,}091 + 2{,}23 \cdot 10^{-3} \cdot T$ with the correlation coefficient 0,998. This means that melting entropy of HCP metals not undergoing the polymorphous transformations is constant and equal to $\frac{\lambda}{T} = 2{,}31 \pm 0{,}02 \frac{cal}{mole} \cdot K$.

The dependence of λ on T for the HCP metals undergoing the polymorphous transformations $(\alpha \to \beta)$ can be described by the empirical formula $\lambda = 1{,}090 + 2{,}47 \cdot 10^{-3} \cdot T$, this that meting entropu $\frac{\lambda}{T} = 1{,}90 \pm 0{,}03 \frac{cal}{mole} \cdot K$ (Fig.2). As it is shown in seen from Fig.2, the values of λ for these metals are by $1 \frac{kcal}{mole}$ less than that for metals not undergoing the polymorphous transformations $(\alpha \to \beta)$ before their melting.

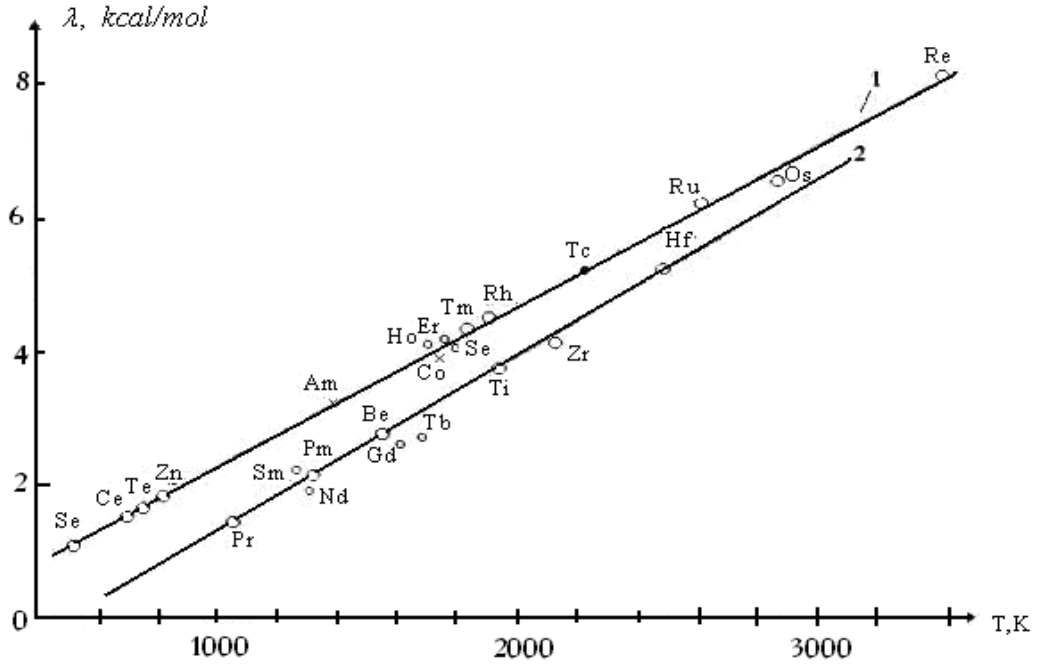

Fig.2. The dependence of liquefaction heat on melting temperature for the HCP metals not undergoing polymorphous transformations (1) and undergoing polymorphous transformations (2).

In our opinion, this difference, characterizes the heat of polymorphous transformations and this can be well seen from the dependencies of λ on T in Fig.2. The difference between the binding energy of an atom in the dense hexagonal lattice and that in the BCC characterizes heat of

polymorphous transformations $(\alpha \to \beta)$ of metals [4], i.e. $\Delta E_{HCP \to BCC} \sim \Delta\lambda_{HCP \to BCC}$. Hence, the energy difference of 12 metallic bonds of an atom with its neighboring ones in the HCP α-lattice, for example titanium (or zirconium), and the same 8 metallic bonds of the central atom with the angular BCC lattice and 6 covalent longer bonds of the central atom with the neighboring ones in the second sphere is equal to $\Delta E_{HCP \to BCC} = 12E_{met.bond} - (8E_{met.bond} + E_{\text{cov.bond}})$.

If the interaction between the atoms with metallic and covalent bonds is supposed to obey the law r^{-6}, then it is possible to estimate the difference in interaction energy for one atom and hence for one mole in the both HCP and BCC lattices [5]. The calculation of the bond energy of atoms of metals was based on the relation $E = \sum \frac{CK_i d_i}{r_i^6}$, where K_i-is the number of metallic and valence bonds, i.e., the number of neighbor atoms, d_i – the number of electrons per bond, r_i – the distance between neighboring atoms and C – interaction energy constant.

MATERIALS AND METHODS

Using data for well studied metals like Nb and Mo, and taking the melting heat $\lambda = \Delta E_{bond} = E_{liq} - E_{sol}$ for these metals is 6,36 kcal/mole and 6,65 kcal/mole respectively, the following value for the constant of interaction is determined:

$$E = 3 \cdot 10^{-79}\ J \cdot m^6 \cdot mole \text{ or } 7{,}15 \cdot 10^{-80}\ cal \cdot m^6 \cdot mole.$$

Using this value of the constant the calculations for determination of the melting heat for Ti, Zr, Hf were provided. These values are listed in the table.

Table

Metals	$T_{trans.}$, K	$T_{mel.}$, K	$\lambda_{mel.}$	$\lambda'_{mel.}$	$\lambda_{trans.}$	$\lambda'_{trans.}$
Ti	1158	1941	3,70	3,86	0,83	0,87
Zr	1135	2128	4,0	3,99	0,92	0,96
Hf	2050	2495	4,42-5,75	4,89	1,38	1,34

Remarks: $\lambda_{mel.}$ and $\lambda_{trans.}$ - are from reference sources, $\lambda'_{mel.}$ and $\lambda'_{trans.}$ - calculated values in kcal/mole.

RESULTS AND DISCUSSION

As we can see, our calculations are in good coincidence with that in [2].

The results obtained by the estimation for titanium and zirconium give the value of about 0.9 kcal/mole which explains sufficiently well the difference in *T*-dependence of λ for metals undergoing and not undergoing polymorphous transformations (Fig.2. curves 1 and 2) and is

well confirmed by experimental data, namely 0.83 cal/mole K for titanium and 0.92 kcal/mole-K for zirconium.

It should be noted that Am and Co undergoes polymorphous transformations $\alpha \to \gamma$, i.e. the structure of these metals changes from the HCP lattice to the FCC one and the heat of polymorphous transformations is less than 0.1 kcal/mole. Therefore, on the curve the values of λ for them are closer to curve 1 in Fig.2. Considerable deviations of λ and T for metals, for example Gd and Tb, are connected with their activity relatively to oxygen and carbon located in them as technological impurities forming stable compounds [6].

CONCLUSION

Thus, on the basis of the above mentioned it is possible to make the following conclusions.

1. For HCP metals undergoing polymorphous transformations, the dependence of liquefaction heat on melting temperature can be described sufficiently well by empirical formula $\lambda = 0{,}091 + 2{,}23 \cdot 10^{-3} \cdot T$, and melting entropy is $\frac{\lambda}{T} = 2{,}31 \pm 0{,}02 \frac{cal}{mole} \cdot K$.

2. For HCP metals undergoing polymorphous transformations $(\alpha \to \beta)$, the dependence of liquefaction heat is satisfactorily described by an empirical formula $\lambda = -1{,}090 + 2{,}47 \cdot 10^{-3} \cdot T$ and melting entropy is equal to $\frac{\lambda}{T} = 1{,}90 \pm 0{,}02 \frac{cal}{mole} \cdot K$.

3. From the difference between the two with the difference in two dependencies of λ on T for undergoing and not undergoing polymorphous transformations metals it is possible to estimate the heats of polymorphous transformations $(\alpha \to \beta)$ for metals with the HCP lattice.

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