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The Study of Regularities of Changing Melting Enthalpy of Intermetallides of Magnesium–Lantanoids Systems Rich in Magnesium

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Abstract: Providing a reasonable forecast of the required properties of intermetallic compounds (hereinafter also referred as intermetallides or IM) is an important scientific and commercial problem, which may be solved by focusing scientific researches and permanent generation of knowledge in this field. To date, researches in chemistry and physics of IM have been developing empirically for a simple reason, due to the complexity of describing the relationship between the crystal structure and chemical bonds, and, therefore, between all the properties of IM. IM is mainly characterized by metal type of chemical bond, as well as specific metallic properties. At the same time, among IM, there are also salt-like compounds with ionic bond, i.e. valency compounds formed from elements of different chemical nature, being stoichiometric compounds. The examples of such compounds are compounds with intermediate bond type, i.e. ion-metal and covalently-metal, as well as covalent bond types (e.g., NaAu). In the series of compounds of Mg with elements of the IV subgroup, along with decreasing the difference in the electrochemical characteristics of the components, the change in the IM properties is observed, from those peculiar to ionic compounds (for example, Mg_2Si, Mg_2Ge) to the properties typical of metals (Mg_2Pb), etc. Due to the fact that lanthanides form the largest group of elements of the periodic system occurring in nature, and Mg is a relatively active chemical element in terms of IM formation (for example, it forms three IM with cadmium - Mg_3Cd, MgCd and $MgCd_3$), its oxides in slag provide decreasing average silicon content and increasing the stability of the silicon content in iron, being an important process indicator in the course of physicochemical reactions occurring in a blast furnace (for example, in the process of iron production). The presence of Si impurity (along with O, Au, Ti, V, Zr) produces the greatest effect on efficiency of solar cells, etc. [1–3]. Based on the foregoing, it is very important to study the state function, i.e. enthalpy of magnesium-lanthanide systems, rich in magnesium, and, based on the results of computer simulation, taking into account molecular dynamics method and other similar studies [4–8], to model regularities of changes in melting enthalpy of IM of the mentioned systems. The issue of modeling the pattern of change in melting enthalpy of IM of magnesium-lanthanide (Mg-Ln) magnesium-rich systems is considered based on systematic analyzing melting enthalpy of IM of Mg-Ln magnesium-rich system, including Mg_2Ln, Mg_3Ln and equimolar compound MgLn, implemented using semi-empirical method developed by N.S. Poluektov.

Keywords: regularity, intermetallides, correlation, lanthanides, magnesium, lanthanide composition, enthalpy of melting, electronic structure, semi-empirical method.

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Моделирование закономерности изменения энтальпии плавления интерметаллидов систем магний-лантаноиды, богатых магнием

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Аннотация: Обеспечение обоснованного прогноза необходимых свойств интерметаллидов (ИМ), являющегося важным направлением науки и определенных отраслей промышленности, достигается научно-исследовательскими работами и постоянной генерацией знаний в этом направлении. Проводимые до сегодняшнего дня исследования по химии и физике ИМ развиваются эмпирически по простой причине – в связи со сложностью описания взаимосвязи между кристаллическим строением и химическими связями, а следовательно, и между всеми свойствами ИМ. Для ИМ в основном характерны металлический тип химической связи, а также специфические металлические свойства. В то же время среди ИМ имеются также солеобразные соединения с ионной связью, т.е. валентные соединения, образующиеся из элементов различной химической природы, представляющие собой стехиометрические соединения. Примером таких соединений являются соединения с промежуточным характером связи, т.е. ионно-металлической и ковалентно-металлической, а также с ковалентной (например, NaAu). В ряду соединений Mg с элементами IV подгруппы вместе с уменьшением различия в электрохимических характеристиках компонентов наблюдается и изменение свойств ИМ – от характерных для ионных соединений (например, Mg_2Si, Mg_2Ge) до свойств, типичных для металлов (Mg_2Pb), и т.д. В связи с тем что лантаноиды образуют самую большую группу элементов периодической системы, находящихся в природе, а элемент Mg является относительно активным химическим элементом по образованию ИМ (например, с кадмием образует три ИМ – Mg_3Cd, MgCd и $MgCd_3$), – его оксиды в шлаке обеспечивают снижение среднего значения и повышение устойчивости содержания кремния в чугуне, – а это важный технологический показатель в ходе физико-химических реакций, происходящих в горне доменной печи (например, при выплавке чугуна). Наличие его примеси (наряду с O, Au, Ti, V, Zr) оказывает наибольшее влияние на эффективность солнечных элементов и т.д. [1–3]. Исходя из изложенного весьма важным является исследование функции состояния, т.е. энтальпии систем магний–лантаноиды, богатых магнием, и на основе полученных путем компьютерного моделирования результатов, с учетом метода молекулярной динамики и других подобных исследований [4–8], моделирование закономерности изменения энтальпии плавления ИМ упомянутых систем. Рассматривается вопрос моделирования закономерности изменения энтальпии плавления ИМ систем магний–лантаноиды (Mg–Ln), богатых магнием, путем системного анализа энтальпии плавления ИМ систем Mg–Ln, богатых магнием составов Mg_2Ln, Mg_3Ln и эквимолярного состава MgLn, проведенного с помощью полуэмпирического метода, разработанного Н.С.Полуэктовым.

Ключевые слова: закономерность, интерметаллиды, корреляция, лантаноиды, магний, состав лантанидов, энтальпия плавления, электронное строение, полуэмпирический метод.

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Introduction Intermetallides (IM), the most important minerals of rare-earth metals (elements) in nature, are characterized by predominantly metallic bonding between atoms in the lattice, but at the same time, there are intermetallic compounds with ionic and covalent chemical bonds, as well as intermediate cases, i.e. ion-metallic and covalent-metallic bonding. This rather diverse bonding between atoms in the IM lattice provides them with: low to high hardness; chemical resistance, as well as an active chemical reactivity (for example, the reaction of zinc and nickel at a temperature above 1000 ° C is of explosive nature); higher melting point than the that of the source metals in a range from 804 °C for cerium and 1700 °C for lutetium); the formation of an eutectic alloy (based on the smallest crystals of two metals, each of which has an independent crystal lattice), which melts at lower temperature than these pure metals (for example, an eutectic alloy consisting of 24.4 atomic % Pb (melting point of 327 °C) and 75.6 atomic % Sn (melting point of 232 °C), melts at 181 °C); relatively lower plasticity than the source metals, but appropriate ductility; increased brittleness of the alloys in the structure of which the elements are included; semiconductor properties; shape memory (after hardening, the product can be deformed mechanically, but will take its original shape after heating a little); weakening the contact mechanical strength and deterioration of electrical characteristics (for example, in soldered joints); division into two groups based on their density (light, below 8 g/cm^3, and heavy, from 8.272 to 9.482 cm^3), etc. [9–15].

Thematic justification Despite the fact that the term lanthanides appeared about a century ago (in 1925 it was first used by V. Goldschmidt), the importance and relevance of the use of lanthanides (Ln) are still required expansion and deepening of studies to identify their thermomechanical and thermodynamic characteristics, and also prospecting and exploration of deposits to produce Ln concentrates. Lanthanides find growing application in modern industries, actively developing over the past 40 years, especially in Japan, China, and other industrialized countries. The published data show that the demand for rare earth elements (REE) from 1980 to the present has grown from 30,000 tons to 120,000 tons and the annual average rate of their consumption growth is projected at 4%, which in turn justifies the relevance of further research in this direction.

Review of the historical studies shows that light alloys based on magnesium, alloyed with rare-earth metals, in particular lanthanides, have important application characteristics. In turn, reliable information on the physicochemical and thermal characteristics of these alloys contribute to their widespread use in modern branches of science, engineering and technological processes. Phase equilibrium diagrams of magnesium-based systems (silicate systems), as well as Mg – Ln systems, have been studied by many researchers [16–30]. The findings of these and other studies, summarized in [31], indicate that MgLn, Mg_2Ln, Mg_3Ln, $Mg_{12}Ln$, and $Mg_{24}Ln_5$ intermetallides (IM) are formed in Mg – Ln systems. Currently, there is no published information on an important indicator of the system internal energy (state function) – melting enthalpy (EP) of these IM, which characterizes the thermal effect of the process proceeding at constant pressure.

This paper presents the findings of a systematic analysis of melting enthalpy of the IM of Mg – Ln systems, magnesium-rich compounds Mg_2Ln, Mg_3Ln, and the equimolar MgLn. The analysis was carried out using the semi-empirical method developed by N. S. Poluektov and et. al. [32, 33]. The calculation (hereinafter calculation 1) is produced using the following correlation equation:

$$A_{(\mathrm{Mg\ xLny})} = A_{(\mathrm{Mg\ xLay})} + \alpha N_f + \beta S + \gamma' L_{(\mathrm{Ce\text{-}Eu})}(\gamma'' L_{(\mathrm{Tb\text{-}Yb})}), \qquad (1)$$

where coefficient α – takes into account the share effect of 4*f* electrons, β-spin (*S*) - and γ-orbital (*L*) moments of Ln atom motion (γ' for Ln-cerium and γ" for Ln-yttrium subgroups) on the values of the IM melting enthalpy (ΔH_{melt}).

The mentioned method is widely used, and we have also successfully applied it for many Ln compounds [34–36].

Determined and/or refined values of the melting temperature of Mg–Ln system IM made it possible to determine melting enthalpy of IM of the above-mentioned compositions (hereinafter referred as Calculation 2) using the following equation [37, 38]:

$$\Delta H^{0}_{\text{пл,}}\mathrm{Mg}_x\mathrm{Ln}_y = T_{\text{пл.}}^{\text{им}}(n\Delta H_{\text{пл.}}^{\mathrm{Ln}}/T_{\text{пл.}}^{\mathrm{Ln}} + \\ + m\Delta H_{\text{пл.}}^{\mathrm{Mg}}/T_{\text{пл.}}^{\mathrm{Mg}})/n+m. \qquad (2)$$

The values of the coefficients of the correlation equation (1) given in Table 1 allow to determine the share effect of each component of the equation on the values of melting enthalpy of Mg–Ln system IM.

The most complete data obtained on melting enthalpy of intermetallides of the studied compositions are given in Table 2.

The data given in Table 2 show satisfactory coincidence of the melting enthalpy values obtained by the two methods. This indicates the validity of the applied semi-empirical methods and the reliability of the obtained results. The only exception is data for few MI. Perhaps this is due to some experimental conditions and insufficiently pure reagents.

Table 1

The values of the coefficients of equation (1) for the determination of melting enthalpy of intermetallides

IM	Parameter	α	β	γ'	γ''
MgLn	$\Delta H^{0}_{\text{пл}}$	−0.096	0.02	−0.127	0.410
$\mathrm{Mg_2Ln}$	$\Delta H^{0}_{\text{пл}}$	−0.26	0.43	−0.09	0.005
$\mathrm{Mg_3Ln}$	$\Delta H^{0}_{\text{пл}}$	−0.018	−0.365	0.1652	0.062

Table 2

The most complete information obtained on melting enthalpy of intermetallides of the studied compositions

IM	$\mathrm{Mg_3Ln}$			$\mathrm{Mg_2Ln}$			MgLn		
	$\Delta H^{\circ}_{\text{пл.}}$		Discrepancy, %	$\Delta H^{\circ}_{\text{пл.}}$		Discrepancy, %	$\Delta H^{\circ}_{\text{пл.}}$		Discrepancy, %
Ln	Calculation 1	Calculation 2		Calculation 1	Calculation 2		Calculation 1	Calculation 2	
La	10190	10190	–	9950	9950	–	10610	10610	–
Ce	10670	10410	2.4	9550	9370	1.9	9000	9560	5.8
Pr	10290	10520	2.1	8530	9130	6.6	8779	8910	1.47
Nd	9870	10560	6.5	8530	9000	5.2	8466	8530	0.75
Pm	9954	10360	3.91	9270	8590	7.3	9010	8440	6.3
Sm	9080	9990	9.1	9420	9000	4.4	8333	8640	3.55
Eu	7800	8110	3.8	9520	9520	–	7080	7140	0.8
Gd	9040	9040	–	9650	9650	–	10010	10010	–
Tb	9024	9120	1.0	8150	8900	8.4	11140	11140	–
Dy	9073	9400	3.4	9330	8410	9.8	11220	11750	4.5
Ho	9260	9630	3.8	8020	7930	1.1	11170	12050	7.5
Er	10190	9800	3.9	8260	7450	9.8	10906	11950	8.37
Tm	9260	9900	6.46	6820	6980	2.2	10767	11430	5.80
Yb	8156	8420	3.13	8980	8980	–	6790	7020	3.27
Lu	9940	9940	–	6530	6530	–	9270	9270	–

The obtained most complete values of melting enthalpy of the studied IM compounds made it possible to determine the regularities of changing the melting enthalpy depending on the nature of Ln. As seen from Fig. 1-3, the dependencies are complex in nature within the entire group and are divided into the Ln subgroups, cerium and yttrium, with the manifestation of the "tetrad effect". The following features should be noted:

–for IM of MgLn and Mg_2Ln compositions (cerium subgroup), the similar curves are observed. Increasing Ln atomic number within the subgroups leads to decreasing the IM melting enthalpy, with a minimum for the Pm compound.

For the IM of the composition Mg_2Ln (yttrium subgroup), increasing Ln atomic number leads to practically linear decreasing the IM melting enthalpy, with the exception of the ytterbium compound;

–the similar curve character is observed for IM of MgLn (yttrium subgroup) and Mg_3Ln (both subgroups) compositions. The curves have a bulge up with a maximum in the middle of the subgroups;

–the deviation of the characteristics of europium and ytterbium IM from the found regularities is due to the partial and complete filling by electrons of the 4*f* orbitals of these elements atoms.

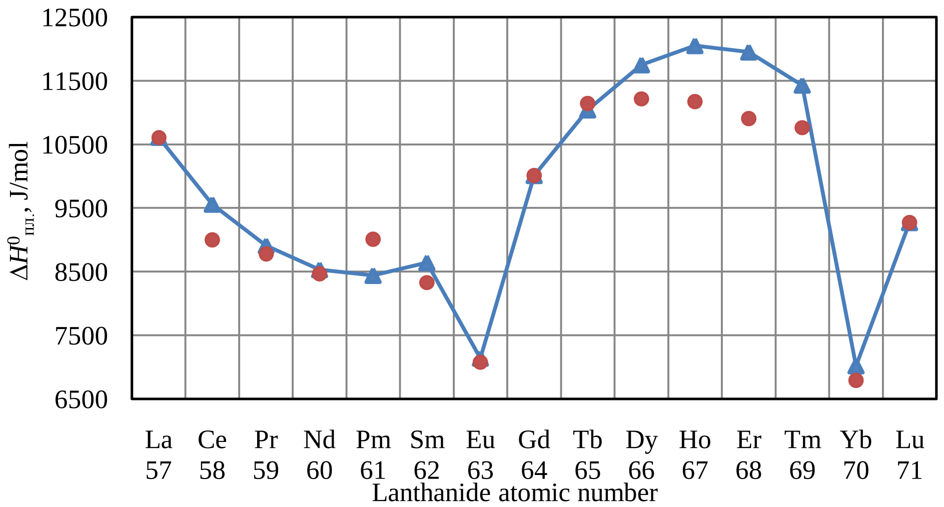


Fig. 1. Plot of melting enthalpy of intermetallides of MgLn composition as function of Ln sequence number. Hereinafter ● – calculation 1, ▲ – calculation 2

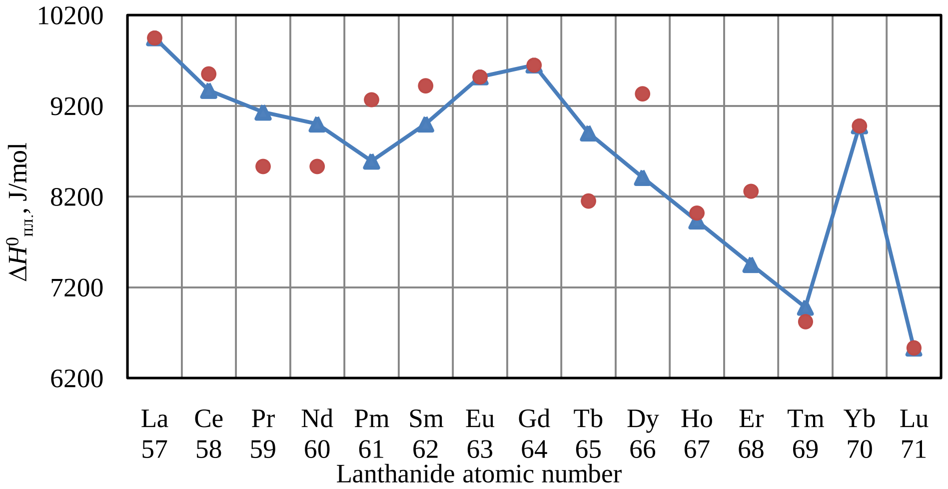


Fig. 2. Plot of melting enthalpy of intermetallides of Mg_2Ln composition as function of Ln sequence number

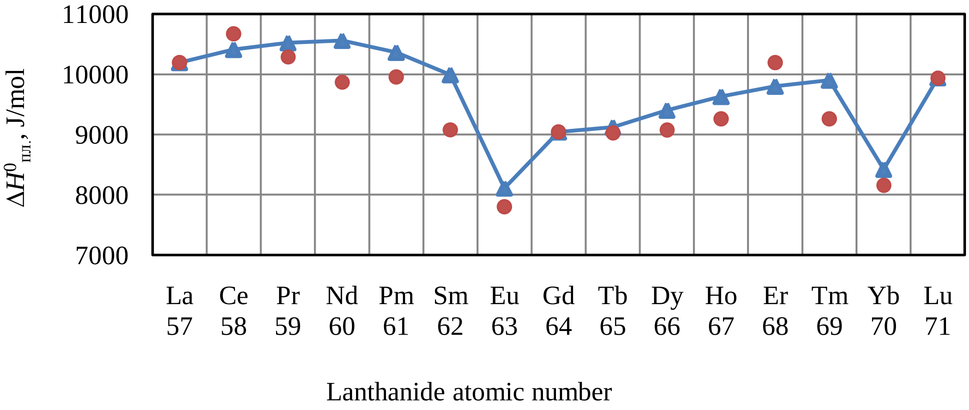


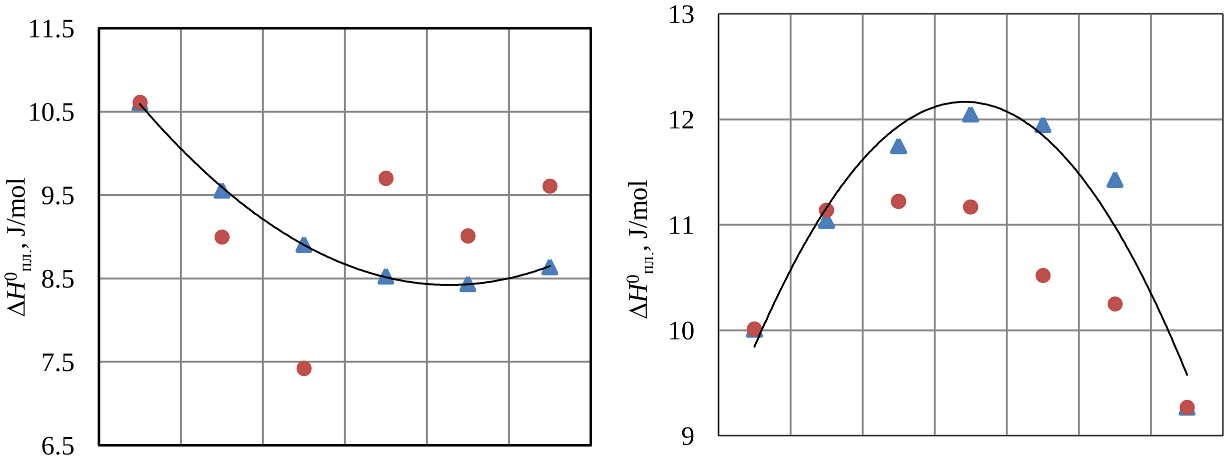
Fig. 3. Plot of melting enthalpy of intermetallides of Mg_3Ln composition as function of Ln sequence number

Table 3

The equations describing change of thermal characteristics of intermetallides depending on nature of lanthanides

IM composition	Parameter		Equation	R^{2*}
MgLn	$\Delta H^0_{пл.}$	(*a*)	$y = 0.1516x^2 - 1.4495x + 11.889$	0.9994
		(*b*)	$y = -0.2726x^2 + 2.1367x + 7.9771$	0.9412
Mg_2Ln	$\Delta H^0_{пл.}$	(*a*)	$y = 0.0763x^2 - 0.74x + 10.607$	0.9211
		(*b*)	$y = 0.019x^2 - 0.6581x + 10.23$	0.998
Mg_3Ln	$\Delta H^0_{пл.}$	(*a*)	$y = -0.0748x^2 + 0.492x + 9.751$	0.9806
		(*b*)	$y = -0.0145x^2 + 0.2826x + 8.7071$	0.9782

Notes: (*a*) – cerium; (*b*) – yttrium subgroups; R^2 is the degree of confidence; x is atomic number of a metal; y is melting enthalpy of an IM.



(*a*) Lanthanide atomic number

(*b*) Lanthanide atomic number

Fig. 4. Plot of melting enthalpy of intermetallides as function of the nature of lanthanides: – trend line

Table 4

The equations describing change of ΔH^0_{melt} of intermetallides depending on their composition

Lanthanide	Trend equation	Lanthanide	Trend equation
La	$y = 450x^2 - 2010x + 12170$	Gd	$y = -125x^2 + 15x + 10120$
Ce	$y = 285x^2 - 305x + 9020$	Tb	$y = 740x^2 - 5210x + 15610$
Pr	$y = 325x^2 + 135x + 6960$	Dy	$y = -230x^2 - 1200x + 12650$
Nd	$y = 1255x^2 - 4935x + 13380$	Ho	$y = 2195x^2 - 9735x + 18710$
Pm	$y = -340x^2 + 1280x + 8070$	Er	$y = 2095x^2 - 8545x + 16970$
Sm	$y = -75x^2 + 35x + 9650$	Tm	$y = 2715x^2 - 11575x + 19110$
Eu	$y = -2080x^2 + 8680x + 480$	Yb	$y = -2250x^2 + 8940x + 100$
		Lu	$y = 3075x^2 - 11965x + 18160$

***Notes to Table 4**: $R^2 = 1$ – for all the IM; $x = m : n$ and is determined based on $Mg_{(m)}Ln_{(n)}$ composition of IM; y – IM melting enthalpy ΔH^0_{melt}

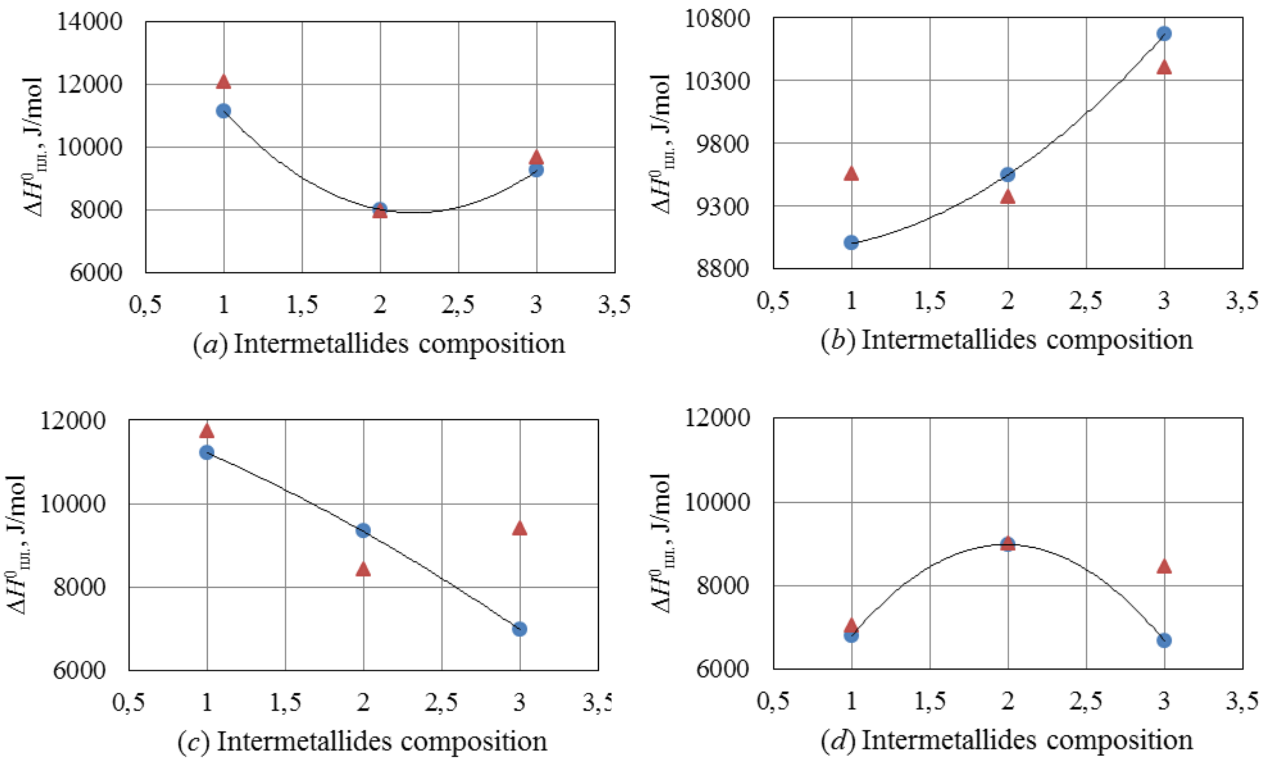


Fig. 5. Plot of melting enthalpy (ΔH^0_{melt}) of intermetallides of $Mg_{(m)}Ln_{(n)}$ system as function of their composition (m/n): — trend line

Mathematical modeling of the IM melting enthalpy for the studied compositions of Mg–Ln system was carried out using the standard Microsoft Excel program. The calculation results are given in Table 3. The data processing was performed separately for cerium and yttrium Ln subgroups. The calculations did not take into account the melting enthalpy values for europium and ytterbium IM.

Fig. 4 shows the characteristic curves of the IM melting enthalpy depending on the nature of Ln for the subgroups: 4 (*a*) – cerium, 4 (*b*) – yttrium.

Equations of the IM $\Delta H^{0}_{\text{melt}}$ dependence on the IM composition and the characteristic curves reflecting the IM melting enthalpy in Mg-Ln system depending on their composition are given in Table 4 and in Fig. 5, respectively.

The graphs present the melting enthalpy curves for the lanthanide IM of: 5 (*a*) – yttrium subgroups, 5 (*b*) – Ce, Pr, and Nd; 5 (*c*) – Pm, Sm, and Eu; 5 (*d*) – La, Gd, and Lu. The changes in the properties of the IM of La, Gd, and Lu are mainly due to the linear nature of electron replenishment of 4*f* orbitals (N_f Eq. (1)), the similarity of the electronic structure, and the possibility of 4f electron transfer to 5d orbitals in these atoms. In other subgroups, spin (*S*)-orbital (*L*) interactions have a decisive effect.

Conclusion

Analytical and graphical interpretations of the study results using the above methods and mathematical modeling of the IM compounds melting enthalpy allowed drawing the following conclusions:

1. Based on the use of the semi-empirical method, the values of the correlation equation coefficients were determined, enabling determining the share effect of each component on melting enthalpy of the Mg–Ln system IM.

2. The most complete data have been obtained on the melting enthalpy of the Mg – Ln system IM of the studied compositions, showing a fairly satisfactory convergence of the melting enthalpy values obtained by two methods, indicating the validity of the applied semi-empirical methods and the reliability of the study results (with the exception of few IM, large discrepancy for which was possibly connected with some experimental conditions and insufficiently pure reagents).

3. The regularities of changing the calculated IM melting enthalpy depending on Ln nature were determined: within the whole group, the regularities are of complex nature, with division into Ln subgroups, cerium and yttrium, with the "tetrad effect" manifestation, and with the following features: for the cerium group (IM of MgLn and Mg_2Ln composition), the similar curve shape is observed. Increasing Ln atomic number within the subgroups leads to decreasing the IM melting enthalpy, with a minimum for the Pm compound.

3.1. For the IM of Mg_2Ln composition (yttrium subgroup), increasing Ln atomic number leads to practically linear decreasing the IM melting enthalpy, with the exception of the ytterbium compound.

4. The determination of the regularities of changing the melting enthalpy of the Mg – Ln system IM (rich in Mg) depending on Ln nature, taking into account their important application characteristics, expands a database on: prognostic properties of the IM of different their structures and compositions; physicochemical and thermal characteristics of IM; as well as allows simplifying and refining system analyzes and solving other important applied problems.

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