The method of quantitative assessment of galaxite dissociation degree in the oxide $MnO–Al_2O_3$ melt based on the Bjerrum-Guggenheim coefficient concept

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At present time, taking into account the existing situation in the raw material base of production of manganese ferroalloys, the technologies for obtaining new carbon reducing agents for metals from weakly coking, long-flaming and high-ash coals instead of metallurgical coke are developed intensively. It was caused first of all by the fact, that chemical compositions vary cardinally and become low-melting during the process of development of deposits (in particular manganese ores). As a result, technological violations and decrease of production volumes of manganese alloys occur in the furnaces of manganese production shops. Respectively, establishment of regularities in phases interaction, in forming of their crystallization fields and in reducing reactions of the elements by carbon from liquid melts in multi-component systems is especially important. At the same time, the obtained results allow to optimize their manufacturing technologies from different kinds of raw materials and to predict searching ways or rational charge compositions for processing of different low-melting manganese and other raw materials. The aim of this research is to reveal the features of forming of the crystallization fields of galaxite phase $MnO–Al_2O_3$ as the most important metallurgical phase and to determine dissociation degree in molten state, as well as to assess influence of these appearances of completeness of extraction of the aimed elements (Mn) from raw materials into metal to stabilize the technological process. The numerical results of dissociation degree for galaxite congruent compound were obtained using Gibbs energy of dissociation reaction and equilibrium constant of this reaction. Material on behaviour of the osmotic coefficient of Bjerrum-Guggenheim is demonstrated as a criterion of melt structure assessment. It was established that dissociation degree of $MnO–Al_2O_3$ compound increases with temperature rise and makes 50 % at the melting temperature.
Key words: phase diagram, congruent compound, monovariant phase equilibrium lines, Bjerrum-Guggenheim coefficient, activity, dissociation degree, melt structure.
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Introduction

To develop the reliable scientific grounds of technological processes for production of manganese-based complex alloys, it is required to evaluate behaviour of melt components: either high-temperature compounds will be formed, or, on the contrary, dissociation of compounds will take place.

The phase diagrams are very important in development of new high-efficient compositions of alloys and materials and their manufacturing technologies. These diagrams are especially interesting due to direct link between thermodynamic properties of initial components and equilibrium phases in them. At the same time the observed phase equilibrium lines in all classes and types of systems are caused by chemical interaction between primary components. This circumstance allows to formulate the task for decoding of phase diagrams with obtaining thermodynamic properties of melts and solid solutions [1–4].

The aim of this work is to establish the features of forming the crystallization fields of galaxite phase ($MnO–Al_2O_3$), which is the most important for metallurgy, as well as to determine dissociation degree in molten state and to evaluate influence of these appearances on extraction completeness for the aimed elements (Mn) from raw material to metal, in order to stabilize technological process.

Simple analysis of crystallization fields for phases in different systems is based on location of the liquidus line and practically does not provide information about the melt features and about reliability of experimental data (except weak or strong melting temperature lowering for the examined phase under the effect of the second component. The picture varies cardinally, if these appearance of effect are considered from the point of view of the osmotic coefficient of Bjerrum-Guggenheim. This coefficient is a very good structurally sensitive melt parameter; when analysis of crystallization lines of the phases is based on real possibility of behaviour

evaluation of melt compounds and features of inter-particle interaction in liquid phase using the osmotic coefficient of Bjerrum-Guggenheim (Φ_i), such analysis allows also to determine data reliability in phase diagrams of these systems and stability of compounds themselves in melts.

The presented article continues theoretical researches of behaviour of the components in metallurgical melts based on the concept of the Bjerrum-Guggenheim osmotic coefficient [5–7].

Materials and methods

Consideration of complicated systems, which can be characterized by different chemical transformations with variation of composition, requires introduction of new variables describing these variations [5–8]. Degree of the process completeness is one of such parameters [9, 10]. It can be expressed with assistance of dissociation degree or reversed process (association); mathematical description is the same and difference is formed in calculation of the equilibrium constant, i.e. reaction products and initial substances [1, 11, 12].

Dissociation degree α is a relation of number of dissociated molecules of substance at the equilibrium moment to total number of molecules of this substance before dissociation, because the part of substance, which has dissociated until the equilibrium moment is equal to;

$$\alpha = \frac{\mathrm{d}n_i}{n_i^0} \quad , \tag{1}$$

where $\mathrm{d}n_i$ – number of dissociated molecules;

n_i^o – initial number of molecules.

Let us consider calculation of location of the lines of multi-variant phase equilibriums via degree of forming the chemical compound on the example of congruently melting *AB* compound:

$$A + B = AB \tag{2}$$

Then we calculate number of miles of substances for the system equilibrium state:

$$\begin{aligned} n_A &= z_A - \alpha \\ n_B &= z_B - \alpha \\ n_{AB} &= \alpha \end{aligned} \tag{3}$$

where n_{AB}, n_A, n_B – number of moles of substances *AB*, *A*, *B* in equilibrium state;

z_B, z_A – number of moles of substances *B* and *A* in initial state;

α – dissociation degree.

Total amount of *AB*, *A*, *B* moles in the mixture will be equal to:

$$\sum n = z_A - \alpha + z_B - \alpha + \alpha = 1 - \alpha \tag{4}$$

Molar part for each component makes:

$$\begin{aligned} x_A &= \frac{z_A - \alpha}{1 - \alpha} \\ x_B &= \frac{z_B - \alpha}{1 - \alpha} \\ x_{AB} &= \frac{\alpha}{1 - \alpha} \end{aligned} \tag{5}$$

To determine the degree of forming the congruently melting compound, it is necessary to know the value of equilibrium constant for association reaction as a temperature function:

$$\ln K_p = \frac{-\Delta G_p(T)}{RT} \quad , \tag{6}$$

$$K_P = \frac{x_{A_B}}{x_A x_B} = \exp\left(\frac{-\Delta G(T)}{RT}\right) \tag{7}$$

Then we express the equilibrium constant in dissociation reaction via molar parts of the mixture components:

$$K_P = \frac{\alpha(1-\alpha)(1-\alpha)}{(1-\alpha)(z_A-\alpha)(z_B-\alpha)} = \frac{\alpha - \alpha^2}{(z_A-\alpha)(z_B-\alpha)} \tag{8}$$

The degree of association of the congruently melting compound will be determined from the following equation:

$$\alpha_{1,2} = \frac{\left(1+K_p\right) \pm \sqrt{K_p^2\left(1-4Z_AZ_B\right)+2K_p\left(1-2Z_AZ_B\right)+1}}{2+2K_p}$$

or

$$\alpha_{1,2} = \frac{\sqrt{1+K_p} \pm \sqrt{1+K_p-4K_pZ_AZ_B}}{2\sqrt{1+K_p}} \tag{9}$$

The above-presented calculation formulas for composition of equilibrium phases via dissociation degree of different chemical compounds allow to obtain new regularities of the Bjerrum-Guggenheim osmotic coefficient in the form of correlation line and to present description of liquidus curves in analytical form, taking into account dissociation degree [2–4].

The algorithm of dissociation degree calculation via Gibbs energy and equilibrium constant is displayed on the example of dissociation of the congruently melting compound $MnO{\cdot}Al_2O_3$.

Obtained results and their analysis

The researches of dissociation degree of the congruently melting compound $MnO{\cdot}Al_2O_3$ are presented, as well as the results of conducted thermodynamic calculations.

$MnO–Al_2O_3$ equilibrium diagram is classified to eutectic systems with forming $MnO{\cdot}Al_2O_3$ congruent compound (**Fig. 1**). It is rather simple at the first glance, having no component solubility in solid state, with only one congruent compound. Attention should be paid to the fact that all crystallization areas in this figure are marked with dotted lines; it means that crystallization areas of the system components arise some doubts for researchers, and there is no categorical answer in graphic image of this system at present time. It can be explained only by high melting temperatures of manganese and aluminium oxides. It makes 1800 °C for MnO and it exceeds 2100 °C for Al_2O_3 [4].

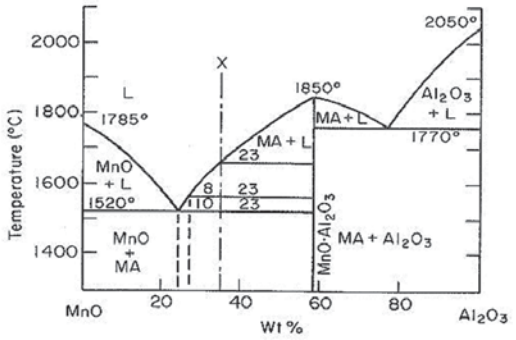


Fig. 1. $MnO–Al_2O_3$ equilibrium diagram

Simple analysis of crystallization fields in different systems gives practically no results about features of melts and about reliability of experimental data based on mutual location of liquidus lines, except weak or strong lowering of melting temperature of the examined phase under effect of the second component. This picture changes cardinally, if we shall examine this effect based on the Bjerrum-Guggenheim osmotic coefficient Φ_i [13]. This coefficient is considered as rather good structurally sensitive melt parameter. Taking into account the real possibility of behaviour evaluation for compounds in melts and the features of inter-particle interaction in liquid phase using the Bjerrum-Guggenheim osmotic coefficient , analysis of crystallization lines of phases allows also to determine data reliability about equilibrium diagrams of these systems and stability of the compounds themselves in melts.

$MnO·Al_2O_3$ congruent compound is characterized by the definite melting point 1849.85 °C [14–16]; melting enthalpy $H_{MnO·Al_2O_3}$ at preset temperature was equal to 167,296.77 J/mol [14]. In this case the compound is characterized by behaviour of individual chemical compound, and the general diagram can be separated to two partial systems: the first diagram is located to the left of the solidus line of congruent compound, it relates to the system MnO–$MnO·Al_2O_3$, and the second diagram – to the right of this line, it relates to the system $MnO·Al_2O_3$– Al_2O_3.

Initial data for temperature and composition were taken from the experimental equilibrium diagram (see Fig. 1) for galaxite crystallization area of the partial system $MnO·Al_2O_3$–MnO. It means that each composition (in vertical) corresponds to each temperature (in horizontal). The initial data for the left part of this equilibrium diagram for the congruent compound $MnO·Al_2O_3$ are presented in the **Table 1**.

Then we build the graph of relationship between the Bjerrum-Guggenheim osmotic coefficient $\Phi_{MnO·Al_2O_3}$ and activity correlation using the data from the Table 1 (**Fig. 2**).

This graph displays non-linear relationship with apparently expressed concave interaction feature, what testifies about non-stability of a chemical compound. Respectively, dissociation process of the congruent compound $MnO·Al_2O_3$ takes place with its quick increase depending on melting temperature, which is characterized by a maximal value and then harshly decreased dissociation process.

Mathematical description of crystallization line for the chemical compound $MnO·Al_2O_3$, for the partial system $MnO·Al_2O_3$–MnO is presented as follows:

$$lnX^{L}_{MnO·Al_2O_3} = \frac{\frac{167296,77}{8,3143}\left(\frac{1}{2123}-\frac{1}{T}\right)+\int_T^{T_m}\left[\frac{1}{RT^2}\int_T^{T_m}C_p dT\right]dT}{5,042-4,666+0,472\cdot exp\left[\frac{167296,77}{8,3143}\left(\frac{1}{2123}-\frac{1}{T}\right)+\int_T^{T_m}\left[\frac{1}{RT^2}\int_T^{T_m}C_p dT\right]dT\right]} \quad (10)$$

Initial parameters for Gibbs energy calculation during galaxite dissociation reaction is presented in the **Table 2**.

Gibbs energy values for dissociation reaction of the chemical compound $MnO·Al_2O_3$ were calculated according to the developed software for heterogeneous and homogeneous reactions with obtaining the data on the equilibrium constant (K_p) and dissociation degree (α). These data are obtained via the Bjerrum-Guggenheim osmotic coefficient for congruently melting compounds during galaxite dissociation reaction. The equilibrium constant along the line of multi-variant phase equilibriums and dissociation degree of congruently melting compounds were also calculated.

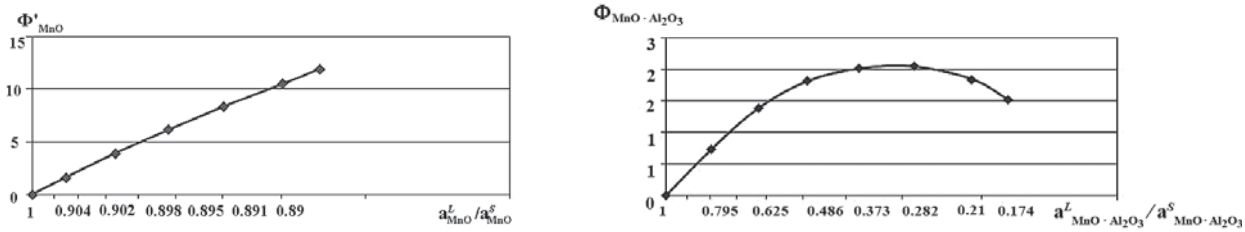
Calculated thermodynamic data about the system $MnO·Al_2O_3$–MnO for dissociation degree of the galaxite compound $MnO·Al_2O_3$ are presented in the **Table 3**. This

Table 1. **Initial data of crystallization area in oxide melt of galaxite $MnO·Al_2O_3$ for the partial system "galaxite – manganese oxide" $MnO·Al_2O_3$–MnO**

Temperature T, °C	$X^{L(0)}_{MnO}$ Liquidus of substance (MnO)	$X^{S(0)}_{MnO}$ Solidus of substance (MnO)	$X^{L(1)}_{MnO·Al_2O_3}$ Liquidus of substance ($MnO·Al_2O_3$)	$X^{S(1)}_{MnO·Al_2O_3}$ Solidus of substance ($MnO·Al_2O_3$)	$\ln a^{L}_{MnO·Al_2O_3}/a^{S}_{MnO·Al_2O_3}$ Logarithm of activity correlation	$a^{L}_{MnO·Al_2O_3}/a^{S}_{MnO·Al_2O_3}$ Activity correlation	$\Phi_{MnO·Al_2O_3}$ Osmotic coefficient
1849.85	0.5	0.5	1	1.000	0	1	0
1799.85	0.578	0.5	0.7956	1.000	–0.2286	0.7956	0.7267
1749.85	0.584	0.5	0.6259	1.000	–0.4685	0.6259	1.3811
1699.85	0.598	0.5	0.4865	1.000	–0.7206	0.4865	1.8144
1649.85	0.62	0.5	0.3732	1.000	–0.9857	0.3732	2.0135
1599.85	0.65	0.5	0.2822	1.000	–1.2651	0.2822	2.0436
1549.85	0.7	0.5	0.2102	1.000	–1.5597	0.2102	1.8408
1519.85	0.76	0.5	0.1748	1.000	–1.7444	0.1748	1.5133

Table 2. **Initial parameters for Gibbs energy calculation during galaxite dissociation reaction [4, 13, 18]**

Substance	Stoichiometric coefficient	Temperature T, °C	Enthalpy dH_o kJ/mol	Entropy S_o kJ/mol grad	A	B	C
MnO	1	25	–385.1856	0.059871	46.515	8.122	–3.684
		1874.85	54.4284	0.025339	56.522	0	0
		3126.85	383.15672	0.142105	35.376	1.256	–3.643
Al_2O_3	1	25	–1674.72	0.051079	114.56	12.89	–34.31
		2053.85	118.48646	0.050918	144.947	0	0
$MnAl_2O_4$	1	25	–2098.0055	0.105507	110.532	54.01	0
Galaxite		1559.85	150	0.075	230.486	0	0



(*a*) (*b*)

Fig. 2. Relationship between the Bjerrum-Guggenheim osmotic coefficient Φ'_{MnO} (*a*), $\Phi_{MnO \cdot Al_2O_3}$ (*b*) and activity correlation $a^L_{MnO \cdot Al_2O_3} / a^S_{MnO \cdot Al_2O_3}$ for the partial system $MnO \cdot Al_2O_3$–MnO

compound is unstable, dissociation degree makes 50 % (according to the calculated data), i.e. both galaxite molecules and oxides of manganese and aluminium are presented in the melt in equal amounts.

The new values of the Bjerrum-Guggenheim osmotic coefficient in the form of correlation line (**Fig. 3**) were obtained according to the equilibrium calculation method for dissociation (association) parameters of a congruent compound on the base of analysis of the mono-variant equilibrium line (see Table 3). Examination of behaviour of the Bjerrum-Guggenheim osmotic coefficient near the melting temperature of the compound [16] displayed that the relation is presented by a straight line if all existing components in the melt are taken into account.

Crystallization area $MnO \cdot Al_2O_3$ for the partial system $MnO \cdot Al_2O_3$–MnO (see Fig. 1) was also examined according to the processing technique for experimental data along the crystallization line of $MnO \cdot Al_2O_3$ compound [19–21]. The initial data for concluding the correlation relationship of the Bjerrum-Guggenheim osmotic coefficient are presented in the **Table 4** [22].

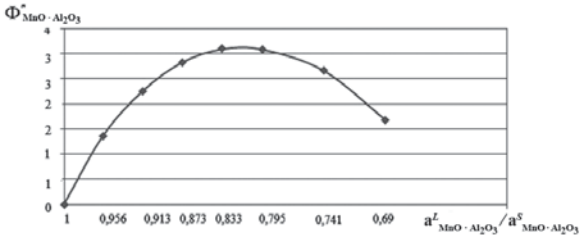


Fig. 3. Graph of relationship between the Bjerrum-Guggenheim osmotic coefficient (Φ") and activity correlation for the partial system $MnO \cdot Al_2O_3$–Al_2O_3

Based on the obtained experimental data on $\Phi''_{MnO \cdot Al_2O_3}$ and $a^L_{MnO \cdot Al_2O_3}/a^S_{MnO \cdot Al_2O_3}$, and according to the calculated data (see Table 4), the graph of relationship between the Bjerrum-Guggenheim osmotic coefficient and activity relation was built (**Fig. 3**).

Dissociation process of the chemical compound $MnO \cdot Al_2O_3$ (graph concavity) can be seen distinctly in the Fig. 3; the compound is weak, dissociation starts from the

Table 3. **Calculated thermodynamic data of the "galaxite – manganese oxide" system $MnO \cdot Al_2O_3$–MnO**

T, °C Temperature	ΔG, J Gibbs energy	K_p Direct properties	A Activity	$X_{(new)}$ $a^L_{MnO \cdot Al_2O_3}$ Substance	$\Phi''_{MnO \cdot Al_2O_3\ new}$ Osmotic coefficient
1849.85	157535	0.000132995	0.5000665	0.00013	0
1799.85	158290	0.000102642	0.5000236	0.00010	0.329823
1749.85	158050	0.000082974	0.5000176	0.00008	0.675939
1699.85	158417	0.000063943	0.5000110	0.00006	1.039583
1649.85	158589	0.000049211	0.5000056	0.00005	1.422129
1599.85	158643	0.000037633	0.5000015	0.00004	1.825094
1549.85	158642	0.000028461	0.5000020	0.00003	2.250186
1519.85	158640	0.000023891	0.5000044	0.00002	2.516636

Table 4. **Initial data of crystallization area in galaxite $MnO{\cdot}Al_2O_3$ for the partial system "galaxite – aluminium oxide" $MnO{\cdot}Al_2O_3$– Al_2O_3**

Temperature T, °C	$X^{L(0)}_{MnO}$ Liquidus of substance (MnO)	$X^{S(0)}_{MnO}$ Solidus of substance (MnO)	$X^{L(1)}_{MnO\cdot Al_2O_3}$ Liquidus of substance ($MnO{\cdot}Al_2O_3$)	$X^{S(1)}_{MnO\cdot Al_2O_3}$ Solidus of substance ($MnO{\cdot}Al_2O_3$)	$\ln a^L_{MnO\cdot Al_2O_3}/a^S_{MnO\cdot Al_2O_3}$ Logarithm of activity	$a^L_{MnO\cdot Al_2O_3}/a^S_{MnO\cdot Al_2O_3}$ Activity correlation	$\Phi_{MnO\cdot Al_2O_3}$ Osmotic coefficient
1849.85	0.5	0.5	1.0000	1.0	0	1.0000	0
1839.85	0.4918	0.5	0.9677	1.0	–0.0449	0.9561	1.3674
1829.85	0.49	0.5	0.9608	1.0	–0.0901	0.9138	2.2531
1819.85	0.488	0.5	0.9531	1.0	–0.1358	0.8730	2.8297
1809.85	0.4853	0.5	0.9429	1.0	–0.1820	0.8336	3.0944
1799.85	0.4815	0.5	0.9286	1.0	–0.2286	0.7956	3.0878
1784.85	0.472	0.5	0.8939	1.0	–0.2993	0.7413	2.6699
1769.85	0.445	0.5	0.8018	1.0	–0.3711	0.6900	1.6801

first minutes of temperature lowering and achieves maximal values within the temperature range 1816.85–1786.85 °C.

Mathematical description of the crystallization line of the chemical compound $MnO{\cdot}Al_2O_3$ for the partial system $MnO{\cdot}Al_2O_3$– Al_2O_3 is presented as the following equation:

$$lnX^L_{MnO\cdot Al_2O_3} = \frac{\frac{167296,77}{8,3143}\left(\frac{1}{2123}-\frac{1}{T}\right)+\int_T^{Tm}\left[\frac{1}{RT^2}\int_T^{Tm}C_p dT\right]dT}{123,982-74,834+48,779.exp\left[\frac{167296,77}{8,3143}\left(\frac{1}{2123}-\frac{1}{T}\right)+\int_T^{Tm}\left[\frac{1}{RT^2}\int_T^{Tm}C_p dT\right]dT\right]} \quad (11)$$

According to the developed technique for quantitative evaluation of forming degree for compound associates depending on curvature of the liquidus line [22], numerical results of dissociation degree for the congruent compound $MnO{\cdot}Al_2O_3$ were obtained using Gibbs energy values in dissociation and the reaction constant (**Table 5**).

Calculating dissociation degree of the compound $MnO{\cdot}Al_2O_3$ (see Table 5), it is possible to calculate the real composition parameters for this crystallization area of the compound, i.e. to solve the reverse problem after introduction of α values in the equations (5) [7, 23].

Based on the obtained experimental data, the diagram of relationship between the Bjerrum-Guggenheim osmotic coefficient and activity relation was built (**Fig. 4**).

Fig. 4 displays strictly correlation relationship between the Bjerrum-Guggenheim osmotic coefficient $\Phi_{MnO\cdot Al_2O_3}$ and activity correlation $a^L_{MnO\cdot Al_2O_3}/a^S_{MnO\cdot Al_2O_3}$; it means that molecules of dissociation process – oxides MnO and Al_2O_3 are presented in the melt, in addition to $MnO{\cdot}Al_2O_3$ molecules. This dissociation process increases from the eutectic temperature to melting temperature up to 50 %. Practically straight feature of variation of $\Phi_{MnO\cdot Al_2O_3}$ testifies about presence of mainly van der Waals interaction forces between particles in the melt, as well as about constant feature of galaxite dissociation during varying the melt composition along the liquidus line.

Comparative literature analysis of the experimental data and obtained calculated data on dissociation degree of galaxite alloys can be executed in accordance with the only work [9], separately for manganese oxides and aluminium oxides. Dissociation degree at the temperature 1599,85 °C was 83 % for manganese oxides, while dissociation constants of liquid and solid alumina ($LgKp_{(Al_2O_3)}$) for aluminium oxides were 23.21 and 45.78 respectively [9, 10]. The obtained

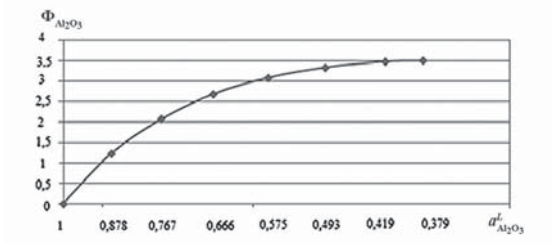


Fig. 4. Diagram of relationship between the Bjerrum-Guggenheim osmotic coefficient (Φ") and activity correlation for the partial system $MnO{\cdot}Al_2O_3$–Al_2O_3

Table 5. **Calculated thermodynamic parameters of the system $MnO{\cdot}Al_2O_3$– Al_2O_3**

T, °C Temperature	ΔG, J Gibbs energy	K_p Direct properties	A Activity	$X_{(new)}\, a^L_{MnO\cdot Al_2O_3}$ Substance	$\Phi''_{MnO\cdot Al_2O_3\ new}$ Osmotic coefficient
1849.85	156900	0.00013780	0.5000689	0.000137781	0
1839.85	157556	0.00012730	0.5000596	0.000127284	0.064723
1829.85	155708	0.00013560	0.5000625	0.000135582	0.130062
1819.85	156377	0.00012500	0.5000567	0.000124984	0.196022
1809.85	156964	0.00011580	0.5000513	0.000115787	0.262613
1799.85	157475	0.00010760	0.5000461	0.000107588	0.329845
1784.85	159912	0.00010035	0.5000395	0.000100340	0.397725
1769.85	158315	0.00008956	0.5000270	0.000089554	0.535472

numerical results of dissociation degree for a galaxite congruent compound made 50 %, using Gibbs energy of dissociation and equilibrium constant of the reaction.

Conclusion

The features of forming the crystallization fields for the phases of galaxite congruent compound ($MnO{\cdot}Al_2O_3$) are characterized by more complicated parameters of relationship between the Bjerrum-Guggenheim osmotic coefficient and activity. Analytical relationships of crystallization phases in congruent compounds show the enormous positive deviation from an ideal relationship (Φ'_i values exceed 1.0 significantly) occurring in the melt, thus dissociation process strengthens with temperature decrease. Respectively, analysis of graphs characterizing relationship between the Bjerrum-Guggenheim osmotic coefficients Φ'_i and activity allows to mark location of the most low-melting and high-melting compounds in multi-component systems and then, based on the results of thermodynamic properties of melts after examination of the Bjerrum-Guggenheim osmotic coefficient, to evaluate structural and energetic state of oxide melts in general and oxides of manganese, silicon and aluminium in particular. It will provide assessment of dissociation degree within the temperature range 1399.85–2099.85 °C.

Numerical results of dissociation degree of galaxite congruent compound were obtained using Gibbs energy of dissociation and equilibrium constant of the reaction. Behaviour of the Bjerrum-Guggenheim osmotic coefficient as a criterion of melt structure evaluation is demonstrated. It is established that dissociation degree of $MnO{\cdot}Al_2O_3$ compound increases with temperature rise and makes 50 % at the melting temperature.

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