

APPLICATION OF THE POLYMER THEORY TO MULTICOMPONENT SILICATE AND  
ALUMINOSILICATE MELTS

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Synopsis: Methods of ionic composition and components activities calculation in  $MeO^1 \dots MeO^n - SiO_2$  system were examined considering cation environment of various silicon-oxygen anions, and  $CaO-Al_2O_3$  based on the polymeric theory of oxides melts structure. For melts of  $CaO-Al_2O_3$  various aluminum coordination in the form of  $Al^+$ ,  $AlO^+$  and anion environment of  $Al \times O^y$  were taken into account. Calculation results of ionic composition and components activities in the system under study are given.

Key words: oxygen anions, alumo-oxygen anions, complex formation, polymerization constant.

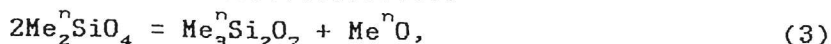
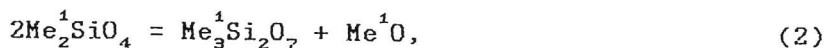
1. MULTICOMPONENT SILICATE MELTS

At present methods are elaborated which allow to calculate ionic composition and components activity in triple system of  $MeO^1 - MeO^2 - SiO_2$  [1] type and in multicomponent oxides melts of  $MeO^1 \dots MeO^n - SiO_2$ , based on the polymeric theory. In [2] all cations in the melts are energetically averaged, i.e. binary system of  $MeO - SiO_2$  with averaged polymerization constant  $k$  is examined:

$$\ln k_n = N_{MeO^1} \ln k_{2,0}^1 \left[ \sum_{i=0}^n N_{MeO^i} \right]^{-1} + \dots + N_{MeO^n} \ln k_{2,0}^n \left[ \sum_{i=0}^n N_{MeO^i} \right]^{-1}, \quad (1)$$

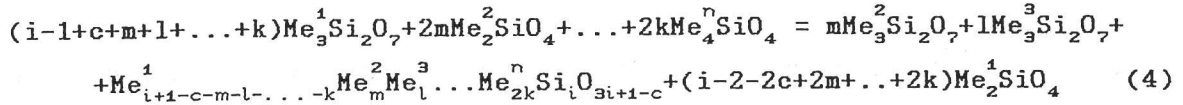
where  $N_{MeO^1}, \dots, N_{MeO^n}$  are mole fractions of  $MeO^1, \dots, MeO^n$  oxides respectively;  $k_{2,0}^1, \dots, k_{2,0}^n$  are polymerization constants in binary systems of  $MeO^1 - SiO_2, \dots, MeO^n - SiO_2$ .

This study, based on O.A. Yesin's approach, suggests methods of ionic composition and components activities calculation in melts of  $MeO^1 \dots MeO^h - MeO^{h+1} \dots MeO^2 - SiO_2$  considering cation environment composition of complex anions. In the binary melts cation of Me are neighbors to all anions whereas in n-component system anions of  $SiO_{3i+1-c}$  have cation environment cationing various quantities of  $Me^1 \dots Me^n$ , which corresponds to ionic groups of  $Me_{i+1-c-m}^1 \dots Me_m^2 \dots Me_{2k}^n \times SiO_{3i+1-c}$  type. Suppose  $k_{2,0}^1, k_{2,0}^2, \dots, k_{2,0}^n$  are balance constants of the following reactions:

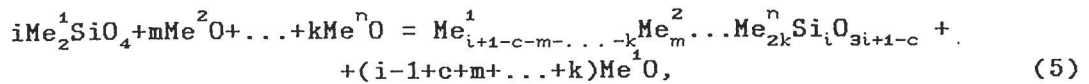


We can disregard energetic differences in attaching and self-locking of  $SiO_4$  groups, i.e. suppose  $k_{2,0}^1, k_{2,0}^2, \dots, k_{2,0}^n$  values are irrespective

of  $i$  and  $c$  as this was in [1,3-5]. In consequence of assumption of  $k_{2,O}^1$ ,  $k_{2,O}^2, \dots, k_{2,O}^n$  being irrespective of  $i$  and  $c$  for any polymerization reaction including reaction of the following type:



standard change of Gibb's energy is proportional to mole quantity  $MeO$  ( $n_{MeO}$ ) taking part in the reaction. Since for equations (4)  $n_{MeO} = 0$ ,  $\Delta G^0$  in the limits of the accepted assumptions is equal to zero and  $k_{(4)} = 1$ . Whereas for reaction (5) being a sum of reactions (2-4),



in approximation of perfect ionic solution, equation of complex anions distributions is equal to:

$$N_{i,c,m,\dots,k} = \frac{N_O^{2-}}{k_{2,O}^1} \left[ \frac{k_{2,O}^1 N_{1,4}^1}{N_O^{2-}} \right]^i \left[ \frac{k_{2,O}^1}{N_O^{2-}} \right]^c \left[ \frac{k_{2,O}^2 N_O^{2-}}{k_{2,O}^1 N_O^{2-}} \right]^m \dots \left[ \frac{k_{2,O}^n N_O^{2-}}{k_{2,O}^1 N_O^{2-}} \right]^k, \quad (6)$$

where  $N_O^{2-}, \dots, N_O^{2-}$  are ionic fractions of free oxygen connected with cations of  $Me^1, \dots, Me^n$  respectively;  $N_{1,4}^1$  - ionic fraction of  $SiO_4^{4-}$  anion, cation environment of which includes only  $Me^1$  cations.

Indicate, as in [1],  $N_{1,4}^1 = U$ ,  $k_{2,O}^1/N_O^{2-} = V$ ,  $(k_{2,O}^2 N_O^{2-}/k_{2,O}^1 N_O^{2-}) = t, \dots$   $(k_{2,O}^n N_O^{2-}/k_{2,O}^1 N_O^{2-}) = f$ . Then

$$N_{i,c,m,\dots,k} = V^{c-1} (UV)^i t^m \dots f^k. \quad (7)$$

Expression (8) contains variables  $(N_O^{2-}, N_O^{2-}, \dots, N_O^{2-}, N_{1,4}^1)$ . To find these variables, we may use the following equations:

$$\sum_{c=0}^{\infty} \sum_{i=c+1}^{\infty} \sum_{m=0}^{i+1-c} \dots \sum_{k=0}^{i+1-c-m-\dots-p} N_{i,c,m,\dots,k} + \sum_{j=1}^n N_O^{2-} = 1; \quad (8)$$

$$1 + \sum_{c=0}^{\infty} \sum_{i=c+1}^{\infty} \sum_{m=0}^{i+1-c} \dots \sum_{k=0}^{i+1-c-m-\dots-p} (2i-c) N_{i,c,m,\dots,k} = D; \quad (9)$$

$$\left[ N_O^{2-} + \sum_{c=0}^{\infty} \sum_{i=c+1}^{\infty} \sum_{m=0}^{i+1-c} \dots \sum_{k=0}^{i+1-c-m-\dots-p} (i+1-c-m-\dots-k) N_{i,c,m,\dots,k} \right]^{-1} D = N_{MeO}^1; \quad (10)$$

$$\left[ N_O^{2-} + \sum_{c=0}^h \sum_{i=c+1}^{\infty} \sum_{m=0}^{i+1-c} \dots \sum_{k=0}^{i+1-c-m-\dots-p} \varepsilon(h) N_{i,c,m,\dots,k} \right]^{-1} D = N_{MeO}^h; \quad (11)$$

$$h = \{2, 3, \dots, n\}; \quad \varepsilon(h) = \{m, l, \dots, k\}; \quad (12)$$

Study [6] contains finite expression for a four-component system. However, sum values in equations (8-11) we may determine on recurrent

dependence:

$$S_j = \left[ S_j(x, y, t_1, \dots, t_{n-1}) - t_n S_j(t_n, x, y, y/t_n, t_1/t_n, \dots, t_{n-1}/t_n) \right], \quad (13)$$

where  $x = N_{1,4}^1 k_{2,o}^1 / N_0^{1,2-}$ ,  $y = k_{2,o}^2 / N_0^{1,2-}$ ,  $S_j^n$  - n-dimensional sum of

$$\sum_{c=0}^{\infty} \sum_{i=c+1}^{\infty} \sum_{m=0}^{i+1-c} \dots \sum_{k=0}^{i+1-c-m-\dots-p} j N_{i,c,m,\dots,k} = S_j^n, \quad j = \{1, i, c, m, \dots, k\}, \quad (14)$$

let's note that

$$S_p^3 = \left[ t_l (S_i^2 + 2S_1^2 - S_c^2) - (S_i^2 + 2S_1^2 - S_c^2) \right] (1 - t_l)^{-2}, \quad p = \{m, \dots, k\}, \quad l = \{1, 2, \dots, n\}. \quad (15)$$

As in [1] reactivities of basic oxides of molten metal are equal to  $a_{MeO} = N_0^{1,2-}$ . Activity of silica was calculated according to the following

equation  $a_{SiO_2} = N_{1,4}^1 (k_{2,o}^1 / N_0^{1,2-})^2$ . Let's illustrate the elaborated method

following the example of system FeO-MnO-MgO-CaO-SiO<sub>2</sub> and FeO-MgO-CaO-SiO<sub>2</sub>. Table 1 shows ionic composition and activity of FeO in melts FeO-MnO-MgO-CaO-SiO<sub>2</sub> at 1873K. Calculations are made at the following polymerization constant values:  $k_{2,o}^1 = 0.9$ ,  $k_{2,o}^2 = 0.2$ ,  $k_{2,o}^3 = 0.03$ ,  $k_{2,o}^4 = 0.003$  [1].

Table 1 Ionic Composition and Activity FeO in the System

FeO-MnO-MgO-CaO-SiO<sub>2</sub> at 1873K

N <sub>s</sub>	Slag composition, mas%				N <sub>1,4</sub> <sup>1</sup>	N <sub>0</sub> <sup>1,2-</sup>	N <sub>0</sub> <sup>2-</sup>	N <sub>0</sub> <sup>3-</sup>	N <sub>0</sub> <sup>4-</sup>	a <sub>FeO</sub> [7] <sub>exp</sub>
	CaO	SiO <sub>2</sub>	FeO	MgO						
1	16.78	5.73	67.79	4.71	2.32 · 10 <sup>-4</sup>	0.745	0.026	0.074	4.74 · 10 <sup>-2</sup>	0.765
2	0.32	2.52	62.24	1.82	2.30 · 10 <sup>-3</sup>	0.633	0.312	0.021	6.71 · 10 <sup>-4</sup>	0.581
3	0.34	13.74	42.48	5.68	1.01 · 10 <sup>-2</sup>	0.490	0.248	0.025	1.65 · 10 <sup>-4</sup>	0.477
4	0.28	22.12	28.63	12.57	4.39 · 10 <sup>-3</sup>	0.410	0.299	0.055	1.76 · 10 <sup>-4</sup>	0.396

Table 2 shows ionic composition of melts FeO-MgO-CaO-SiO<sub>2</sub>. From Table 2 we can see that increase of SiO<sub>2</sub> contents in slags causes significant increase of Mg<sub>2</sub>SiO<sub>4</sub> and Ca<sub>2</sub>SiO<sub>4</sub> contents and appearance of complex Fe<sub>i+1-c-m-k</sub>Mg<sub>m</sub>Ca<sub>k</sub>xSiO<sub>3i+1-c</sub> containing a number of cations. In Table 3 calculation results on equation (8-12) are compared to experimental data. It should be noted that in studies [8,9] data for systems (MnO+MgO+CaO)+FeO+(SiO<sub>2</sub>+P<sub>2</sub>O<sub>5</sub>) are given. It may be the reason of discrepancy, especially when MgO quantities are high (25 and 40 mole %). Activities of FeO and SiO<sub>2</sub> in [8,9] are rated on pure liquid non-stoichiometric FeO and pure solid SiO<sub>2</sub>.

Table 2 Ionic Composition in the System FeO-MgO-CaO-SiO<sub>2</sub> at 1873K

N <sub>s</sub>	Slag comps., mol%			N <sub>0</sub> <sup>1,2-</sup>	N <sub>0</sub> <sup>2-</sup>	N <sub>0</sub> <sup>3-</sup>	N <sub>1,4</sub> <sup>1</sup>	N <sub>1,4</sub> <sup>2</sup>	N <sub>1,4</sub> <sup>3</sup>
	FeO	MgO	CaO						
1	53.0	10.0	10.0	0.646	9.3 · 10 <sup>-3</sup>	1.6 · 10 <sup>-4</sup>	0.120	0.022	6.6 · 10 <sup>-4</sup>
2	61.0	10.0	10.0	0.760	2.1 · 10 <sup>-2</sup>	2.8 · 10 <sup>-3</sup>	0.036	0.025	4.4 · 10 <sup>-2</sup>
3	30.0	15.0	10.0	0.386	8.5 · 10 <sup>-3</sup>	9.4 · 10 <sup>-5</sup>	0.096	0.042	5.1 · 10 <sup>-4</sup>
4	20.0	10.0	30.0	0.446	6.9 · 10 <sup>-3</sup>	4.2 · 10 <sup>-4</sup>	0.110	0.024	8.8 · 10 <sup>-3</sup>
5	35.0	10.0	30.0	0.673	1.1 · 10 <sup>-2</sup>	2.1 · 10 <sup>-4</sup>	0.120	0.029	1.1 · 10 <sup>-3</sup>
6	80.0	5.0	5.0	0.879	1.8 · 10 <sup>-2</sup>	3.2 · 10 <sup>-3</sup>	0.021	0.004	2.5 · 10 <sup>-2</sup>
7	25.0	10.0	10.0	0.228	5.5 · 10 <sup>-3</sup>	7.2 · 10 <sup>-4</sup>	0.042	0.022	3.8 · 10 <sup>-2</sup>
8	20.0	25.0	15.0	0.350	1.2 · 10 <sup>-2</sup>	1.1 · 10 <sup>-3</sup>	0.055	0.058	4.9 · 10 <sup>-2</sup>
9	15.0	40.0	10.0	0.445	1.5 · 10 <sup>-2</sup>	8.8 · 10 <sup>-4</sup>	0.073	0.075	2.6 · 10 <sup>-2</sup>

Table 3 follows that the calculated values of activities are in good conformity with experimental data. According to evaluations of root - mean - square deviations (R) of the calculated activities of FeO and SiO<sub>2</sub>

from the experimental ones, calculation of cation environment composition of anions is 3-7 times more than calculation accuracy.

Table 3 Activities of Components in the system FeO-MgO-CaO-SiO<sub>2</sub> at 1873K

N <sub>s</sub>	a <sub>FeO</sub>	a <sub>FeO</sub> [7]	a <sub>FeO</sub> [10]	*	**	exp.	a <sub>SiO<sub>2</sub></sub>	*	**	exp.
				a <sub>FeO</sub> [2]	a <sub>FeO</sub> [2]	a <sub>FeO</sub> [8]		a <sub>S</sub> [2] <sub>2</sub>	a <sub>S</sub> [2] <sub>2</sub>	a <sub>S</sub> [8] <sub>2</sub>
1	0.646	0.784	1.090	0.433	0.451	0.690	0.254	0.081	0.077	0.26
2	0.760	0.800	1.280	0.566	0.581	0.83	0.055	0.041	0.039	0.08
3	0.386	0.678	0.244	0.105	0.107	0.44	0.568	0.34	0.33	0.51
4	0.466	0.638	0.246	0.075	0.071	0.42	0.488	0.12	0.11	0.47
5	0.673	0.722	0.664	0.446	0.529	0.70	0.230	0.006	0.004	0.10
6	0.879	0.860	0.901	0.746	0.750	0.94	0.024	0.043	0.029	0.05
7	0.228	0.555	0.126	0.047	0.048	0.23	0.713	0.672	0.667	0.70
8	0.350	0.638	0.239	0.084	0.096	0.41	0.396	0.136	0.124	0.36
9	0.445	0.533	0.201	0.106	0.112	0.45	0.325	0.043	0.038	0.25
R	0.045	0.17	0.24	0.29	0.27	-	0.056	0.179	0.185	-

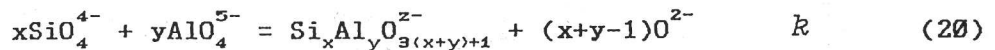
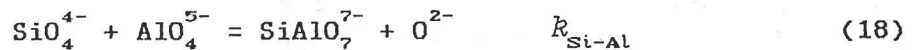
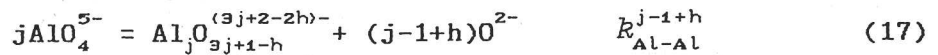
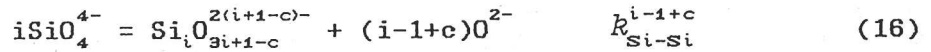
\* -  $k_{2,O}^1=0.9, k_{2,O}^2=0.2, k_{2,O}^3=0.003$ ; \*\* -  $k_{2,O}^1=0.9, k_{2,O}^2=0.25, k_{2,O}^3=0.0016$ [2]

## 2. ALUMINOSILICATE MELTS

It is known that structural units of polymerized anions in the system under consideration are the AlO<sub>4</sub> complexes, which make up chains, rings and other forms of aluminium oxygen anions. Since Al<sub>2</sub>O<sub>3</sub> is an amphoteric oxide, one can expect the appearance of free cations Al<sup>3+</sup> in the melt, or according to some other data, AlO<sup>+</sup> [11].

The absence of data about the real ionic constitution of such melts permits to judge about the correctness of this and some other calculation schemes only in an indirect way, i.e. through the proximity of calculated and experimental values of activities of the components.

Let us assume the following complex formation reactions for systems MeO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> :



where  $K$  is the equilibrium constant the reaction (20).

In this case calculation equations will be as follows:

$$N_{\xi, \sigma, \eta}^1 = K_{\text{Si-Si}}^\xi K_{\text{Si-Al}}^{2\sigma} K_{\text{Al-Al}}^\eta \frac{N_{1,4,\text{Si}}^{\xi+\sigma+1} N_{1,4,\text{Al}}^{\xi+\sigma}}{N_{\text{O}^{2-}}^{2\sigma+\xi+\eta}} \quad (21)$$

$$N_{\xi, \sigma, \eta}^2 = K_{\text{Si-Si}}^\xi K_{\text{Si-Al}}^{2\sigma} K_{\text{Al-Al}}^\eta \frac{N_{1,4,\text{Si}}^{\xi+\sigma} N_{1,4,\text{Al}}^{\xi+\sigma+1}}{N_{\text{O}^{2-}}^{2\sigma+\xi+\eta}} \quad (22)$$

$$N_{\xi, \sigma, \eta}^3 = K_{\text{Si-Si}}^\xi K_{\text{Si-Al}}^{2\sigma+1} K_{\text{Al-Al}}^\eta \frac{N_{1,4,\text{Si}}^{\xi+\sigma+1} N_{1,4,\text{Al}}^{\xi+\sigma+1}}{N_{\text{O}^{2-}}^{2\sigma+\xi+\eta+1}} \quad (23)$$

$$N_{i,c} = k_{\text{Si-Si}}^{i-1+c} N_{1,4,\text{Si}}^i N_{\text{O}^{2-}}^{-(i-1+c)} \quad (24)$$

$$N_{j,h} = k_{\text{Al-Al}}^{j-1+h} N_{1,4,\text{Al}}^j N_{\text{O}^{2-}}^{-(j-1+h)} \quad (25)$$

$$\sum_{c=0}^{\infty} \sum_{i=c+1}^{\infty} N_{i,c} + \sum_{h=0}^{\infty} \sum_{j=h+1}^{\infty} N_{j,h} + \sum_{\sigma=1}^{\infty} \sum_{\xi=0}^{\infty} \sum_{\eta=0}^{\infty} N_{\xi,\sigma,\eta}^1 + \sum_{\sigma=1}^{\infty} \sum_{\xi=0}^{\infty} \sum_{\eta=0}^{\infty} N_{\xi,\sigma,\eta}^2 + \sum_{\sigma=0}^{\infty} \sum_{\xi=0}^{\infty} \sum_{\eta=0}^{\infty} N_{\xi,\sigma,\eta}^3 + N_{\text{O}^{2-}} = 1 \quad (26)$$

- balance for silica atoms :

$$\sum C^- \left[ \sum_{c=0}^{\infty} \sum_{i=c+1}^{\infty} i N_{i,c} + \sum_{\sigma=0}^{\infty} \sum_{\xi=0}^{\infty} \sum_{\eta=0}^{\infty} (\xi+\sigma+1) N_{\xi,\sigma,\eta}^3 + \sum_{\sigma=1}^{\infty} \sum_{\xi=0}^{\infty} \sum_{\eta=0}^{\infty} (\xi+\sigma+1) N_{\xi,\sigma,\eta}^1 + \sum_{\sigma=1}^{\infty} \sum_{\xi=0}^{\infty} \sum_{\eta=0}^{\infty} (\xi+\sigma) N_{\xi,\sigma,\eta}^2 \right] = C_{\text{SiO}_2} \quad (27)$$

- balance for aluminium atoms :

$$\sum C^- \left[ \sum_{h=0}^{\infty} \sum_{j=h+1}^{\infty} j N_{j,h} + \sum_{\sigma=0}^{\infty} \sum_{\xi=0}^{\infty} \sum_{\eta=0}^{\infty} (\eta+\sigma+1) N_{\xi,\sigma,\eta}^3 + \sum_{\sigma=1}^{\infty} \sum_{\xi=0}^{\infty} \sum_{\eta=0}^{\infty} (\eta+\sigma+1) N_{\xi,\sigma,\eta}^2 + \sum_{\sigma=1}^{\infty} \sum_{\xi=0}^{\infty} \sum_{\eta=0}^{\infty} (\eta+\sigma) N_{\xi,\sigma,\eta}^1 \right] = C_{\text{Al}_2\text{O}_3} \quad (28)$$

- balance for electricity :

$$\sum C^- \left[ 2N_{\text{O}^{2-}} + \sum_{c=0}^{\infty} \sum_{i=c+1}^{\infty} 2(i+1-c) N_{i,c} + \sum_{h=0}^{\infty} \sum_{j=h+1}^{\infty} (3j+2-2h) N_{j,h} + \sum_{\sigma=1}^{\infty} \sum_{\xi=0}^{\infty} \sum_{\eta=0}^{\infty} (3\eta+5\sigma+2\xi+4) N_{\xi,\sigma,\eta}^1 + \sum_{\sigma=1}^{\infty} \sum_{\xi=0}^{\infty} \sum_{\eta=0}^{\infty} (3\eta+5\sigma+2\xi+5) N_{\xi,\sigma,\eta}^2 + \sum_{\sigma=0}^{\infty} \sum_{\xi=0}^{\infty} \sum_{\eta=0}^{\infty} (3\eta+5\sigma+2\xi+7) N_{\xi,\sigma,\eta}^3 \right] = 2C_{\text{MeO}} + C_{\text{Al}_2\text{O}_3} \left[ 1 + \frac{2k_{\theta}}{k_{\theta} + N_{\text{O}^{2-}}} \right] \quad (29)$$

where  $\sum C^-$  is the sum of the concentrations of all anions in mole/m<sup>3</sup>;  $C_{\text{MeO}}$ ,  $C_{\text{Al}_2\text{O}_3}$ ,  $C_{\text{SiO}_2}$  are respectively, concentrations of MeO, Al<sub>2</sub>O<sub>3</sub> and SiO<sub>2</sub> in mole/m<sup>3</sup>;  $N_{1,4,\text{Si}}$ ,  $N_{1,4,\text{Al}}$  are the ionic fractions of the anions SiO<sub>4</sub><sup>4-</sup> and AlO<sub>4</sub><sup>5-</sup>. We find activities of the components of the melt, within the assumed scheme, from the expressions:

$$a_{\text{SiO}_2} = k_{\text{Si-Si}}^2 N_{1,2,\text{Si}} N_{\text{O}^{2-}}^{-2}; \quad (30)$$

$$a_{\text{Al}_2\text{O}_3} = k_{\text{Al-Al}}^2 N_{\text{AlO}} + N_{1,4,\text{Al}} N_{\text{O}^{2-}}; \quad (31)$$

$$a_{\text{CaO}} = N_{\text{O}^{2-}} N_{\text{Ca}^{2+}}; \quad (32)$$

where  $N_{\text{AlO}^+}$ ,  $N_{\text{Ca}^{2+}}$  are the ionic fractions of the anions AlO<sup>+</sup> and Ca<sup>2+</sup> respectively.

Table 4 shows ionic compositions and activities components in the

systems CaO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> at 1823K with  $k_{Si-Si} = 0.003[1]$ ,  $k_{Al-Al} = 0.04[11]$ ,  $k_0 = 0.012[11]$ ,  $k_{Si-Al} = 0.003$ .

Further development of the proposed methods is connected with taking into account the presence of other complex-forming oxides (TiO<sub>2</sub>, Cr<sub>2</sub>O<sub>3</sub> and other) in the melt and the imperfection of an ionic melt.

Table 4 Ionic Composition and Activities Components in the System CaO - Al<sub>2</sub>O<sub>3</sub> - SiO<sub>2</sub> at 1823K

Mole fractions			N <sub>O<sup>2-</sup></sub>	N <sub>1,4, Si</sub>	N <sub>1,4, Al</sub>	N <sub>AlO<sup>+</sup></sub>	a <sub>CaO</sub>	a <sub>SiO<sub>2</sub></sub>	a <sub>Al<sub>2</sub>O<sub>3</sub></sub>
CaO	AlO <sub>3/2</sub>	SiO <sub>2</sub>					exp a <sub>CaO</sub>	exp a <sub>SiO<sub>2</sub></sub>	exp a <sub>Al<sub>2</sub>O<sub>3</sub></sub>
0.4	0.1	0.5	1.98·10 <sup>-3</sup>	0.253	2.24·10 <sup>-3</sup>	1.71·10 <sup>-2</sup>	0.0066 0.005	0.58 0.40	0.056 —
0.3	0.1	0.6	1.40·10 <sup>-3</sup>	0.163	1.16·10 <sup>-3</sup>	1.62·10 <sup>-2</sup>	0.0035 0.0045	0.74 0.70	0.051 —
0.4	0.2	0.4	2.98·10 <sup>-3</sup>	0.360	4.73·10 <sup>-3</sup>	4.18·10 <sup>-2</sup>	0.0086 0.010	0.38 0.25	0.136 0.10
0.2	0.2	0.6	1.25·10 <sup>-3</sup>	0.138	9.59·10 <sup>-4</sup>	3.36·10 <sup>-2</sup>	0.0031 —	0.78 0.68	0.117 —
0.6	0.3	0.1	2.66·10 <sup>-1</sup>	0.287	4.12·10 <sup>-1</sup>	2.06·10 <sup>-1</sup>	0.794 0.80	6·10 <sup>-1</sup> 0.0001	0.0069 —
0.4	0.3	0.3	5.55·10 <sup>-3</sup>	0.526	1.62·10 <sup>-2</sup>	9.22·10 <sup>-2</sup>	0.015 0.022	0.15 0.10	0.28 0.30
0.3	0.3	0.4	2.41·10 <sup>-3</sup>	0.305	3.40·10 <sup>-3</sup>	5.92·10 <sup>-2</sup>	0.0059 0.0045	0.47 0.32	0.20 0.26
0.5	0.4	0.1	5.47·10 <sup>-2</sup>	0.370	3.40·10 <sup>-1</sup>	2.50·10 <sup>-1</sup>	0.145 0.20	0.001 0.0005	0.17 0.26
0.4	0.4	0.2	1.23·10 <sup>-2</sup>	0.580	6.54·10 <sup>-2</sup>	1.80·10 <sup>-1</sup>	0.03 0.05	0.034 0.02	0.45 0.50
0.4	0.5	0.1	2.59·10 <sup>-2</sup>	0.400	1.97·10 <sup>-1</sup>	2.78·10 <sup>-1</sup>	0.06 0.10	0.0054 0.003	0.47 0.50
0.3	0.5	0.2	8.75·10 <sup>-3</sup>	0.550	3.87·10 <sup>-2</sup>	2.01·10 <sup>-1</sup>	0.018 0.02	0.065 0.05	0.60 0.75
0.2	0.5	0.3	3.92·10 <sup>-3</sup>	0.390	6.34·10 <sup>-3</sup>	1.25·10 <sup>-1</sup>	0.0052 0.003	0.32 0.30	0.42 —

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