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APPLICATION OF THE POLYMER THEORY TO MULTICOMPONENT SILICATE AND ALUMINOSILICATE MELTS

N.I.Zalomov*, V.N.Boronenkov**

*Ural Polytechnic Institute & CANPO Corporation Ltd., Ekaterinburg, Russia
**Ural Polytechnic Institute Russia

Synopsis: Methods of ionic composition and components activities calculation in MeO^1-...-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^{3+}, AlO^+ and anion environment of $Al_xO_y^{z-}$ 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-...-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:

$$\ln k_n = N_{MeO^1} \ln k^1_{2,0}\left[\sum_{i=0}^{n} N_{MeO^i}\right]^{-1} + \ldots + N_{MeO^n} \ln k^n_{2\ 0}\left[\sum_{i=0}^{n} N_{MeO^i}\right]^{-1}, \qquad (1)$$

where $N_{MeO^1},\ldots,N_{MeO^n}$ are mole fractions of $MeO^1,\ldots,MeO^n$ oxides respectively; $k^1_{2,0},\ldots,k^n_{2,0}$ are polymerization constants in binary systems of MeO^1-SiO_2,..., 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-...-MeO^h-MeO_2^{h+1}-...-MeO_2^n-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 $Si_iO_{3i+1-c}^{2(i+1-c)}$ have cation environment cationing various quantities of Me^1-...-Me^n, which corresponds to ionic groups of $Me^1_{i+1-c-m-\ldots-k}Me^2_m \ldots Me^n_{2k} x SiO_{3i+1-c}$ type. Suppose $k^1_{2,0}$, $k^2_{2,0}$,..., $k^n_{2,0}$ are balance constants of the following reactions :

$$2Me^1_2SiO_4 = Me^1_3Si_2O_7 + Me^1O, \qquad (2)$$

....

$$2Me^n_2SiO_4 = Me^n_3Si_2O_7 + Me^nO, \qquad (3)$$

We can disregard energetic differences in attaching and self-locking of SiO_4^{4-} groups, i.e suppose $k^1_{2,0}$, $k^2_{2,0}$,..., $k^n_{2,0}$ values are irrespective of i and c as this was in [1,3-5]. In consequence of assumption of $\overset{1}{k}_{2,0}$, $\overset{2}{k}_{2,0}, \ldots, \overset{n}{k}_{2,0}$ being irrespective of i and c for any polymerization reaction including reaction of the following type:

$$(i-1+c+m+l+\ldots+k)\overset{1}{Me}_3Si_2O_7+2m\overset{2}{Me}_2SiO_4+\ldots+2k\overset{n}{Me}_4SiO_4 = m\overset{2}{Me}_3Si_2O_7+l\overset{3}{Me}_3Si_2O_7+$$
$$+\overset{1}{Me}_{i+1-c-m-l-\ldots-k}\overset{2}{Me}_m\overset{3}{Me}_l\ldots\overset{n}{Me}_{2k}Si_iO_{3i+1-c}+(i-2-2c+2m+\ldots+2k)\overset{1}{Me}_2SiO_4 \qquad (4)$$

standard change of Gibb´s energy is proportional to mole quantity MeO (n_{MeO}) taking part in the reaction. Since for equations (4) $n_{MeO}= 0$, ΔG^o 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),

$$i\overset{1}{Me}_2SiO_4+m\overset{2}{Me}O+\ldots+k\overset{n}{Me}O = \overset{1}{Me}_{i+1-c-m-\ldots-k}\overset{2}{Me}_m\ldots\overset{n}{Me}_{2k}Si_iO_{3i+1-c} +$$
$$+(i-1+c+m+\ldots+k)\overset{1}{Me}O, \qquad (5)$$

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

$$N_{i,c,m,\ldots,k}=\frac{\overset{1}{N}_{O^{2-}}}{\overset{1}{k}_{2,0}}\left(\frac{\overset{1}{k}_{2,0}N_{1,4}}{\overset{1}{N}_{O^{2-}}}\right)^i\left(\frac{\overset{1}{k}_{2,0}}{\overset{1}{N}_{O^{2-}}}\right)^c\left(\frac{\overset{1}{k}_{2,0}\overset{2}{N}_{O^{2-}}}{\overset{2}{k}_{2,0}\overset{1}{N}_{O^{2-}}}\right)^m\ldots\left(\frac{\overset{1}{k}_{2,0}\overset{n}{N}_{O^{2-}}}{\overset{n}{k}_{2,0}\overset{1}{N}_{O^{2-}}}\right)^k, \qquad (6)$$

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

Indicate, as in [1], $\overset{1}{N}_{1,4}= U$, $\overset{1}{k}_{2,0}/\overset{1}{N}_{O^{2-}}= V$, $(\overset{1}{k}_{2,0}\overset{2}{N}_{O^{2-}}/\overset{2}{k}_{2,0}\overset{1}{N}_{O^{2-}})= t,\ldots$ $(\overset{1}{k}\ \overset{n}{N}{}^{2-}/\overset{n}{k}\ \overset{1}{N}{}^{2-})= f$. Then

$$N_{i,c,m,\ldots,k} = V^{c-1}(UV)^it^m\ldots f^k. \qquad (7)$$

Expression (8) contains variables $(\overset{1}{N}_{O^{2-}},\overset{2}{N}_{O^{2-}},\ldots,\overset{n}{N}_{O^{2-}},\overset{1}{N}_{1,4})$. To find these variables, we may use the following equations:

$$\sum_{c=0}^{\infty}\sum_{i=c+1}^{\infty}\sum_{m=0}^{i+1-c}\ldots\sum_{k=0}^{i+1-c-m-\ldots-p} N_{i,c,m,\ldots,k} + \sum_{j=1}^{n}\overset{j}{N}_{O^{2-}} = 1; \qquad (8)$$

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

$$\left[\overset{1}{N}_{O^{2-}}+\sum_{c=0}^{\infty}\sum_{i=c+1}^{\infty}\sum_{m=0}^{i+1-c}\ldots\sum_{k=0}^{i+1-c-m-\ldots-p} (i+1-c-m-\ldots-k)N_{i,c,m,\ldots,k}\right]D^{-1} =\overset{1}{N}_{MeO}; \qquad (10)$$

$$\left[\overset{h}{N}_{O^{2-}}+\sum_{c=0}^{\infty}\sum_{i=c+1}^{\infty}\sum_{m=0}^{i+1-c}\ldots\sum_{k=0}^{i+1-c-m-\ldots-p} \overset{h}{\varepsilon(h)}N_{i,c,m,\ldots,k}\right]D^{-1} =\overset{h}{N}_{MeO}; \qquad (11)$$

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

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

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

where $x = N^1_{1,4} k^1_{2,o}/N^1_{O^{2-}}$, $y = k^1_{2,o}/N^1_{O^{2-}}$, S_j^n - n-dimensional sum of

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

let's note that

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

As in [1] reactivities of basic oxides of molten metal are equal to $a_{MeO}{}^{i} = N^{i}_{O^{2-}}$. Activity of silica was calculated according to the following equation $a_{SiO_2} = N^1_{1,4}(k^1_{2,o}/N^1_{O^{2-}})^2$. Let's illustrate the elaborated method following the example of system FeO-MnO-MgO-CaO-SiO_2 and FeO-MgO-CaO-SiO_2. Table 1 shows ionic composition and activity of FeO in melts FeO-MnO-MgO-CaO-SiO_2 at 1873K, Calculations are made at the following polymerization constant values: $k^1_{2,o}=0.9$, $k^2_{2,o}=0.2$, $k^3_{2,o}=0.03$, $k^4_{2,o}=0.003$[1].

Table 1 Ionic Composition and Activity FeO in the System FeO-MnO-MgO-CaO-SiO_2 at 1873K

N_s	Slag composition, mas%				$N^1_{1,4}$	$N^1_{O^{2-}}$	$N^2_{O^{2-}}$	$N^3_{O^{2-}}$	$N^4_{O^{2-}}$	a_{FeO}[7] exp
	CaO	SiO_2	FeO	MgO						
1	16.78	5.73	67.79	4.71	$2.32\cdot10^{-4}$	0.745	0.026	0.074	$4.74\cdot10^{-2}$	0.765
2	0.32	2.52	62.24	1.82	$2.30\cdot10^{-3}$	0.633	0.312	0.021	$6.71\cdot10^{-4}$	0.581
3	0.34	13.74	42.48	5.68	$1.01\cdot10^{-2}$	0.490	0.248	0.025	$1.65\cdot10^{-4}$	0.477
4	0.28	22.12	28.63	12.57	$4.39\cdot10^{-3}$	0.410	0.299	0.055	$1.76\cdot10^{-4}$	0.396

Table 2 shows ionic composition of melts FeO-MgO-CaO-SiO_2. From Table 2 we can see that increase of SiO_2 contents in slags causes significant increase of Mg_2SiO_4 and Ca_2SiO_4 contents and appearance of complex $Fe_{i+1-c-m-k}Mg_mCa_k\times SiO_{3i+1-c}$ 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_2+P_2O_5) are given. It may be the reason of discrepancy, especially when MgO quantities are high (25 and 40 mole %). Activities of FeO and SiO_2 in [8,9] are rated on pure liquid non-stechiometric FeO and pure solid SiO_2.

Table 2 Ionic Composition in the System FeO-MgO-CaO-SiO_2 at 1873K

N_s	Slag comps., mol%			$N^1_{O^{2-}}$	$N^2_{O^{2-}}$	$N^3_{O^{2-}}$	$N^1_{1,4}$	$N^2_{1,4}$	$N^3_{1,4}$
	FeO	MgO	CaO						
1	53.0	10.0	10.0	0.646	$9.3\cdot10^{-3}$	$1.6\cdot10^{-4}$	0.120	0.022	$6.6\cdot10^{-4}$
2	61.0	10.0	10.0	0.760	$2.1\cdot10^{-2}$	$2.8\cdot10^{-3}$	0.036	0.025	$4.4\cdot10^{-2}$
3	30.0	15.0	10.0	0.386	$8.5\cdot10^{-3}$	$9.4\cdot10^{-5}$	0.096	0.042	$5.1\cdot10^{-4}$
4	20.0	10.0	30.0	0.446	$6.9\cdot10^{-3}$	$4.2\cdot10^{-4}$	0.110	0.024	$8.8\cdot10^{-3}$
5	35.0	10.0	30.0	0.673	$1.1\cdot10^{-2}$	$2.1\cdot10^{-4}$	0.120	0.029	$1.1\cdot10^{-3}$
6	80.0	5.0	5.0	0.879	$1.8\cdot10^{-2}$	$3.2\cdot10^{-3}$	0.021	0.004	$2.5\cdot10^{-2}$
7	25.0	10.0	10.0	0.228	$5.5\cdot10^{-3}$	$7.2\cdot10^{-4}$	0.042	0.022	$3.8\cdot10^{-2}$
8	20.0	25.0	15.0	0.350	$1.2\cdot10^{-2}$	$1.1\cdot10^{-3}$	0.055	0.058	$4.9\cdot10^{-2}$
9	15.0	40.0	10.0	0.445	$1.5\cdot10^{-2}$	$8.8\cdot10^{-4}$	0.073	0.075	$2.6\cdot10^{-2}$

Table 3 follows that the calculated values of activities are in good conformity with with experimental data. According to evaluations of root - mean - square deviations (R) of the calculated activities of FeO and SiO_2

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-SiO2 at 1873K

N_s	a_{FeO}	a_{FeO}[7]	a_{FeO}[10]	* a_{FeO}[2]	** a_{FeO}[2]	exp. a_{FeO}[8]	a_{SiO_2}	* a_{SiO_2}[2]	** a_{SiO_2}[2]	exp. a_{SiO_2}[8]
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	–

* - $k^1_{2,0}=0.9, k^2_{2,0}=0.2, k^3_{2,0}=0.003$; ** - $k^1_{2,0}=0.9, k^2_{2,0}=0.25, k^3_{2,0}=0.0016$[2]

2. ALUMINOSILICATE MELTS

It is known that structural units of polymerized anions in the system under consideration are the AlO_4^{5-} complexes, which make up chains, rings and other forms of aluminium oxygen anions. Since Al_2O_3 is an amphoteric oxide, one can expect the appearance of free cations Al^{3+} in the melt, or according to some other date, AlO^+ [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 $MeO-Al_2O_3-SiO_2$:

$$iSiO_4^{4-} = Si_iO_{3i+1-c}^{2(i+1-c)-} + (i-1+c)O^{2-} \qquad k^{i-1+c}_{Si-Si} \tag{16}$$

$$jAlO_4^{5-} = Al_jO_{3j+1-h}^{(3j+2-2h)-} + (j-1+h)O^{2-} \qquad k^{j-1+h}_{Al-Al} \tag{17}$$

$$SiO_4^{4-} + AlO_4^{5-} = SiAlO_7^{7-} + O^{2-} \qquad k_{Si-Al} \tag{18}$$

$$AlO^+ = Al^{3+} + O^{2-} \qquad k_{\partial} \tag{19}$$

$$xSiO_4^{4-} + yAlO_4^{5-} = Si_xAl_yO_{3(x+y)+1}^{2-} + (x+y-1)O^{2-} \qquad k \tag{20}$$

where k is the equilibrium constant the reaction (20).

In this case calculation equations will be as follows:

$$N^1_{\xi,\sigma,\eta} = k^{\xi}_{Si-Si} k^{2\sigma}_{Si-Al} k^{\eta}_{Al-Al} \frac{N^{\xi+\sigma+1}_{1,4,Si} N^{\xi+\sigma}_{1,4,Al}}{N^{2\sigma+\xi+\eta}_{O^{2-}}} \tag{21}$$

$$N^2_{\xi,\sigma,\eta} = k^{\xi}_{Si-Si} k^{2\sigma}_{Si-Al} k^{\eta}_{Al-Al} \frac{N^{\xi+\sigma}_{1,4,Si} N^{\xi+\sigma+1}_{1,4,Al}}{N^{2\sigma+\xi+\eta}_{O^{2-}}} \tag{22}$$

$$N^3_{\xi,\sigma,\eta} = k^{\xi}_{Si-Si} k^{2\sigma+1}_{Si-Al} k^{\eta}_{Al-Al} \frac{N^{\xi+\sigma+1}_{1,4,Si} N^{\xi+\sigma+1}_{1,4,Al}}{N^{2\sigma+\xi+\eta+1}_{O^{2-}}} \tag{23}$$

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

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

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

- balance for silica atoms :

$$\sum C^{-} \left[\sum_{c=0}^{\infty}\sum_{i=c+1}^{\infty} iN_{i,c} + \sum_{\sigma=0}^{\infty}\sum_{\xi=0}^{\infty}\sum_{\eta=0}^{\infty} (\xi+\sigma+1)N^{3}_{\xi,\sigma,\eta} + \sum_{\sigma=1}^{\infty}\sum_{\xi=0}^{\infty}\sum_{\eta=0}^{\infty} (\xi+\sigma+1)N^{1}_{\xi,\sigma,\eta} + \right.$$
$$\left. + \sum_{\sigma=1}^{\infty}\sum_{\xi=0}^{\infty}\sum_{\eta=0}^{\infty} (\xi+\sigma)N^{2}_{\xi,\sigma,\eta} \right] = C_{SiO_2} \qquad (27)$$

- balance for aluminium atoms :

$$\sum C^{-} \left[\sum_{h=0}^{\infty}\sum_{j=h+1}^{\infty} jN_{j,h} + \sum_{\sigma=0}^{\infty}\sum_{\xi=0}^{\infty}\sum_{\eta=0}^{\infty} (\eta+\sigma+1)N^{3}_{\xi,\sigma,\eta} + \sum_{\sigma=1}^{\infty}\sum_{\xi=0}^{\infty}\sum_{\eta=0}^{\infty} (\eta+\sigma+1)N^{2}_{\xi,\sigma,\eta} + \right.$$
$$\left. + \sum_{\sigma=1}^{\infty}\sum_{\xi=0}^{\infty}\sum_{\eta=0}^{\infty} (\eta+\sigma)N^{1}_{\xi,\sigma,\eta} \right] = C_{Al_2O_3} \qquad (28)$$

- balance for electricity :

$$\sum C^{-} \left[2N_{O^{2-}} + \sum_{c=0}^{\infty}\sum_{i=c+1}^{\infty} 2(i+1-c)N_{i,c} + \sum_{h=0}^{\infty}\sum_{j=h+1}^{\infty} (3j+2-2h)N_{j,h} + \right.$$
$$+ \sum_{\sigma=1}^{\infty}\sum_{\xi=0}^{\infty}\sum_{\eta=0}^{\infty} (3\eta+5\sigma+2\xi+4)N^{1}_{\xi,\sigma,\eta} + \sum_{\sigma=1}^{\infty}\sum_{\xi=0}^{\infty}\sum_{\eta=0}^{\infty} (3\eta+5\sigma+2\xi+5)N^{2}_{\xi,\sigma,\eta} +$$
$$\left. \sum_{\sigma=0}^{\infty}\sum_{\xi=0}^{\infty}\sum_{\eta=0}^{\infty} (3\eta+5\sigma+2\xi+7)N^{3}_{\xi,\sigma,\eta} \right] = 2C_{MeO} + C_{Al_2O_3}\left[1 + \frac{2k_{\partial}}{k_{\partial} + N_{O^{2-}}}\right] \qquad (29)$$

where $\sum C^{-}$ is the sum of the concentrations of all anions in mole/m^3; C_{MeO}, $C_{Al_2O_3}$, C_{SiO_2} are respectively, concentrations of MeO, Al_2O_3 and SiO_2 in mole/m^3; $N_{1,4,Si}$, $N_{1,4,Al}$ are the ionic fractions of the anions SiO_4^{4-} and AlO_4^{5-}. We find activities of the components of the melt, within the assumed scheme, from the expressions:

$$a_{SiO_2} = k^{2}_{Si-Si} N_{1,2,Si} N^{-2}_{O^{2-}}; \qquad (30)$$

$$a_{Al_2O_3} = k^{2}_{Al-Al} N_{AlO^{+}} N_{1,4,Al} N_{O^{2-}}; \qquad (31)$$

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

where $N_{AlO^{+}}$, $N_{Ca^{2+}}$ are the ionic fractions of the anions AlO^{+} and Ca^{2+} respectively.

Table 4 shows ionic compositions and activities components in the systems $CaO-Al_2O_3-SiO_2$ at 1823K with k_{Si-Si} = 0.003[1], k_{Al-Al} = 0.04[11], k_{∂} = 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_2, Cr_2O_3 and other) in the melt and the imperfection of an ionic melt.

Table 4 Ionic Composition and Activities Components in the System $CaO - Al_2O_3 - SiO_2$ at 1823K

Mole fractions			$N_{O^{2-}}$	$N_{1,4,Si}$	$N_{1,2,Al}$	N_{AlO^+}	a_{CaO} a^{exp}_{CaO}	a_{SiO_2} $a^{exp}_{SiO_2}$	$a_{Al_2O_3}$ $a^{exp}_{Al_2O_3}$
CaO	$AlO_{\frac{3}{2}}$	SiO_2							
0.4	0.1	0.5	$1.98\cdot10^{-3}$	0.253	$2.24\cdot10^{-3}$	$1.71\cdot10^{-2}$	0.0066 0.005	0.58 0.40	0.056 —
0.3	0.1	0.6	$1.40\cdot10^{-3}$	0.163	$1.16\cdot10^{-3}$	$1.62\cdot10^{-2}$	0.0035 0.0045	0.74 0.70	0.051 —
0.4	0.2	0.4	$2.98\cdot10^{-3}$	0.360	$4.73\cdot10^{-3}$	$4.18\cdot10^{-2}$	0.0086 0.010	0.38 0.25	0.136 0.10
0.2	0.2	0.6	$1.25\cdot10^{-3}$	0.138	$9.59\cdot10^{-4}$	$3.36\cdot10^{-2}$	0.0031 —	0.78 0.68	0.117 —
0.6	0.3	0.1	$2.66\cdot10^{-1}$	0.287	$4.12\cdot10^{-1}$	$2.06\cdot10^{-1}$	0.794 0.80	$6\cdot10^{5}$ 0.0001	0.0069 —
0.4	0.3	0.3	$5.55\cdot10^{-3}$	0.526	$1.62\cdot10^{-2}$	$9.22\cdot10^{-2}$	0.015 0.022	0.15 0.10	0.28 0.30
0.3	0.3	0.4	$2.41\cdot10^{-3}$	0.305	$3.40\cdot10^{-3}$	$5.92\cdot10^{-2}$	0.0059 0.0045	0.47 0.32	0.20 0.26
0.5	0.4	0.1	$5.47\cdot10^{-2}$	0.370	$3.40\cdot10^{-1}$	$2.50\cdot10^{-1}$	0.145 0.20	0.001 0.0005	0.17 0.26
0.4	0.4	0.2	$1.23\cdot10^{-2}$	0.580	$6.54\cdot10^{-2}$	$1.80\cdot10^{-1}$	0.03 0.05	0.034 0.02	0.45 0.50
0.4	0.5	0.1	$2.59\cdot10^{-2}$	0.400	$1.97\cdot10^{-1}$	$2.78\cdot10^{-1}$	0.06 0.10	0.0054 0.003	0.47 0.50
0.3	0.5	0.2	$8.75\cdot10^{-3}$	0.550	$3.87\cdot10^{-2}$	$2.01\cdot10^{-1}$	0.018 0.02	0.065 0.05	0.60 0.75
0.2	0.5	0.3	$3.92\cdot10^{-3}$	0.390	$6.34\cdot10^{-3}$	$1.25\cdot10^{-1}$	0.0052 0.003	0.32 0.30	0.42 —

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