A thermodynamic model has been developed for the representation of ternary liquid silicate systems \( \text{SiO}_2-\text{AO}-\text{BO} \), where A and B are metals such as Ca, Fe, Mn, etc. It is based on a structural model which assumes that each metallic oxide produces the depolymerization reaction \( O^\circ + O^{2-} = 2O^- \) with a characteristic free energy change. The model can calculate the properties of ternary systems solely from data of the binary sub-systems. No ternary terms are required.

The model is used to calculate the activities of the components in complex silicates such as \( \text{SiO}_2-\text{FeO}-\text{CaO} \) where the behavior of \( \text{Fe}^{2+} \) is very different from that of \( \text{Ca}^{2+} \) in the silicate structure. This model has been also used to calculate the activities in the systems \( \text{SiO}_2-\text{MgO}-\text{FeO}, \text{SiO}_2-\text{MgO}-\text{CaO}, \text{SiO}_2-\text{MgO}-\text{MnO}, \text{SiO}_2-\text{Na-O}-\text{MgO} \) and \( \text{SiO}_2-\text{Na}_2\text{O}-\text{CaO} \). Good agreement is obtained between calculated and experimental results.

KEY WORDS: molten silicates, ternary systems, thermodynamic model.
atoms (each associated with four oxygen atoms bonded to it):

$$\Delta S^c = -R \left[ X_{SiO} \ln \left( \frac{X_{SiO}}{X_{SiO} + N_{O^2}} \right) + N_{O^2} \ln \left( \frac{N_{O^2}}{X_{SiO} + N_{O^2}} \right) \right]$$

$$- R N_{O^2} \ln \left( \frac{N_{O^2}}{N_{Si-Si}} \right) + (N_{Si-Si} - N_{O^2}) \ln \left( \frac{N_{Si-Si} - N_{O^2}}{N_{Si-Si}} \right)$$

(5)

where $N_{Si-Si}$ is the number of moles of neighboring Si–Si pairs per mole of solution:

$$N_{Si-Si} = \frac{4X_{SiO}}{2} \left( \frac{X_{SiO}}{X_{SiO} + N_{O^2}} \right)$$

(6)

The structural model assumes that Reaction (1) is associated with a Gibbs energy change containing an enthalpic ($\omega$) and entropic ($\eta$) term:

$$\Delta H = \frac{N_{O^2}}{2} \omega$$  

(7)

$$S^\omega = \frac{N_{O^2}}{2} \eta$$  

(8)

Finally, $\omega$ and $\eta$ are expanded as polynomials:

$$\omega = \omega_0 + \omega_1 X_{SiO} + \omega_2 X_{SiO}^2 + \ldots$$  

(9)

$$\eta = \eta_0 + \eta_1 X_{SiO} + \eta_2 X_{SiO}^2 + \ldots$$  

(10)

The coefficients $\omega_i$ and $\eta_i$ are the parameters of the model which are obtained by optimization of the data. Given a composition, $X_{SiO}$, and values of the parameters $\omega_i$ and $\eta_i$, the actual value of $N_{O^2}$ can be calculated by minimizing the Gibbs energy at constant $X_{SiO}$, $\omega$ and $\eta$:

$$\Delta G = \Delta H - T(\Delta S^c + S^\omega)$$  

(11)

$$2 \frac{\partial \Delta G}{\partial N_{O^2}} \bigg|_{X_{SiO}, \omega, \eta} = (\omega - \eta T) - RT \left[ \ln \left( \frac{N_{O^2}}{1 - X_{MO} + N_{O^2}} \right) + \frac{N_{O^2}}{N_{Si-Si}} \ln \left( \frac{N_{Si-Si} - N_{O^2}}{N_{Si-Si}} \right) \right] = 0$$

(12)

Substitution of Eqs. (3), (4) and (6) into Eq. (12) gives an equation in terms of $X_{MO}$ (or $X_{SiO}$) and $N_{O^2}$, which can be solved numerically at a fixed composition and for given values of the parameters $\omega_i$ and $\eta_i$ to give $N_{O^2}$. This value can then be substituted back into Eqs. (3), (4), (5), (7) and (8) to give $\Delta S$ and $\Delta H$.

3. Binary Metallic Oxide Systems

The main goal of this paper is to apply the model to analyse SiO₂–AO–BO ternary systems. Thus, a model is necessary to represent the thermodynamic properties of the liquid binary metallic oxides (AO–BO). In this work the following expression was chosen:

$$G_{AO-BO} = X_{SiO}X_{BO}(a_1 + a_2 T) + (b_1 + b_2 T)X_{BO} + (c_1 + c_2 T)X_{BO}$$

(13)

where $a_i$, $b_i$ and $c_i$ are constant parameters.

4. Ternary Equations

Let us consider the general SiO₂–AO–BO ternary system where A and B are divalent cations. It is assumed that there are 5 kinds of oxygens:

1. $O^\circ$ : Bridge oxygens
2. $O_A^\circ$ : “Free oxygens ions” introduced in the system by the AO species
3. $O_B^\circ$ : “Free oxygens ions” introduced in the system by the BO species
4. $O_A^\circ$ : Broken bridges for the AO species
5. $O_B^\circ$ : Broken bridges for the BO species

That is, there are two depolymerization reactions given by:

$$\text{Si–O–Si} \rightarrow \text{Si–Si} \hspace{1cm} (14)$$

$$\text{Si–O–Si} \rightarrow \text{Si±Si} \hspace{1cm} (15)$$

The mass balance considerations requires now that:

$$N_{O^\circ} = 2X_{SiO} - \frac{N_{O_A^\circ} + N_{O_B^\circ}}{2}$$  

(16)

$$N_{O_A^\circ} = X_{AO} - \frac{N_{O_A^\circ}}{2}$$  

(17)

$$N_{O_B^\circ} = X_{BO} - \frac{N_{O_B^\circ}}{2}$$  

(18)

Combination of Eqs. (17) and (18) gives:

$$N_{O_A^\circ} + N_{O_B^\circ} = (X_{AO} + X_{BO}) - \frac{N_{O_A^\circ} + N_{O_B^\circ}}{2}$$  

(19)

The number of moles of neighboring Si–Si pairs per mole of solution ($N_{Si-Si}$) in the ternary system is expressed by:

$$N_{Si-Si} = 4X_{SiO} \left( \frac{X_{SiO}}{X_{SiO} + N_{O_A^\circ} + N_{O_B^\circ}} \right)$$

(20)

4.1. Configurational Entropy

The expression of the entropy is obtained making two statistical distributions:

$$S^w = S^w_I + S^w_II$$  

(21)

Where $S^w_I$ is estimated through the distribution of $O_A^\circ$, $O_B^\circ$, and Si in a quasilattice:

$$S^w_I = -R \left[ N_{O_A^\circ} \ln \left( \frac{N_{O_A^\circ}}{N_{O_A^\circ} + N_{O_B^\circ} + X_{SiO}} \right) + N_{O_B^\circ} \ln \left( \frac{N_{O_B^\circ}}{N_{O_A^\circ} + N_{O_B^\circ} + X_{SiO}} \right) \right]$$
\( S^\parallel \) is estimated through the distribution of \( O^\circ \) over the neighboring Si–Si pairs:

\[
S^\parallel = -RT \left( N_{O^\circ} \ln \left( \frac{N_{O^\circ}}{N_{Si-Si}} \right) + (N_{Si-Si} - N_{O^\circ}) \ln \left( \frac{N_{Si-Si} - N_{O^\circ}}{N_{Si-Si}} \right) \right)
\]

.........................(23)

4.2. Excess Free Energy

The excess free energy expression for the ternary system is obtained by the addition of the interaction energy terms \((\omega - \eta T)\) for each bridge breaking reaction, Eqs. (14) and (15), which are known in the two binary systems (AO–SiO\(_2\) and BO–SiO\(_2\)) from the binary optimizations. This expression also must include the contribution of the excess free energy for the AO–BO binary system, \(G_{AO-BO}^E\), which is multiplied by the fraction of free oxygen ions in the quasi lattice whose sites are occupied by O\(^2\)– ions and Si atoms.

\[
G^E = \frac{N_{O^\circ}}{2} (\omega - \eta T)_{AO} + \frac{N_{O^\circ}}{2} (\omega - \eta T)_{BO}
\]
\[
+ \frac{N_{O^\circ} - N_{O^\circ}^*}{N_{O^\circ} + N_{O^\circ}^* + X_{SiO_2}} G_{AO-BO}^E
\]

.........................(24)

The Gibbs free energy of mixing is then obtained joining the expressions (22) to (24)

\[
\Delta g^{mix} = RT \left\{ N_{O^\circ} \ln \left( \frac{N_{O^\circ}}{N_{O^\circ} + N_{O^\circ}^* + X_{SiO_2}} \right) + N_{O^\circ} \ln \left( \frac{N_{O^\circ}^*}{N_{Si-Si}} \right) + (N_{Si-Si} - N_{O^\circ}) \ln \left( \frac{N_{Si-Si} - N_{O^\circ}}{N_{Si-Si}} \right) + \frac{N_{O^\circ}}{2} (\omega - \eta T)_{AO}ight.
\]
\[
+ \frac{N_{O^\circ} - N_{O^\circ}^*}{N_{O^\circ} + N_{O^\circ}^* + X_{SiO_2}} G_{AO-BO}^E \right\}
\]

.........................(25)

This expression is thermodynamically consistent with the Gibbs–Duhem and Gibbs–Helmholtz equations. Equation (25) reduces to the respective expressions for the binary sub-systems:

a) If \( X_{AO} = 0 \) or \( X_{BO} = 0 \)

\[
\Delta g^{mix} = RT \left\{ N_{O^\circ} \ln \left( \frac{N_{O^\circ}}{N_{O^\circ} + X_{SiO_2}} \right) \right\}
\]

b) If \( X_{SiO_2} = 0 \)

\[
N_{O^\circ} = X_{AO}, N_{O^\circ}^* = X_{BO}, \text{ and } \\
\Delta g^{mix} = RT \left\{ X_{AO} \ln \left( \frac{N_{O^\circ}}{N_{Si-Si}} \right) + X_{BO} \ln \left( \frac{N_{O^\circ}}{N_{Si-Si}} \right) + G_{AO-BO}^E \right\}
\]

The expression of \( \Delta g^{mix} \) depends on two parameters (\( N_{O^\circ} \) and \( N_{O^\circ}^* \) or \( N_{O^\circ} \) and \( N_{O^\circ}^* \)). Their values will be calculated by minimizing the expression of the free energy. Choosing the first pair of parameters one obtains:

\[
\frac{\partial \Delta g^{mix}}{\partial N_{O^\circ}} \bigg|_{X_{AO}, X_{BO}, N_{O^\circ}^*}
\]

.........................(28)

Minimizing \( \Delta g^{mix} \) with respect to \( N_{O^\circ} \) one obtains:

\[
\frac{\partial \Delta g^{mix}}{\partial N_{O^\circ}} = RT \left\{ \ln \left( \frac{N_{O^\circ}}{N_{O^\circ} + N_{O^\circ}^* + X_{SiO_2}} \right) \ln \left( \frac{N_{O^\circ}}{N_{Si-Si}} \right) + \left( \frac{\partial N_{Si-Si}}{\partial N_{O^\circ}} - 1 \right) \ln \left( \frac{N_{Si-Si} - N_{O^\circ}}{N_{Si-Si}} \right) \right.
\]
\[
- (\omega - \eta T)_{AO} + \frac{X_{SiO_2}}{(N_{O^\circ} + N_{O^\circ}^* + X_{SiO_2})^2} G_{AO-BO}^E \right\}
\]

.........................(29)

Minimizing \( \Delta g^{mix} \) with respect to \( N_{O^\circ} \) one obtains:

\[
\frac{\partial \Delta g^{mix}}{\partial N_{O^\circ}} = RT \left\{ \ln \left( \frac{N_{O^\circ}}{N_{O^\circ} + X_{SiO_2}} \right) \ln \left( \frac{N_{O^\circ}}{N_{Si-Si}} \right) + \left( \frac{\partial N_{Si-Si}}{\partial N_{O^\circ}} - 1 \right) \ln \left( \frac{N_{Si-Si} - N_{O^\circ}}{N_{Si-Si}} \right) \right.
\]
\[
- (\omega - \eta T)_{BO} + \frac{X_{SiO_2}}{(N_{O^\circ} + N_{O^\circ} + X_{SiO_2})^2} G_{AO-BO}^E \right\}
\]

.........................(30)

Minimizing \( \Delta g^{mix} \) with respect to \( N_{O^\circ} \) one obtains:

\[
\frac{\partial \Delta g^{mix}}{\partial N_{O^\circ}} = RT \left\{ \ln \left( \frac{N_{O^\circ}}{N_{O^\circ} + N_{O^\circ} + X_{SiO_2}} \right) \ln \left( \frac{N_{O^\circ}}{N_{Si-Si}} \right) + \left( \frac{\partial N_{Si-Si}}{\partial N_{O^\circ}} - 1 \right) \ln \left( \frac{N_{Si-Si} - N_{O^\circ}}{N_{Si-Si}} \right) \right.
\]
\[
- (\omega - \eta T)_{BO} + \frac{X_{SiO_2}}{(N_{O^\circ} + N_{O^\circ} + X_{SiO_2})^2} G_{AO-BO}^E \right\}
\]

.........................(31)

Now minimizing \( \Delta g^{mix} \) with respect to \( N_{O^\circ} \) one obtains:

\[
\frac{\partial \Delta g^{mix}}{\partial N_{O^\circ}} = RT \left\{ \ln \left( \frac{N_{O^\circ}}{N_{O^\circ} + N_{O^\circ} + X_{SiO_2}} \right) \ln \left( \frac{N_{O^\circ}}{N_{Si-Si}} \right) + \left( \frac{\partial N_{Si-Si}}{\partial N_{O^\circ}} - 1 \right) \ln \left( \frac{N_{Si-Si} - N_{O^\circ}}{N_{Si-Si}} \right) \right.
\]
\[
- (\omega - \eta T)_{BO} + \frac{X_{SiO_2}}{(N_{O^\circ} + N_{O^\circ} + X_{SiO_2})^2} G_{AO-BO}^E \right\}
\]

.........................(32)

\[
\frac{\partial N_{Si-Si}}{\partial N_{O^\circ}} = -2(X_{SiO_2})^2
\]

.........................(33)
Since Eqs. (30) and (32) are both equal to zero and given that
\[ \Delta N_{\text{Si-Si}}/N_{\text{Si}} - 25 = \Delta N_{\text{Si-Si}}/N_{\text{Si}}\] we can reduce the number
of unknowns through the resulting expression:

\[ \omega = 56.143 - 1.791 X_{\text{SiO}_2} + 116.820 X_{\text{SiO}_2}^2 \]
\[ \eta = -15.11 + 16.638 X_{\text{SiO}_2} \]

\[ \omega = 55.140 - 76.333 X_{\text{SiO}_2} + 245.570 X_{\text{SiO}_2}^2 \]
\[ \eta = -47.99 X_{\text{SiO}_2} + 16.638 X_{\text{SiO}_2}^2 \]

\[ \omega = 6.770 - 122.724 X_{\text{SiO}_2} + 183.040 X_{\text{SiO}_2}^2 + 106.539 X_{\text{SiO}_2}^3 \]
\[ \eta = -34.59 X_{\text{SiO}_2} + 87.366 X_{\text{SiO}_2} \]

\[ \omega = -57.738 - 258.739 X_{\text{SiO}_2} + 262.548 X_{\text{SiO}_2}^2 + 89.325 X_{\text{SiO}_2}^3 \]
\[ \eta = -35.5 X_{\text{SiO}_2} + 70.71 X_{\text{SiO}_2}^2 \]

\[ \omega = -90.841 - 473.168 X_{\text{SiO}_2} + 297.835 X_{\text{SiO}_2}^2 \]
\[ \eta = -31.38 \]

Thus, it is required to solve only a non-linear equation
with one unknown in order to estimate the amount of differ-
ent kind of oxygens as well as the mixing free energy.

This model is also applied to systems of the type SiO₂–
A₂O–BO, for example SiO₂–Na₂O–MgO, in the silica rich
region. In this case, we assume A^+ cations associate in
pairs and remain so in the silicate structure.

5. Applications

The test of the model have been made for the following
ternary systems SiO₂–FeO–CaO, SiO₂–FeO–MgO, SiO₂–
MgO–CaO, SiO₂–MnO–MgO, SiO₂–Na₂O–MgO and SiO₂–
Na₂O–CaO. The parameters \( \omega \) and \( \eta \) for the binary sili-
cate systems MO–SiO₂ (M = Fe, Ca, Mg, Mn, Na₂) are
given in Table 1 and the parameters of the excess free en-
ergy for the binary liquid metallic oxides AO–BO are
shown in Table 2.

5.1. SiO₂–FeO–CaO

Activities of FeO in the liquid phase were determined by
Timucin and Morris at 1823 K by equilibration of the
melts, held in thin-walled platinum crucibles, with CO/CO₂
mixtures. The experimental and calculated activities of
FeO, shown in Fig. 1, are in good agreement, especially be-
tween 0.4 and 0.8.

5.2. SiO₂–FeO–MgO

The calculated curves of activities of FeO at 1873 K
plotted in Fig. 2 are consistent with the concentration de-
pendence of the experimental data obtained by Ban-ya et al. by equilibration of the melts with H₂–H₂O mixtures.

5.3. SiO₂–MgO–CaO

Activities of SiO₂ in the liquid phase (relative to the solid
as standard state) were determined by Rein and Chipman at 1873 K by measuring the distribution of Si between the
slag and an Fe–Si–C alloy saturated either with graphite or
SiC. The experimental activities of SiO₂ are shown in Fig.
3 along with the calculated values by the model. The Gibbs
energy of fusion of pure SiO₂ was taken as:

\[ \Delta G^\circ_{\text{fusion}} (\text{SiO}_2) = 9581.36 - 4.8003T \quad \text{J/mol} \]

5.4. SiO₂–MnO–MgO

In Fig. 4 is shown the comparison between calculated ac-
tivities of MnO at 1923 K (relative to the solid as standard
state) and the experimental values measured by Metha and
Richardson. In this experimental work the slags contain-

---

**Table 1.** Energy parameters, \( \omega \) and \( \eta \), for the bridge breaking
reaction in binary silicate systems\(^2\) (\( \omega \) in J mol\(^{-1}\) and
\( \eta \) in J mol\(^{-1}\) K\(^{-1}\)).

| SYSTEM     | \( \omega \) parameters | \( \eta \) parameters |
|------------|--------------------------|----------------------|
| MnO–SiO₂   | \( \omega = -56.143 - 1.791 X_{\text{SiO}_2} + 116.820 X_{\text{SiO}_2}^2 \) | \( \eta = -15.11 + 16.638 X_{\text{SiO}_2} \) |
| MgO–SiO₂   | \( \omega = -55.140 - 76.333 X_{\text{SiO}_2} + 245.570 X_{\text{SiO}_2}^2 \) | \( \eta = -47.99 X_{\text{SiO}_2} + 16.638 X_{\text{SiO}_2}^2 \) |
| FeO–SiO₂   | \( \omega = 6.770 - 122.724 X_{\text{SiO}_2} + 183.040 X_{\text{SiO}_2}^2 + 106.539 X_{\text{SiO}_2}^3 \) | \( \eta = -34.59 X_{\text{SiO}_2} + 87.366 X_{\text{SiO}_2} \) |
| CaO–SiO₂   | \( \omega = -57.738 - 258.739 X_{\text{SiO}_2} + 262.548 X_{\text{SiO}_2}^2 + 89.325 X_{\text{SiO}_2}^3 \) | \( \eta = -35.5 X_{\text{SiO}_2} + 70.71 X_{\text{SiO}_2}^2 \) |
| NaO₂–SiO₂  | \( \omega = -90.841 - 473.168 X_{\text{SiO}_2} + 297.835 X_{\text{SiO}_2}^2 \) | \( \eta = -31.38 \) |

**Table 2.** Excess free energy for the liquid binary metallic
oxide systems.

\[ \Delta G^\circ = X_{\text{SiO}_2}X_{\text{SiO}_2} (a_1 + b_1 T) + (b_2 + b_3 T)X_{\text{SiO}_2} + (c_1 + c_2 T)X_{\text{SiO}_2} \quad \text{J/mol} \]

| SYSTEM     | \( a_1 \) | \( a_2 \) | \( b_1 \) | \( c_1 \) | Ref. |
|------------|----------|----------|----------|----------|------|
| MgO–FeO    | 2810     | 0.0      | 0.0      | 0.0      | 4    |
| CaO–FeO    | 15924    | 0.0      | 0.0      | 0.0      | 5    |
| FeO–MgO    | 24311    | 0.0      | -14490   | 0.0      | 5    |
| MgO–CaO    | 7531     | 0.0      | 0.0      | 0.0      | 4    |
| FeO–CaO    | -107294  | 41.84    | 0.0      | -17442   | 5    |

\( b_2 \) and \( c_2 \) are equal to zero for all the systems.
ing manganese oxide were brought into equilibrium with thin strips of platinum metal at controlled partial pressure of oxygen, obtained from mixtures of carbon dioxide, hydrogen and nitrogen. The Gibbs energy of fusion of pure MnO was taken as:

$$\Delta G_{\text{fusion}}^{\circ}(\text{MnO}) = 54392.0 - 25.71454T \text{ J/mol} \quad (36)$$

### 5.5. SiO$_2$–Na$_2$O–MgO

The model has been also used to estimate the thermodynamic properties of ternary silicate systems with a monovalent cation in the silica rich region. The activities of Na$_2$O were measured by Rego et al.$^{11}$ at 1673 K in the silica rich region of the SiO$_2$–Na$_2$O–CaO system. The experimental and calculated activities of Na$_2$O shown in Fig. 5 are in good agreement.

### 5.6. SiO$_2$–Na$_2$O–CaO

The activities of Na$_2$O were also measured by Rego et al.$^{11}$ at 1673 K in the silica rich region of the SiO$_2$–Na$_2$O–CaO system. The experimental and calculated activities of Na$_2$O are shown in Fig. 6. Agreement is well within the uncertainties.

### 6. Discussion

The amount of different kind of oxygens in the SiO$_2$–FeO–CaO predicted by the model at 1823 K and $X_{\text{SiO$_2$}} = 0.35$ is shown in Fig. 7. Although the experimental evidence is scarce it is clear that there is a complete breakdown of the polymeric structure by the CaO and FeO basic oxides at this composition of SiO$_2$. This Figure also shows that the cations Ca$^{2+}$ are associated to the O$^-$ and the amount of O$_{\text{Ca}}^{2-}$ is negligible along all the composition range, whereas cations Fe$^{2+}$ are partially associated to the O$^-$ especies and free oxygen ions O$_{\text{Fe}}^{2-}$. In this way the
model takes into account the non random mixing of cations in the silicate structure.

The characteristic “c” shape of the FeO activity curves in the SiO2–FeO–CaO system at 1 823 K, shown in Fig. 8, is explained by the amount of broken bridges (O⁻Ca₂ and O₂Fe) produced by the bridge breaking reactions, Eqs. (14) and (15). The bold line separates the regions where the FeO contributes to the breaking oxygen bridges, i.e. where \(N_{O^-Ca}=0\) and \(N_{O^-Fe}>0\), which corresponds with the sharp change in the slope of the curves.

When extended to SiO₂–Na-O–MgO and SiO₂–Na₂O–CaO, the model gives a good representation of the thermodynamic data in the acid region (\(X_{SiO^2}=0.50\)). This supports the assumption of the model, that in the silica rich region, two cations Na⁺ are associated with each broken oxygen bridge.

7. Conclusions

The earlier structural model\(^{1,2}\) for binary silicate melts has been extended to ternary systems for the representation of liquid silicate systems SiO₂–AO–BO, where A and B are metals such as Ca, Fe, Mn, etc. The model assumes that each metallic oxide produces the depolymerization reaction \(O^+ + O^- = 2O^-\) with a characteristic free energy change. The model can calculate the properties of ternary systems solely from data of the binary sub-systems. No ternary terms are required.

The model is used to calculate the activities of the components in complex silicates such as SiO₂–FeO–CaO where the behavior of Fe²⁺ is very different from that of Ca²⁺ in the silicate structure. This model has been also used to calculate the activities in the systems SiO₂–MgO–FeO, SiO₂–MgO–CaO, SiO₂–MgO–MnO, SiO₂–Na₂O–CaO and SiO₂–Na₂O–MgO. Good agreement is obtained between calculated and experimental results.

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