THERMODYNAMIC PROPERTIES OF MgO-SiO$_2$ MELTS

Shornikov S.I. (GEOKHI RAS)
shorn@mail.wplus.net

Key words: MgO-SiO$_2$ system, thermodynamic properties of melts, theory of ideal solutions of complex components

This work presents the calculation of the thermodynamic properties of the MgO-SiO$_2$ melts at temperature from 1700 to 2300 K in the framework of the ideal associated solutions theory. The simplified lattice model as before for CaO-Al$_2$O$_3$ [1], CaO-SiO$_2$ [2] and Al$_2$O$_3$-SiO$_2$ system [3] accounts for the intermolecular interactions using the semi-phenomenological parameters, which were determined on the base of the experimental [4] and reference [5, 6] thermodynamic data.

In contrast to the previous calculations made in the frameworks of the quasichemical model [7], the initial thermodynamic data considers 8 condensed phases (4 solid and 4 liquid) and 11 gas species; these components are listed in the Table.

The same Table gives the calculated values of the Gibbs formation energies for the compounds and the vapor species over the MgO-SiO$_2$ system, which are used for the calculation of the equilibrium conditions in the system at a given composition and temperature. The equation solution for the integral Gibbs energy for the system studied was found by the widely used approach, namely the Gibbs energy minimization method.

Table The Gibbs energies of formation of condensed phases and vapor species over MgO-SiO$_2$ melts at 2000 K calculated in the present study according to data [4-6]

Condensed phases				Gas phase	
Solid phases	$\Delta_f G_{2000}$, kJ/mole	Liquid phases	$\Delta_f G_{2000}$, kJ/mole	Vapor species	$\Delta_f G_{2000}$, kJ/mole
MgO	-376.430	MgO	-349.107	Mg	-57.263
MgSiO$_3$	-956.936	MgSiO$_3$	-963.256	MgO	-108.759
Mg$_2$SiO$_4$	-1363.087	Mg$_2$SiO$_4$	-1357.504	Si	167.228
SiO$_2$	-550.476	SiO$_2$	-550.520	SiO	-254.769
				SiO$_2$	-314.875
				Si$_2$	216.304
				Si$_2$O$_2$	-558.796
				Si$_3$	265.892
				O	121.662
				O$_2$	0.000
				O$_3$	273.851

The obtained results are shown in fig. 1. and compared with the experimental data obtained by the mass spectrometric Knudsen effusion method in the temperature range 1770-1973 K [8-10].

As seen from the figure, the calculated oxide activities at 1873 and 1973 K showed the presence of small liquid phase region according to the phase diagram of MgO-SiO$_2$ system. These values are correlated to the experimental results. The experimental data differ greatly, which might be due to measuring errors amounting to 20%.

The calculated values of Gibbs energies of the magnesium silicate melts formation are deviated of 3-4 kJ/mole with respect to the experimental data heaving the errors of the same order of magnitude.
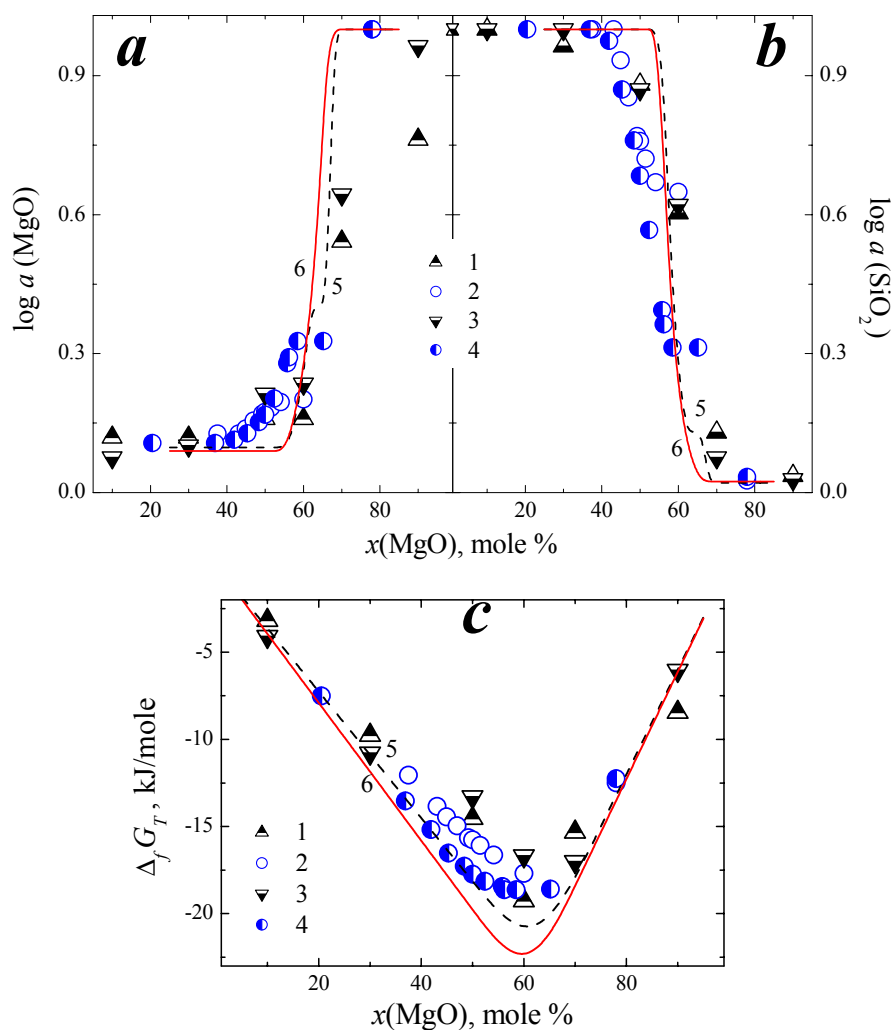
Fig.1. Activities of MgO (*a*), SiO$_2$ (*b*), and the Gibbs energies of formation of the melts of the MgO-SiO$_2$ system (*c*) at 1770 (1), 1873 (2, 5), 1890 (3) and 1973 K (4, 6), obtained by mass spectrometric method (1 and 3 – in [8, 9], 2 and 4 – in [10]) and calculated in the present study (5, 6).

References

1. *Shornikov S.I.* Thermodynamic properties of CaO-Al$_2$O$_3$ melts // Electronic Scientific Information Journal "Herald of the Department of Earth Sciences RAS" №1(21)' 2003.
   http://www.scgis.ru/russian/cp1251/h_dgggms/1-2003/informbul-1_2003/magm-11e.pdf
2. *Shornikov S.I.* // Proc. Intern. Conf. «Science, technology and silicate material production – present and future». M. 2003. V. 4. PP. 196-201.
3. *Shornikov S.I.* Thermodynamic properties of Al$_2$O$_3$-SiO$_2$ melts // Electronic Scientific Information Journal "Herald of the Department of Earth Sciences RAS" № 1(22)' 2004.
   http://www.scgis.ru/russian/cp1251/h_dgggms/1-2004/informbul-1_2004/planet-9e.pdf
4. *Shornikov S.I., Archakov I.Yu., Shultz M.M.* // Russ. J. General Chem. 2000. V. 70. N. 3. PP. 360-370.
5. *Glushko V.P., Gurvich L.V., Bergman G.A., Veitz I.V., Medvedev V.A., Khachkuruzov G.A., Yungman V.S.* Thermodynamic Properties of Individual Substances // Ed.: Glushko V.P. M.: Nauka. V. 1-4. PP. 1978-1982.
6. *Chase M.W.* // J. Phys. Chem. Ref. Data. 1998. Monograph N. 9. PP. 1-1951.

7. *Decterov S.A., Jung I.H., Pelton A.D.* // J. Amer. Ceram. Soc. 2002. V. 85. N. 12. PP. 2903-2910.
8. *Kambayashi S., Kato E.* // J. Chem. Thermodyn. 1983. V. 15. N. 6. PP. 701-707.
9. *Kambayashi S., Kato E.* // J. Chem. Thermodyn. 1984. V. 16. N. 2. PP. 241-248.
10. *Stolyarova V.L., Lopatin S.I., Bondar V.V.* // Dokl. Phys. Chem. 2004. V. 399. N. 1. PP. 82-84.