THERMODYNAMIC PROPERTIES OF Al_2O_3-SiO_2 MELTS

Shornikov S.I.
Center of Isotopic Research, Karpinsky All-Russian Geological Institute (VSEGEI), Saint-Petersburg, Russia
Sergey_Shornikov@vsegei.ru

Key words: Al_2O_3-SiO_2 system, thermodynamic properties of melts, theory of ideal solutions of complex components

For more than 150 years the Al_2O_3-SiO_2 system has remained the focus of physicochemical studies in the fields of geochemistry, petrology, mineralogy, and technology.

This work presents the calculation of the thermodynamic properties of the Al_2O_3-SiO_2 melts at temperature from 1700 to 2500 K in the framework of the ideal associated solutions theory. The simplified lattice model [1, 2] accounts for the intermolecular interactions using the semi-phenomenological parameters, which were determined on the base of the experimental [3-5] and reference [6, 7] thermodynamic data.

In contrast to the previous calculations made in the frameworks of the quasichemical model [8], the initial thermodynamic data considers 8 condensed phases (5 solid and 3 liquid) and 18 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 Al_2O_3-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 Al_2O_3-SiO_2 melts at 2300 K calculated in the present study

Condensed phases				Gas phase	
Solid phases	$\Delta_f G_{2300}$, kJ/mole	Liquid phases	$\Delta_f G_{2300}$, kJ/mole	Vapor species	$\Delta_f G_{2300}$, kJ/mole
Al_2O_3	-937.492	Al_2O_3	-936.202	Al	52.925
$Al_6Si_2O_{13}$	-3871.798	$Al_6Si_2O_{13}$	-3892.411	AlO	-91.574
Al_2SiO_5	-1439.027			AlO_2	-97.395
$Al_2Si_2O_7$	-1872.724			Al_2	154.511
SiO_2	-491.577	SiO_2	-495.065	Al_2O	-294.492
				Al_2O_2	-374.745
				Al_2O_3	-375.705
				AlSi	1230.647
				AlSiO	-226.765
				Si	133.751
				SiO	-268.189
				SiO_2	-305.205
				Si_2	181.835
				Si_2O_2	-520.589
				Si_3	236.819
				O	101.575
				O_2	0.000
				O_3	290.417

The obtained results are shown in Figure and compares with the experimental data obtained by the mass spectrometric Knudsen effusion method in the temperature range 2200-2400 K [5]. As seen from the Figure, the deviations in the calculated oxide activities was less than 8 %, resulting in the errors in the Gibbs energies of the melts formation in the Al_2O_3-SiO_2 system of 2 kJ/mole with respect to the experimental data heaving the errors of the same order of magnitude.

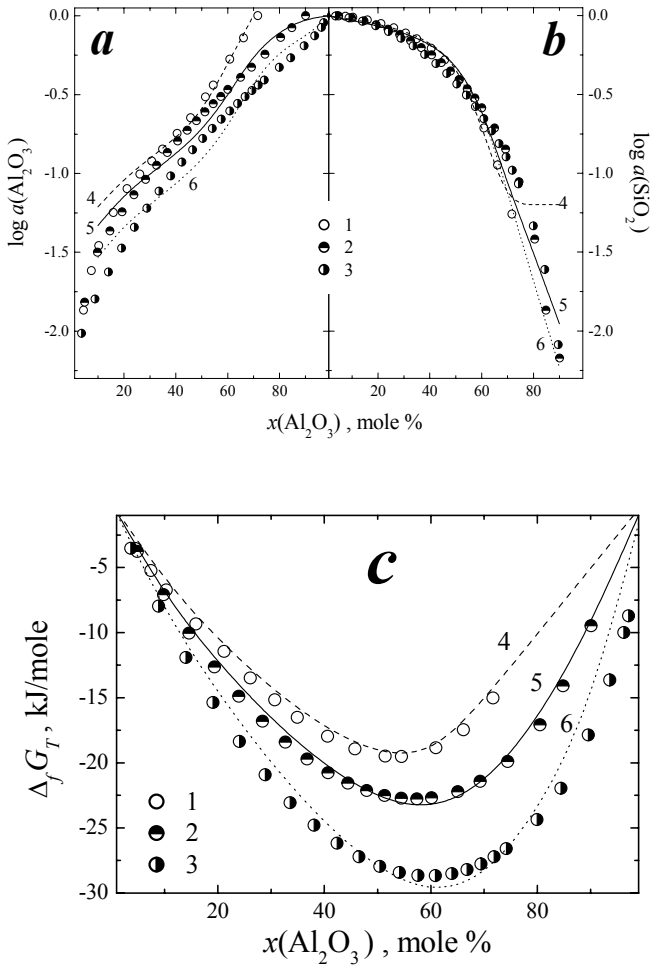

Fig. Activities of Al_2O_3 (*a*), SiO_2 (*b*), and the Gibbs energies of formation of the melts of the Al_2O_3-SiO_2 system (*c*) at 2200 (1, 4), 2300 (2, 5), and 2400 K (3, 6), obtained by mass spectrometric method (1-3 – in [5]) and calculated in the present study (4-6)

References

1. *Shornikov S.I.* // Herald Earth Sci. Dept. RAS. № 1(21)′2003. *http://www.scgis.ru/russian/cp1251/h_dgggms/1-2003/informbul-1/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. *Stearns C.A., Kohl F.J.* // High Temp. Sci. 1973. V. 5. № 2. PP. 113-127.
4. *Shornikov S.I., Stolyarova V.L., Shultz M.M.* // Rapid Commun. Mass Spectr. 1994. V. 8. № 5. PP. 478-480.
5. *Shornikov S.I., Archakov I.Yu.* // Russ. J. Phys. Chem. 2000. V. 74. № 5. PP. 684-688.
6. *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. V.P. Glushko. M.: Nauka. V. 1-4. PP. 1978-1982.
7. *Bale C.W., Chartrand P., Degterov S.A., Eriksson G., Hack K., Ben Mahfoud R., Melançon J., Pelton A.D., Petersen S.* // CALPHAD. 2002. V. 26. № 2. PP. 189-228.
8. *Eriksson G., Pelton A.D.* // Metall. Trans. B. 1993. V. 24. № 4. PP. 807-816.

Electronic Scientific Information Journal "Herald of the Department of Earth Sciences RAS" № 1(22)′2004
Informational Bulletin of the Annual Seminar of Experimental Mineralogy, Petrology and Geochemistry – 2004
URL: http://www.scgis.ru/russian/cp1251/h_dgggms/1-2004/informbul-1_2004/planet-9e.pdf
Published on 1, July, 2004