THERMODYNAMIC PROPERTIES OF CaO-Al_2O_3 MELTS

Shornikov S.I.

*Center of Isotopic Research, Karpinsky All-Russian Geological Institute (VSEGEI), Saint-Peter*sburg

s_shornikov@hotmail.com

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

Thermodynamic properties of the CaO-Al_2O_3 are of interest in ceramic and cement technologies, as well as in metallurgy and material science. The high-alumina region of this system is especially interesting for the cosmochemical study of the selective evaporation and condensation of the primitive solar nebula [1].

This work presents the calculation of the thermodynamic properties of the CaO-Al_2O_3 melts at temperature from 1800 to 2500 K in the framework of the ideal associated solutions theory. The simplified lattice model accounts for the intermolecular interactions using the semi-phenomenological parameters, which were determined on the base of the experimental thermodynamic data [2, 3].

In contrast to the previous calculations made in the frameworks of the sublattice and quasichemical models [4, 5], the initial thermodynamic data considers 12 condensed phases (8 solid and 4 liquid) and 12 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 CaO-Al_2O_3 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 [6].

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 1800-2100 K [7, 8]. As seen from the figure, the deviations in the calculated oxide activities was less than 5 %; resulting in the errors in the Gibbs energies of the melts formation in the CaO-Al_2O_3 system of 1 kJ/mole with respect to the experimental data heaving the errors of the same order of magnitude.

Table

The Gibbs energies of formation of condensed phases and vapor species over CaO-Al_2O_3 melts at 1933 K calculated in the present study on the base of the experimental data [2, 3]

Condensed phases				Gas phase	
Solid phases	$\Delta_f G_{1933}$, kJ/mole	Liquid phases	$\Delta_f G_{1933}$, kJ/mole	Vapor species	$\Delta_f G_{1933}$, kJ/mole
Al_2O_3	-1055.518	Al_2O_3	-1037.330	Al	92.545
CaO	-428.777	CaO	-416.203	AlO	-70.953
$CaAl_2O_4$	-1545.027	$CaAl_2O_4$	-1546.931	AlO_2	-99.424
$CaAl_4O_7$	-2616.481			Al_2	199.593
$CaAl_{12}O_{19}$	-6849.686			Al_2O	-279.329
$Ca_3Al_2O_6$	-2417.464			Al_2O_2	-388.134
$Ca_5Al_6O_{14}$	-5527.788			Al_2O_3	-410.309
$Ca_{12}Al_{14}O_{33}$	-13024.521	$Ca_{12}Al_{14}O_{33}$	-13088.549	Ca	-15.231
				CaO	-71.497
				O	126.135
				O_2	0.000
				O_3	269.935

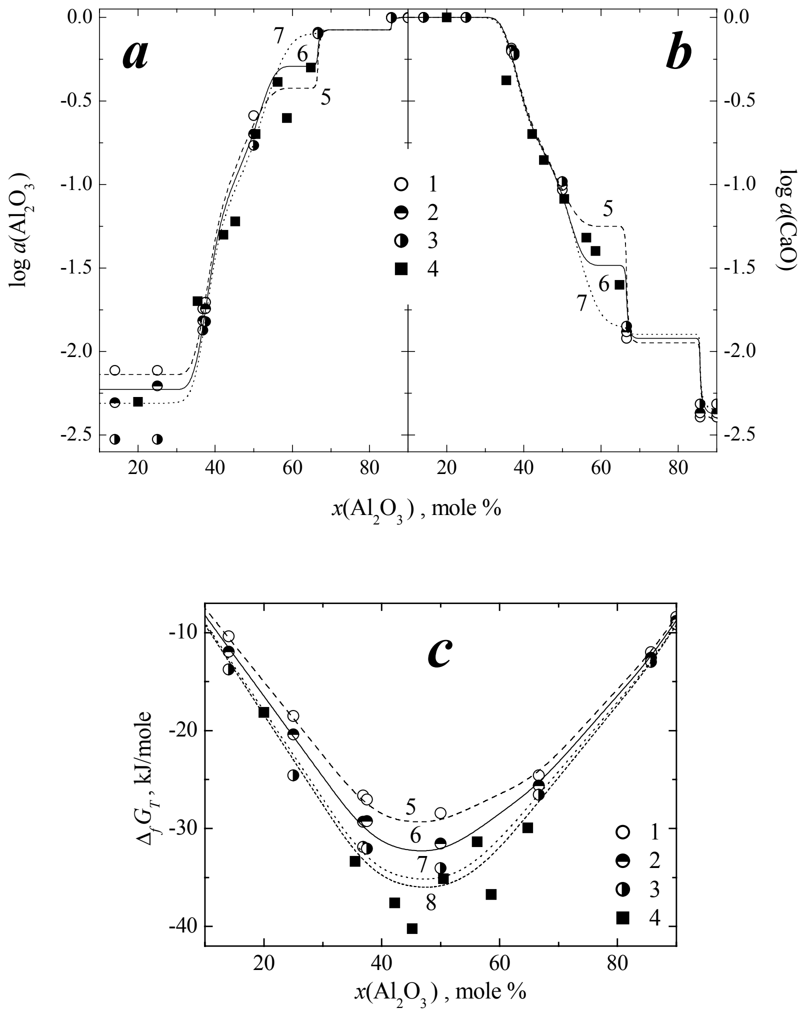

Fig. Activities of Al_2O_3 (*a*), CaO (*b*), and the Gibbs energies of formation of the melts of the CaO-Al_2O_3 system (*c*) at 1833 (1, 5), 1933 (2, 6), 2033 (3, 7), and 2060 K (4, 8), obtained by mass spectrometric method (1-3 – in [7], 4 – in [8]) and calculated in the present study (5-8).

References

1. *Yakovlev O.I., Dikov Yu.P., Gerasimov M.V.* // Geokhimiya. 2000. № 10. P. 1027-1045.
2. *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. 1978-1982.
3. *Shornikov S.I., Stolyarova V.L., Shultz M.M.* // Russian J. Phys. Chem. 1997. V. 71. № 1. P. 23-27
4. *Hallstedt B.* // J. Amer. Ceram. Soc. 1990. V. 73. № 1. P. 15-23.
5. *Eriksson G., Pelton A.D.* // Metall. Trans. B. 1993. V. 24. № 4. P. 807-816.
6. *Saxena S.K.* // Adv. Phys. Geochem. 1982. V. 2. P. 225-241.
7. *Shornikov S.I., Stolyarova V.L., Shultz M.M.* // Russian J. Phys. Chem. 1997. V. 71. № 1. P. 19-22.
8. *Allibert M., Chatillon C., Jacob K.J., Lourtau R.* // J. Amer. Ceram. Soc. 1981. V. 64. № 5. P. 307-314.

Electronic Scientific Information Journal "Herald of the Department of Earth Sciences RAS" № 1(21)'2003
Informational Bulletin of the Annual Seminar of Experimental Mineralogy, Petrology and Geochemistry – 2003
URL: http://www.scgis.ru/russian/cp1251/h_dgggms/1-2003/informbul-1_2003/magm-11e.pdf
Published on July 15, 2003