

THERMODYNAMIC PROPERTIES OF Al_2O_3 - SiO_2 MELTS

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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 |
| $\text{Al}_6\text{Si}_2\text{O}_{13}$ | -3871.798 | $\text{Al}_6\text{Si}_2\text{O}_{13}$ | -3892.411 | AlO | -91.574 |
| Al_2SiO_5 | -1439.027 | | | AlO ₂ | -97.395 |
| $\text{Al}_2\text{Si}_2\text{O}_7$ | -1872.724 | | | Al ₂ | 154.511 |
| SiO_2 | -491.577 | SiO_2 | -495.065 | Al ₂ O | -294.492 |
| | | | | Al ₂ O ₂ | -374.745 |
| | | | | Al ₂ O ₃ | -375.705 |
| | | | | AlSi | 1230.647 |
| | | | | AlSiO | -226.765 |
| | | | | Si | 133.751 |
| | | | | SiO | -268.189 |
| | | | | SiO ₂ | -305.205 |
| | | | | Si ₂ | 181.835 |
| | | | | Si ₂ O 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.

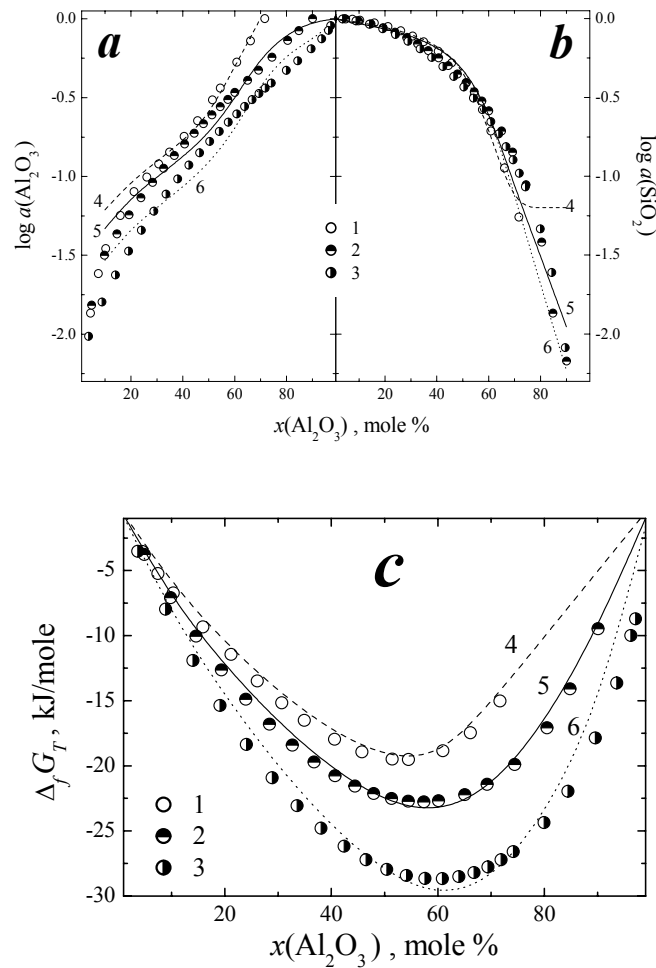


Fig. Activities of Al_2O_3 (a), SiO_2 (b), and the Gibbs energies of formation of the melts of the Al_2O_3 - SiO_2 system (c) at 2200 (1, 4), 2300 (2, 5), and 2400 K (3, 6), obtained by mass spectrometric method (1-3 – in [5]) and calculated in the present study (4-6)

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.

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