THE EFFECT OF CATION SPECIES ON THE SULFUR SOLUBILITY OF CaO-FeO-Al2O3-SiO2 MELTS

Joon Sung Choi, Yonsei University

Dong Joon Min, Yonsei University

The charge compensation effect of Ca2+ and Fe2+ on the sulfur solubility of CaO-FeO-Al2O3-SiO2 melts has been studied. The content of cation species (MO, M=Ca, Fe) and anion groups (AlO45-, SiO44-) were varied to determine the effect of charge compensation [1,2] on the sulfur solubility in high temperature ionic melts. The coordination number of aluminum ion in the super-cooled liquids was identified by deconvolution with PeakFitTM 4.0 of 27Al 500MHz Solid NMR Spectra. [3] The proportion of Qn was analyzed by Raman spectroscopy. [4]

As a result, the sulfide capacity represents a linear relationship according to the MO activity, as an index of the basicity. In the case of the cationic excess region (${M^{2+}}/{Al^{3+}}>1.0$), the sulfide capacity is directly proportional to the basicity due to high S2- stabilization by excess cation. However, in the case of the cation deficient region (${M^{2+}}/{Al^{3+}}<1.0$), the sulfide capacity was shown to be constant depending on the basicity.

Charge Balancing Join $ :{(X\_{Ca^{2+} }+ X\_{Fe^{2+}})}/{(X\_{Fe^{3+}} + 2∙X\_{Al\_{2}O\_{3}})}=1$ (1)

The reason is that S2- activity coefficient of the melts increase due to the absence of M2+ required for charge balancing with AlO45- and FeO45-. Also, the sulfur stabilization region was determined by the kind of the cation species (M2+). The charge balancing region is changed by the stabilization of Al3+ with Fe3+ [5] and influences on the cation substitution effect on the sulfur solubility.

\*Keywords: Sulfur solubility Charge Compensation, Iron Redox Equilibria, Cation Substitution, Aluminosilicate melts

References

[1] Toplis MJ, Dingwell DB. Shear viscosities of CaO-Al2O3-SiO2 and MgO-Al2O3-SiO2 liquids: Implications for the structural role of aluminium and the degree of polymerisation of synthetic and natural aluminosilicate melts. Geochim Cosmochim Acta. 2004;68:5169–5188.

[2] Lee SK, Stebbins JF. The degree of aluminum avoidance in aluminosilicate glasses. Am Mineral. 1999;84:937–945.

[3] Neuville DR, Cormier L, Massiot D. Al environment in tectosilicate and peraluminous glasses: A 27Al MQ-MAS NMR, Raman, and XANES investigation. Geochim Cosmochim Acta. 2004;68:5071–5079.

[4] Mysen BO, Virgo D, Kushiro I. The structural role of aluminum in silicate melts; a Raman spectroscopic study at 1 atmosphere. Am Mineral. 1981;66:678–701.

[5] Yang L, Belton GR. Iron redox equilibria in CaO-Al2O3-SiO2 and MgO-CaO-Al2O3-SiO2 slags. Metall. Mater. Trans. B. 1998;29:837-845.