
The Effect of Cation Species on the Sulfur Solubility of CaO-FeO-Al₂O₃-SiO₂ Melts

Joonsung Choi*¹ and Dongjoon Min†²

¹Yonsei University – 50, Yonsei-ro, Seodaemun-gu, Seoul 03722, South Korea

²Yonsei University – South Korea

Abstract

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 (AlO₄⁻, SiO₄⁻) 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 PeakFit™ 4.0 of ²⁷Al 500MHz Solid NMR Spectra. [3] The proportion of Q_n 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 (M²⁺/Al³⁺ > 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 (M²⁺/Al³⁺ < 1.0), the sulfide capacity was shown to be constant depending on the basicity.

Charge Balancing Join : $(Ca^{2+}+Fe^{2+})/(Fe^{3+}+2XAl_2O_3)=1$ (1)

The reason is that S²⁻ activity coefficient of the melts increase due to the absence of M²⁺ required for charge balancing with AlO₄⁻ and FeO₄⁻. 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.

References

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.

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

Neuvill 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.

*Speaker

†Corresponding author: chemical@yonsei.ac.kr

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.

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.

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