ROLE OF BASICITY AND Al2O3 ON THE NBO/T IN CALCIUM ALUMINOSILICATE MELTS VIA XPS, RAMAN, AND NMR SPECTROSCOPY

Joon Sung Choi, Yonsei University

Dong Joon Min, Yonsei University

The effect of basicity and Al2O3 on the structure of CaO-Al2O3-SiO2 melts has been studied using XPS, Raman and NMR spectroscopy investigation. The content of Al2O3 and basicity (CaO/SiO2) were varied to determine the compositional effect on the structure of high temperature ionic melts. The amount of oxygen ions() in the super-cooled liquids were estimated by deconvolution with PeakFitTM 4.1 of O1s binding energy using X-ray photoelectron spectroscopy (XPS) [1]. The proportion of Qn species were analyzed by Raman [2] and MAS NMR spectroscopy [3]. As a result of the quantitative analysis, the experimental-based NBO/T is shown as follow.

(1)

NBO/T was shown linear relationships to the basicity(CaO/SiO2) including inflection point at CaO/SiO2=1.0. It is due to the stability and Qn dominant unit of melts change around the wollastonite (CaSiO3) congruent point [2]. As Al2O3 increases, the NBO/T converges because of the preference of Q2 chain structure near the anorthite (CaAl2SiO8) congruent point [4]. This is due to the change of the dominant polymeric unit into Al-O-Si and Al-O-Al [5]. Also, iso-NBO/T and lines were derived by comparing XPS and Raman spectroscopy results. The comparative evaluation between the viscosity and the sulfide capacity, which is a representative property of the melts, was carried out.

\*Keywords: NBO/T, XPS, Raman spectroscopy, MAS NMR, Aluminosilicate Slags

References

[1] Park J-H, Rhee. PC-H. Ionic properties of oxygen in slag. J Non-Cryst Solids. 2001;282:7–14.

[2] 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.

[3] Neuville DR, Cormier L, Massiot D. Al coordination and speciation in calcium aluminosilicate glasses: Effects of composition determined by 27Al MQ-MAS NMR and Raman spectroscopy. Chem Geol. 2006;229:173–185.

[4] Navrotsky A, Peraudeau G, McMillan P, et al. A thermochemical study of glasses and crystals along the joins silica-calcium aluminate and silica-sodium aluminate. Geochim Cosmochim Acta. 1982;46:2039–2047.

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