Role of basicity and Al2O3 on the NBO/T in calcium aluminosilicate melts

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Abstract

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(XOn-(n:0,1,2)) 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.
NBO/T=[Qn* (4-n)]/([IV]Al+[IV]Si) (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.

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