American Mineralogist, Volume 101, pages 1232–1235, 2016

LETTER

Ca neighbors from XANES spectroscopy: A tool to investigate structure, redox, and nucleation processes in silicate glasses, melts, and crystals

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ABSTRACT

In this study, Ca *K*-edge X-ray absorption spectroscopy (XAS) has been employed to study the Ca structural role in a set of silicate glasses. For the first time the accurate analysis of the Ca pre-edge peak has been performed, providing information about the different Ca local environments, and on its structural role.

This approach was tested on Ca-aluminosilicate glasses (CAS system) with constant SiO_2 content (50 and 76 mol%), ranging from percalcic to peraluminous domains. In alkali-earth aluminosilicate glasses Al and Si are network formers in a large range of compositions, whereas calcium should act either as network modifier and charge compensator. The results obtained show a different Ca behavior as a function of Al content, which in turn is related to the Al local environment. For example, we observe changes in the pre-edge peak centroid energies depending on the changes in the role of Ca as a network modifier (Al = 0 mol%) to charge compensator (aluminosilicate join) to a more complex role in the peraluminous domain, depending on the fraction of $^{[4],[5],[6]}Al$. This approach was further applied to study Fe-bearing glasses and, a diopside ($CaMgSi_2O_6$) composition at different temperatures. It was possible to correlate the variations occurring in the Ca pre-edge peak centroid positions with both redox state and crystal nucleation mechanism.

Keywords: Calcium, XAS, glass structure, redox, nucleation