American Mineralogist, Volume 95, pages 1580–1589, 2010

AMORPHOUS MATERIALS: PROPERTIES, STRUCTURE, AND DURABILITY†

The structure of crystals, glasses, and melts along the CaO-Al_2O_3 join: Results from Raman, Al *L*- and *K*-edge X-ray absorption, and ^{27}Al NMR spectroscopy

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ABSTRACT

Calcium aluminate glasses are important materials where $AlO_{4/2}^-$ is the only network former. Aluminum in crystals or glasses between CaO and Al_2O_3 can have different environments as a function of the CaO/Al_2O_3 ratio. Using X-ray absorption at the Al *K*- and *L*-edges, Raman and ^{27}Al NMR spectroscopies, we have determined the structural surroundings of Al in glasses, crystals, and melts in this binary system. Aluminum is in octahedral coordination at high-Al_2O_3 content (>80 mol%) and essentially in fourfold coordination with 4 bridging O atoms (BOs) at Al_2O_3 contents between 30 and 75 mol%. At around 25 mol% Al_2O_3, Al is in tetrahedral coordination with two BOs. The presence of higher-coordinated species at high-Al_2O_3 contents and their absence at low Al_2O_3 imply different viscous flow mechanisms for high- and low-concentration Al_2O_3 networks.

Keywords: Aluminate, crystal, glasses, melts, Raman, NMR, XANES