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AMORPHOUS MATERIALS: PROPERTIES, STRUCTURE, AND DURABILITY[†] Structure of Mg- and Mg/Ca aluminosilicate glasses: ²⁷Al NMR and Raman spectroscopy investigations

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ABSTRACT

The structure and properties of glasses and melts in the MgO-Al₂O₃-SiO₂ (MAS) and CaO-MgO-Al₂O₃-SiO₂ (CMAS) systems play an important role in Earth and material sciences. Aluminum has a crucial influence in these systems, and its environment is still questioned. In this paper, we present new results using Raman spectroscopy and ²⁷Al nuclear magnetic resonance on MAS and CMAS glasses. We propose an Al/Si tetrahedral distribution in the glass network in different Q^n species for silicon and essentially in Q^4 and ^VAl for aluminum. For the CMAS glasses, an increase of ^VAl and ^{VI}Al is clearly visible as a function of the increase of Mg/Ca ratio in the (Ca,Mg)₃Al₂Si₃O₁₂ (garnet) and (Ca,Mg)AlSi₂O₈ (anorthite) glass compositions. In the MAS system, the proportion of ^VAl and ^{VI}Al increases with decreasing SiO₂ and, similarly with calcium aluminosilicate glasses, the maximum of ^VAl is located in the center of the ternary system.

Keywords: Aluminosilicate, glasses, NMR, Raman