



Hydrogen speciation in corroded boroaluminosilicate glass: Insights from double-resonance NMR

Kroeker, S.* (1), Brytskyi, M. (1), Paterson, A. (2)

(1) Department of Chemistry, University of Manitoba, Winnipeg, Manitoba, CANADA

(2) NMRFAM, University of Wisconsin, Madison, U.S.A.

The possibility that nuclear glass may eventually come into contact with aqueous fluids in geological repositories demands an understanding of glass corrosion. Since hydrogen is located exclusively within the altered surface layer, ^1H magic-angle-spinning (MAS) nuclear magnetic resonance (NMR) spectroscopy is used to selectively observe the structural impact of aqueous alteration on a sodium boroaluminosilicate glass. The use of dipolar-mediated ^1H -detected double-resonance NMR provides more detailed information about the bonding of H-bearing species formed by alteration. These methods reveal a heterogeneous range of hydroxylated network formers (Si, Al, B) which are hydrogen-bonded to physisorbed water molecules in the altered glass region. There is also evidence of isolated hydroxyl groups and possibly bridging hydroxyls bonded to different network formers. This work shows that aqueous alteration produces a wide variety of H-bearing species in a morphologically complex surface layer.