95Mo Solid State NMR: Structural study of molybdophosphate glasses

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Abstract

Molybdenum oxides are often used in phosphate glasses for its ability to act either as network former and as network modifier. Several other properties are improved when molybdenum is added, such as resistance against devitrification, chemical resistance or electrical conductivity. Solid-State Nuclear Magnetic Resonance (SSNMR) is a powerful tool to probe ordered and disordered materials at the atomic scale which makes this technique ideal to explain the relation between structure and properties in molybdenum phosphate glasses. Meanwhile, 95Mo is an attractive NMR-active isotope with a wide chemical shift range (7000 ppm). Moreover, 95Mo is a quadrupolar nucleus (I=5/2), and as such could provide solid-state NMR spectra dominating by the quadrupolar interaction. This interaction is known to be an invaluable probe to local changes in materials. However, 95Mo is insensitive to NMR due to its low gyromagnetic ratio and low natural abundance (15.92%). This is the reason why few SSNMR studies are dedicated to this nucleus up to now. However, these limitations can be overcome by using high magnetic fields (*i.e.* 18.8T), fast Magic Angle Spinning (MAS) and different pulse sequences such as Q-CPMG. In order to obtain structural information about glasses, 31P and 95Mo NMR experiments are conducted on glassy and crystalline samples. NMR parameters (CQ, ηQ) are extracted thanks to DFT calculation. First results show that molybdenum is a better local probe than phosphorus in molybdenum phosphate glasses.

Keywords: phosphate glasses, 95Mo nuclear magnetic resonance, Quantum chemical calculation

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