The structure of bioactive phosphate glasses using diffraction techniques and EPSR modelling

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Abstract

Neutron and X-ray diffraction, coupled with 23Na and 31P NMR, have been used to investigate the structural effects of substituting CaO with SrO in a 40P2O5·(16-x)CaO·20Na2O·24MgO·xSrO glass, where x is 0, 4, 8, 12 and 16 mol%. Binary metaphosphate glasses were also studied using neutron diffraction and the results were used to guide the analysis of the diffraction data obtained for these complex multi-component glasses. Diffraction data was analysed using direct fitting and EPSR modelling to extract information on the phosphorous and modifier environments. The P-O environment was consistent with NMR results. The M-O coordination environments (M= Mg, Ca, Sr, Na) determined by direct fitting of the neutron data yielded broad asymmetric distributions of bond length, with coordination numbers that were smaller, and bond lengths that were shorter, than in corresponding crystals. The Mg-O coordination number was determined as 5.0(2). EPSR models gave very similar results, but showed the local environments of the modifiers to be even more asymmetric, with higher coordination numbers, closer to those found in published simulations of phosphate glass structure.

Functional properties, including glass transition temperatures, thermal processing windows, dissolution rates and ion release profiles were also investigated. Dissolution studies showed a decrease in degradation rate with initial addition of 4 mol% SrO, but further addition of SrO showed little change. The ion release profiles followed a similar trend to the degradation rates observed. The limited changes in structure and dissolution rates observed for substitution of Ca with Sr in these fixed 40 mol% P2O5 glasses were attributed to their similarities in terms of ionic size and charge.

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