Investigations of Medium-Range Structure of Bioactive Borophosphosilicate Glasses by Solid-State NMR Experiments

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Abstract

Borophosphosilicate (BPS) glasses are promising materials for bone tissue engineering [1]. Such glasses are termed bioactive, because when exposed to body fluids, they bond to bone/tooth by forming a layer of hydroxy-carbonate apatite (HCA) that features a similar composition as bone mineral. Compared with the B-free phosphosilicate counterparts, bioactive BPS glasses exhibit a faster degradation in aqueous solutions and a more complete transformation to HCA [1].

The bone-boding properties of BPS glasses depend on their short-range and medium-range structures. Our previous study on the short-range structures shows that BPS glasses consist primarily of BO3, BO4, and SiO4 units, while P, as a minor component, exists mainly as readily leached orthophosphate groups, with the remaining forming one P–O–Si or P–O–B bridge (*Q1*) [2]. Here we will present results from studies of the medium-range arrangements of the BPS glasses, which were probed by an array of dipolar-coupling-based NMR techniques:

(1) The intermixing of BO3/BO4 units, as revealed by the 11B homonuclear correlation experiments [3].

(2) The distributions of BO3/BO4 units around the orthophosphate groups, and their relative preferences for bonding to *Q1* units, probed by 11B/31P heteronuclear 2D correlation and REDOR dephasing NMR experiments.

(3) The relative contents of P–O–Si and P–O–B bridges, deduced from 31P/11B heteronuclear dephasing experiments, and revealing a slight preference for P to bond to BO4 [3].

(4) The distributions of Na+ cations around BO3/BO4 units and the implications of its roles as network modifiers/charge-compensators, as investigated by the 11B/23Na heteronuclear dephasing experiments compared with the molecular dynamic simulations.

We will also present results on the HCA formation from BPS glasses when subjected to a simulated body fluid (SBF), thereby evaluating the dependence of the *in vitro* bioactivity on the relative amounts of B, Si, and P in the glass matrix.

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