Atomic-level clustering in fluorinated phosphate-based glass

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Abstract

Phosphate-based glasses (PBG) have wide application as biomaterials because they dissolve when implanted into the body, with a composition-dependent dissolution rate that varies over several orders of magnitude. They can be synthesised containing different substances or materials, making them useful for controlled delivery of therapeutically relevant substances. In order to optimise PBGs for these applications, it is vital to understand the dependence of their dissolution rate on the glass composition and structure.
Over the past few years, computer simulation, typically molecular dynamics (MD) simulations, has pioneered our understanding of phosphate glass structure [1], particularly identifying the structural motifs which affect the glass dissolution rate when implanted [2]. Much work has been concentrated on the effects of cation inclusion, but, in this talk, we will discuss recent results on the inclusion of fluorine into PBG for, e.g., dental applications.

In fluorinated *silicate* glasses, local-scale atomic clustering leads to structural inhomogeneity within the glass [3], and there is evidence for [4] and against [5] this in fluorinated phosphate glasses. By developing an accurate polarizable potential which represents the interatomic forces in fluorinated PBG, we propose the existence of significant structural inhomogeneities, which are likely to reduce its bioactivity.

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Keywords: phosphate glass, bioactivity, fluorine, dissolution, molecular dynamics

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