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NMR Studies of Polymer-Nanoparticle Interfaces in Biological and Synthetic Nanocomposites¹ KLAUS SCHMIDT-ROHR, Iowa State University

Nuclear magnetic resonance (NMR) provides unique capabilities for studying buried interfaces in organic-inorganic (specifically phosphate-based) nanocomposites, in terms of local composition as well as distances between, and mobility of, structural units near the interface. The organic-inorganic interface is crucial for the mechanical coupling between the polymer and the inorganic nanoparticles. We have studied the organic-inorganic nanocomposite in bone and characterized the interface between the organic matrix (the triple-helical fibrous polypeptide collagen) and the inorganic, reinforcing bioapatite (a calcium phosphate) that accounts for 45 vol% of the material and is present as ~3-nm thick nanocrystals. By solid-state ¹³C{³¹P} NMR, we can obtain selective spectra of the collagen residues at the interface; ionic and hydroxyproline C-OH groups of significant mobility are dominant. ¹H-³¹P and ¹H-¹³C NMR prove that water with isotropic mobility, which accounts for about 7% of the total volume, forms a monomolecular interfacial layer between apatite and collagen. Its rotational correlation time is about five orders of magnitude longer than that of liquid water. We propose that this water layer can be considered as "viscous glue" that holds the components of the nanocomposite together. It would avoid stress concentration and, by virtue of its flexible H-bonding, reduce the requirement of matched lock-and-key binding sites for collagen sidegroups on the apatite surface. In nanocomposites of phosphate glass with polyamides, ¹H-¹³C NMR reveals a reduced crystallinity of the polyamide near the inorganic particles.

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