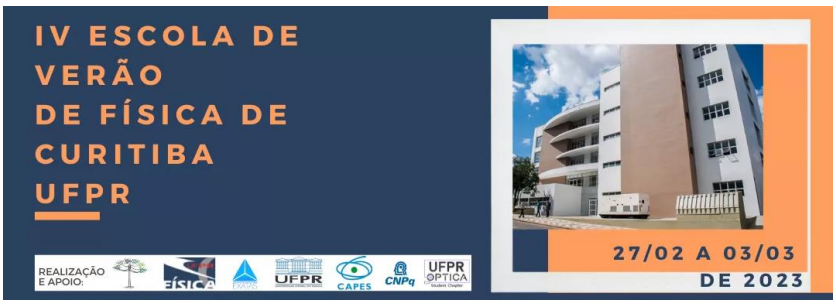

Incorporation of Gallium Into Bioactive Glasses: New Structure/Function Relations Uncovered by Solid State NMR Techniques

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Since the pioneering publication reporting the ability of certain glasses in the SiO_2-CaO-Na_2O-P_2O_5 composition diagram to join bone material without forming fibrous tissue around them or promoting inflation or toxicity (1), research and development of bioactive glasses and glass-ceramics have promoted better quality of life. In bioglasses, gallium stands out for its antibacterial potential, due to the similarity between its Ga^{3+} ions and Fe^{3+} ions (2); so far, however, there is little knowledge about the relation between the details of its structural incorporation and bioactive properties. The present work aimed to study gallium-doped bioactive glasses, melt-quenching and sol-gel process derived, using NMR techniques and additional characterizations. For the melt-derived glasses, 7 samples of Biosilicate® doped with Gallium were produced, with composition $[(49{,}16\text{-}x)SiO_2–(23{,}33)Na_2O–(25{,}79)CaO–(1{,}72)P_2O_5–(x)Ga_2O_3]$, where x= {0,1,2,4,6,8,10} mol%. DSC results show an increase in the glass transition temperature regarding Ga content, indicating there's an increase in network connectivity with the presence of gallium. The NMR spectra indicate that gallium is 4-coordinated and that there is formation of Ga-O-Si linkages with the increase of gallium content in the sample, as well as a proximity/interaction effect of P and Ga atoms. For the sol-gel derived glasses, samples of composition $[(80\text{-}x)SiO_2–(15)CaO–(5)P_2O_5–(x)Ga_2O_3]$ and x={0,2,4,6,8,10} mol% were prepared. The NMR results indicate that, as in the previous set of samples, there may be a formation of Ga-O-Si linkages, since there is a decrease in high-coordinated ^{29}Si and a proportional increase in the lower coordinations. Something curious observed in the ^{29}Si spectra is that there is a stabilization of the components between the 6%, 8% and 10% samples — the spectra are very similar. This may indicate that 6% is an upper bound for gallium incorporated in the sample. In this case, a change in gallium environment should be expected, which will be explored further through ^{71}Ga measurements. This is the focus of the present phase of the research, as well as BET characterization of the other samples. In the future, it is intended to focus on the insertion of sodium in samples derived from sol-gel, on new characterizations and on bioactivity studies (dissolution kinetics in SBF), in order to compare the properties of the different sets of samples.

References: (1) Hench, L. L., Polak J. M. Third-generation biomedical materials. Science. 2002, Feb 8; 295(5557):1014-7. doi:10.1126/science.1067404; **(2)** Kurtuldu, F., Mutlu, M., Boccaccini, A. R., Galusek, D. Gallium containing bioactive materials: A review of anticancer, antibacterial, and osteogenic properties, Bioactive Materials, Volume 17, 2022, Pages 125-146, ISSN 2452-199X, doi: 10.1016/i.bioactmat.2021.12.034.