UNIVERSITÉ DE LORRAINE

CRM² Cristallographie, Résonance Magnétique et Modélisations

Effect of nanostructuring on the structural and physical properties of functional molecular nanomaterials: Applications to bioactive glasses	
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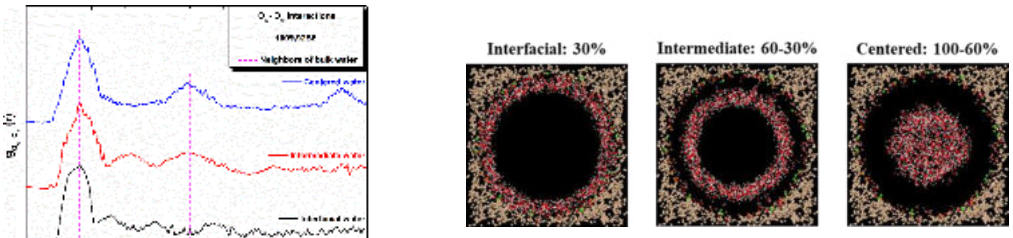
Since the pioneering discovery of the bioactive behaviour of certain silica based glasses by Hench, significant therapeutical progress has been achieved by using these bioactive materials for bone reparation and replacement. The biomedical applications of these materials are mainly due to their high biocompatibility and high reactivity with the human physiological environment, since the reaction products obtained from these bioglasses and the physiological fluids lead to the deposition of a layer of crystalline bone-like carbonate calcium phosphate (*Hydroxy-Carbonate Apatite, HCA*) on their surface shortly after interaction, thus promoting fast integration of the implant with the host and hence reconstruction of damaged bones. Therefore, the glass bioactivity is usually evaluated by measuring the rate of *HCA* formation at its surface on its exposure either to body fluids *in vivo* or to a simulated body fluid (SBF) *in vitro.* The structural analysis of these materials is often accomplished by "conventional" X-ray powder diffraction, and is therefore not sensitive until the formation of the first crystalline *HAC* species. However, it is crucial to understand the different stages from the immersion of the bioactive glass in physiological liquids to the formation of the *HCA*, for improving the bioglasses' properties. Thus, the main goal of this project is the structural characterization of the different species (liquid, amorphous, nanocrystalline...) involved in the glass bioactivity mechanism in order to obtain a full picture of the underlying processes.

The detailed structural analysis of these biomaterials can be performed by using complementary experimental techniques as well as appropriate modelling [1-3]. The approach is based on the multiscale modelling (from sub-Angstrom to several tens of nanometers) of total X-ray scattering data using the pair distribution function (PDF). The PDF analysis allows for the determination of the structural parameters on a local and intermediate length scale and hence the study of ordering effects due to confinement. Complementary information is obtained from solid-state NMR, namely concerning the local structure and light elements such as hydrogen. Further, NMR enables also the study of dynamical behaviour of the encapsulated species.

The thesis project contains a significant experimental part, consisting in collecting and analysing total X-ray scattering data from laboratory or synchrotron experiments as well as neutron diffraction experiments. Further complementary experimental techniques employed are solid-state NMR, NMR relaxometry, and differential scanning calorimetry. An important part of the project is based on Monte Carlo simulation for the reconstruction of the different structural models.



(a) **(b)**

Figure: **(a)** Partial Pair distribution function for confined liquids. **(b)** Snapshot representing the simulated structure for the different species of confined liquids.

Références :
[1] K. Rjiba, H. Khoder et al., *Microporous and Mesoporous Materials* **316**, 110922 (2021)
[2] H. Khoder et al., *Acta Cryst* **A76**, 589 (2020)
[3] E.-E. Bendeif et al., *RSC Advances* **5**, 8895 (2015)

3 year PhD position

Funded by Lorraine University

Application opens from: April 1st 2021 to May 1st 2021

Starting date: October 2021

Candidate profile:

- The PhD candidate must be graduated in Physics and/or Material Science.

- She (He) must show a strong motivation to carry out both experimental and numerical simulation works in collaboration with different research teams.

- An experience in crystallography, total scattering and numerical simulation would be greatly appreciated.

- The candidate must be open-minded and curious, able to learn by her (him) self through bibliographic studies.

Application: Send us as soon as possible

- your CV and a motivation letter

- your Bachelor and Master transcripts

- Assessment letter from the Master2 internship supervisor

- Possibly recommendation letters.

Selected candidates will be interviewed by Visio conference.