Experimental report

19/02/2018

Proposal: 9-12-483 **Council:** 10/2016

Title: The dynamics of aqueous polyacrylic acid solution confined in Dental Cements: From jump diffusion to multiple-state diffusion processes

Research area: Soft condensed matter

This proposal is a continuation of 9-12-407

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Samples: Aqueous solution of polyacrylic acid (Voco Ionofil Molar AC, Voco GmbH, Germany)

Instrument	Requested days	Allocated days	From	To
IN16B	1	1	26/11/2016	28/11/2016

Abstract:

In typical odontological studies water sorption in the restoration material is determined by weighting a freshly mixed cement at regular intervals. These findings were attributed to conformational changes in hydrophilic segments of the polymer on absorption of aqueous sodium chloride. It is considered that in this scenario the molecules form more compact coils than in the presence of pure water.
To improve such evaluation process, to compare different bulk liquids and, at the same time, to develop new materials to be used in dental treatment, insight on the chemical reaction dynamics between the bulk liquid and the glass-silicate particles used in dentistry is important. Such information is usually hard to determine accurately and non-destructively. Here we propose to use QENS to understand how the dynamics of the bulk liquid used in the hydration process in dental cement in order to understand haw it is modified when confined and relate the results to durability.

This work aims to understand the Nano scale dynamics of the free and confined liquid used in the dental cements glass ionomer cements (GIC). The obtain diffusion coefficient was related to cement propertys such as crosslinking and strength. The collected data using IN16B (ΔE=1μeV) of the free liquid PAA solution was part of a bigger investigation and was combined with previously collected quasielastic neutron scattering (QENS) data obtained at IN16B data (of selected GICs cured for 7 and 28 days), IRIS spectrometer at ISIS (ΔE=20μeV) and PELICAN at ANSTO (ΔE=50 μeV), see Figure 1.

For the measurements using IN16B on the free liquid PAA solution used in preparation of GIC the sample was mounted as provided by the manufacture in a flat aluminum sample holder. The QE signal was measured at 220 K (below the glass transition observed in the DSC data), 260 K (between the glass transition and the melting temperature), at 310 K (body temperature) and 10K instrument resolution for four hours at each temperature. Furthermore, we measured an empty can for background subtraction and vanadium for detector calibration. In total 8 different temperature (10K, 220K, 260K, 270K, 280K, 290K, 300K, 310K) were investigated with a doppler speed of 4.4 m/s, corresponding to a energy range of -30 μeV to 30μeV.

The liquid used to prepare a selected GIC, and which dynamics we elucidated using IN16B, is a polyacid solution. As shown in Fig. 1, the analysis of the QENS spectra collected on PELICA IRIS and IN16B confirms that in the Liquid Poly three different hydrogen populations are present and that the dynamical behavior of the liquid is somehow slowed down but maintained in the cement. Further investigation into the polyacid solution was essential to understand how the dynamics at the nanosecond time scale changes when confined. The QENS analysis of the cement data collected using IN16B in November 2015 turned out to be very difficult, since the information on how the liquid behaves on the time scale covered by the spectrometer was still missing. The proposed beam time revealed that a similar deviation from a simple jump diffusion picture could be observed in bulk on the ns time scale. This proposal involved one of the last steps of a multi-disciplinary research project and is part of a PhD thesis. The analyzed data is presented in a manuscript entitled “Nanoscale Mobility of Aqueous Polyacrylic Acid in Dental Restorative Cements” that is currently under review and presented in a completed PhD thesis.

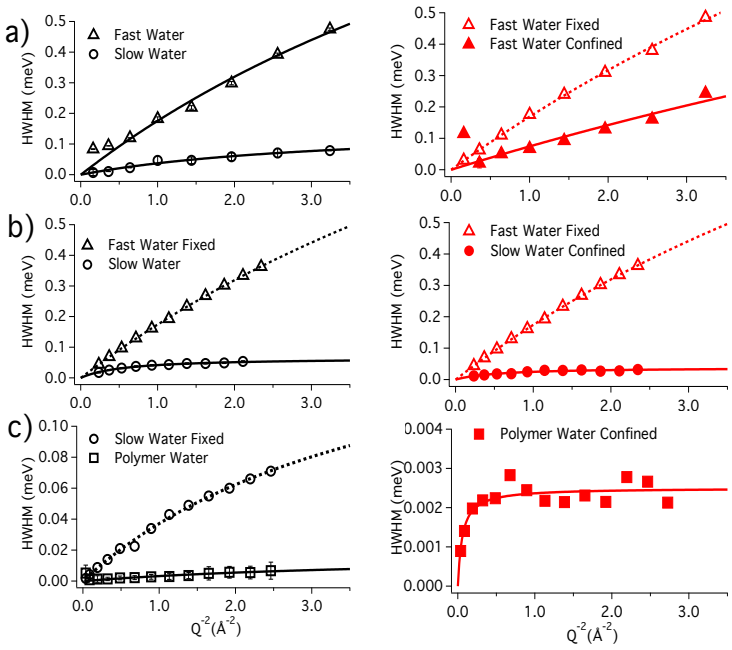

Figure 1 : Obtained diffusion coeficitients for both free PAA solution (left in black) and the confined PAA solution in a GIC (right in red) for the spectrometers PELICAN (a), IRIS (B) and IN16B (C).