Study of atomic motion in rubidium borate glasses

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Introduction
Atomic Scale X-ray Photon Correlation Spectroscopy (aXPCS) uses coherent X-rays to probe the dynamics of materials on an atomic scale. It was applied to study atomic diffusion in crystals [1], but its application was recently extended to glasses as well [2]. Results of dynamics and structural studies studies on high- and low-alkali content rubidium borate glasses are presented here. Structural studies include total scattering experiments, yielding the pair distribution function alongside Small-Angle X-ray Scattering (SAXS) studies giving information about inhomogeneities in the samples.

Theory
Real space structure: changes in time results in different scattering patterns
Space and time dependence described by the Van Hove Pair Correlation Function

\[ g^{(2)}(q,\Delta t) = \frac{\langle f(q, t) f(q, t + \Delta t) \rangle}{\langle f(q, t) \rangle^2} \]

Intensity Auto Correlation Function (ACF)

\[ \tau^{coh}(q) = \frac{1}{\langle f^2(q, t) \rangle} \]

Structure
Scattering function in general includes both Bragg and diffuse scattering → for amorphous substances only diffuse scattering occurs.
Pair distribution function (PDF) is the probability of finding two atoms separated by a distance \( r \).
Connection of the PDF \( G(r) \) to the measured scattered intensity \( S(Q) \) via Fourier sine transform

\[ G(r) = 2 \sum_{m=0}^{\infty} \int_0^{\infty} dQ \mathcal{O}(S(Q)-1) \sin(qr) \]

The scattered intensity is related to the total (static) structure factor by

\[ I(q) = N \left[ \langle f^2(q) \rangle - \langle f(q) \rangle^2 + \langle f(q) \rangle^2 \sin^2(qr) \right] \]

Total structure factor and pair distribution function

\[ \tau_{coh}(q) = \frac{1}{\langle f^2(q, t) \rangle} \]

Pair distribution function as a function of radial distance

\[ g^{(2)}(q) = 1 + \beta e^{-\chi(q)} \]

SAXS

SAXS intensities as a function of momentum transfer

\[ \sigma_{\text{SAXS}}(q) \]

Conclusion

- Diffusion in low rubidium content borate glasses best described by two-jump model
- Large difference in diffusivity between low and high alkali glass
- Diffusion at 20K still too fast to be measured in high alkali glass
- Large difference in diffusivity between low and high alkali glass
- Inhomogeneities are much larger in high alkali sample
- Inhomogeneities in the samples.