Temporal correlations in liquid water using x-rays: from seconds to femtoseconds

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It has been postulated that the observed high- and low-density amorphous ice forms of water, HDA and LDA, can be related to two hypothesized high- and low-density liquids, HDL and LDL, through two distinct glass transitions in the ultraviscous regime. Here, we study experimentally the structure and dynamics of HDA ice as it is heated up and relaxes into the low-density form. Is this a transition between two amorphous ice forms, i.e., an HDA-to-LDA transition, or is this transition occurring between two liquid states, inferring instead an HDL-to-LDL transition in the ultraviscous regime? The unique aspect of this work is the combination of two X-ray methods, where Wide-Angle X-ray Scattering (WAXS) provides the evidence for the structural changes at the atomic level and X-ray Photon Correlation Spectroscopy (XPCS) in the small-angle X-ray scattering (SAXS) geometry provides insight about the motion at the nanoscale, respectively [1]. The diffusive character of both the high- and low-density forms is discussed among different interpretations and the results are most consistent with the hypothesis of a liquid–liquid transition in the ultraviscous regime. In addition, we will discuss of future outlook and possibilities of extending such measurements in obtaining the dynamics of liquids from seconds to femtoseconds [2] by combining Diffraction Limited Storage Rings (DLSR) with X-ray Free-electrons Lasers (XFELs).

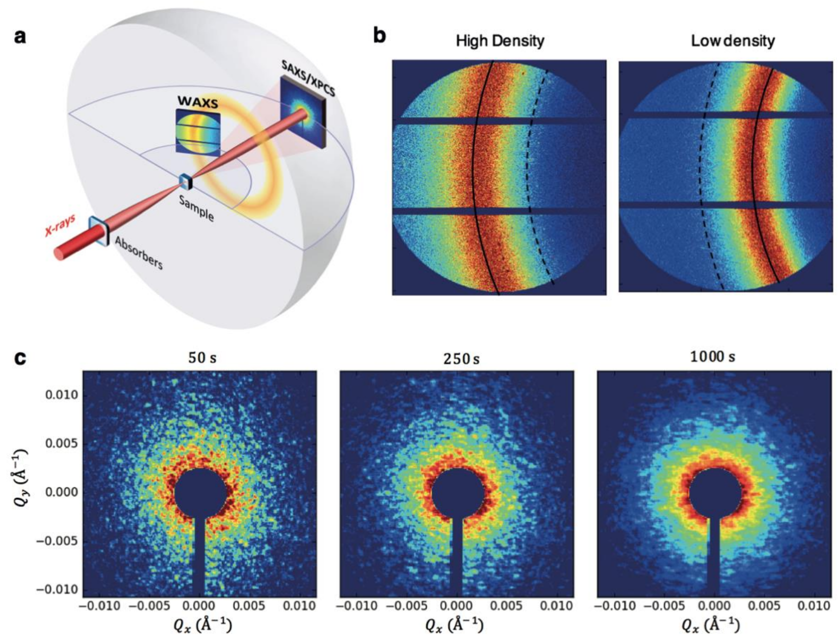

Figure 1: (a) The experimental setup combining (b) WAXS with (c) XPCS in SAXS.

References

[1] F. Perakis *et al.*, "Diffusive dynamics during the high-to-low density transition in amorphous ice," *PNAS*, **114**, 31, p. 8193–8198, (2017)

[2] F. Perakis et al., "Coherent X-rays reveal the influence of cage effects on ultrafast water dynamics," Nat. Commun., vol. 9, no. 1, p. 1917, (2018).