Neutron Diffraction and Raman Studies of the Pressure-Induced LDA-HDA Transition of Ice

Strässle Th.[1], S. Klotz S.[1], G. Hamel G.[1], Nelmes R.J.[2], Loveday J.S.[2], Rousse G.[1], B. Canny B.[1], Chervin J.C.[1], Saitta M.[1]

[1]*Physique des Milieux Condensés, Université P&M Curie, B77, 75252 Paris, France*
[2]*School of Physics and Centre for Science at Extreme Conditions, University of Edinburgh, Edinburgh EH9 3JZ, U.K.*
thierry.strassle@pmc.jussieu.fr

The transition between low density and high density amorphous ice (LDA and HDA respectively) observable below ~135 K figures among the textbook examples of a polyamorphic phase transition [1]. However, for purely experimental reasons, this transition has up to present been studied almost exclusively on quenched-recovered samples, from which various, partly contradicting conclusions have been drawn [2]. Here we present the first in-situ neutron diffraction study of the transition between LDA and HDA under pressure at ~0.3 GPa, at 130 K. It is shown that all the intermediate diffraction patterns can be accurately decomposed into a linear combination of the patterns of the end members, i.e., pure LDA and HDA just before and after the transition, respectively. This gives direct evidence of phase coexistence, as seen in a classical first-order transition. We also report in-situ Raman measurements and visual observation of this transition under the same conditions which strongly support these conclusions. These findings have implications for models of water and the proposed second critical point in the undercooled region of liquid water.

References

[1] O. Mishima et al., J. Chem. Phys. 100, 5910, (1994).
[2] O. Mishima and Y. Suzuki, *Nature* **419**, 599, (2002); C.A. Tulk et al., *Science* **297,** 1320, (2002).