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Report:

The microscopic structure of the hydrogen bond network of water at ambient and in supercooled conditions is controversially discussed, e.g. with respect to a mixture of low density and high density water phases [1]. It is widely believed that strenghthening of the water's hydrogen bond network is responsible for the properties of supercooled water [1]. Thus the question about the local molecular structure of supercooled water is of fundamental interest and may lead to a deeper understanding of the water properties in general.

In Experiment SC-3813 we measured x-ray Raman spectra at the oxygen K-edge of supercooled water for temperatures ranging from 293 K to 255 K. We used the spectrometer for non-resonant inelastic x-ray scattering studies with 72 crystal analysers, arranged in six independent modules. The average scattering angles were chosen to three times 41° (3 modules), two times 121° (2 modules) and one time 85° (1 module) for meausuring x-ray Raman scattering spectra in the vicinity of the oxygen K-edge for different momentum transfers. The water was supercooled in a custom-built sample cell. It was filled in glass capillaries of 2 mm thickness that were vacuum-sealed afterwards. The temperature was controlled via a chiller and heating foils.

Figure 1 shows first results of a series of oxygen K-edge spectra for low momentum transfers (3.55 $Å^{-1}$) and difference profiles between all spectra to the spectrum of 293 K. All spectra were background subtracted and area normalized between 533 eV and 550 eV. Changes in the pre-edge (around 535 eV), the main-edge (around 538 eV) and the post-edge (around 541

eV) regions are observable for decreasing temperatures. The behavior of the pre-edge and the post-edge regions indicate an increase of tetrahedral order with decreasing temperature, while the changes in the main-edge regions reflect the density decrease with decreasing temperatures [2].

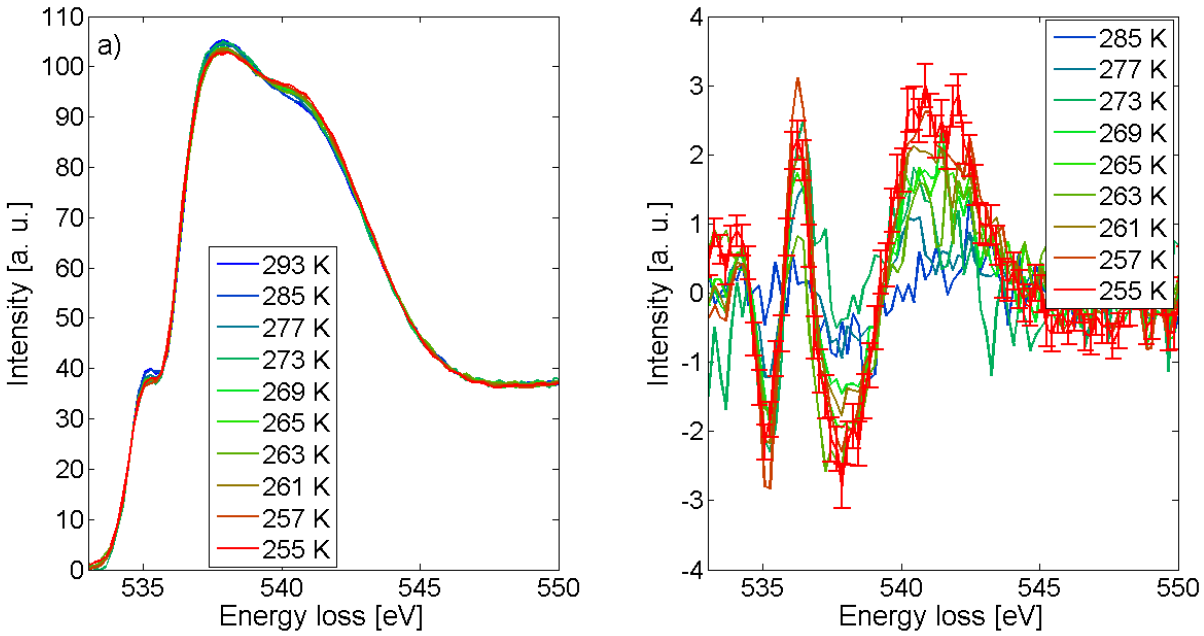

Figure 1: Oxygen K-edge spectra of supercooled water for a momentum transfer of 3.55 $Å^{-1}$ (a) and difference profiles between all spectra to the spectrum of 293 K (b).

For further analysis this results will be compared to structural snaphshots obtained from molecular dynamics simulation and compared to results which we obtained for the local structure of supercooled water via Compton scattering experiments.

[1] A. Nilsson & L.G.M. Pettersson, Chem. Phys. 389, 1 (2011)
[2] T. Pylkkänen, A. Sakko, M. Hakala, K. Hämäläinen, G. Monaco, and S. Huotari, J. Phys. Chem. B 115 (49),14544–14550 (2011)