# Prospects for structural studies on ice phases and clathrate hydrates

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The "old" D2B has been used in the past years for a number of neutron powder diffraction studies in the field of ices and gas hydrates [1]. The "new" D2B offers additional advantages for a number of open questions in these fields. It is the purpose of this presentation to discuss a number of relevant questions concerning these materials and to indicate how diffraction studies on the upgraded D2B may help to answer them.

Recently, the transition of so-called cubic ("ice Ic") ice into ordinary hexagonal ice ("ice ih") has received renewed attention. By neutron diffraction studies it was found that ice Ic persists to much higher temperatures than previously thought [2]. This finding is relevant for atmospheric issues and definitely needs further attention. High-resolution neutron powder diffraction will be crucial to establish the defective crystal structure of ice Ic and help towards a better understanding of the mechanisms of the final transition into ice Ih.

The original goal of *in-situ* neutron diffraction studies on high-pressure ices was to provide critical tests for empirical water-water potential [1984]. For more than twenty years these test largely failed. Recently, DFT and CPMD calculations have demonstrated their capabilities in reproducing structural features including the (partial) ordering in high-pressure ices and orientational disorder patterns in ice Ih [3]. This is remarkable and further detailed crystallographic data are now needed to refine the agreement eventually leading to a better understanding of water-water interactions.

Water-gas interactions are equally interesting. Initial experiments have shown remarkable changes in the lattice constants of ice Ih upon inclusion of He. Similar changes have been found in ice II with He or Ne inclusions. The determination of the pressure-dependent filling of these "stuffed" ices needs excellent neutron diffraction data and will provide critical tests for gas-water interaction potentials.

Gas hydrates are of considerable interest in chemical engineering and geosciences. A large number of questions remain open. The cage filling in other gas hydrates depend critically on the gas-water interactions and provide critical test for improved versions of the classical statistical thermodynamic theory used in hydrate prediction by chemical engineers in the petrol industry. Excellent diffraction data are needed to determine the cage filling under *in-situ* conditions with the necessary precision and accuracy. Neutron powder diffraction is the method of choice to study the cage filling in the recently found $H_2$-THF-hydrates which shows some promise in $H_2$ storage applications [4].

The new D2B is in an excellent position to tackle these and a large number of related questions and will undoubtedly continue to contribute to the advances in these fields.

**References**

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