

Recent Technical and Scientific Advances in High Pressure Neutron Scattering

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There have been significant improvements in the operation of the high pressure diffractometer, SNAP, at the Spallation Neutron Source over the past two years. This talk will highlight the current capacities which include low temperature systems, high temperature systems, and the introduction of new pressure cell technology that is based on supported diamond anvils and, with advances in software, is particularly suited for powder diffraction. Specific examples include our recent attempts to perform neutron powder diffraction at 1 Mbar. The design of the new pressure cell and data from ice VII samples collected at 80 GPa will be discussed.

Specific scientific examples of our recent research focus on high pressure transitions in hydrogen bonded systems such as methane and CO₂ hydrate. The high pressure hexagonal phase of methane hydrate is studied to determine the nature of the hydrate cage loading, this provides detailed experimental data that will lead to better intermolecular potentials for methane – methane interactions, particularly when methane molecules are in close contact and strongly repelling. The high pressure structural systematics of carbon dioxide hydrate is reported. While the structural transformation sequence of most hydrates progress from sl (or sII) to the hexagonal form then to a filled ice structure, CO₂ hydrate is an example of a system that skips the hexagonal phase and may transform directly into the filled ice structure. Finally examples of using SNAP to study disorder in amorphous systems will be given. Particularly amorphous methane hydrate produced by compression of sl hydrate at low temperature and the structural evolution of the amorphous form upon annealing and recovery to ambient pressure.