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Structure of high-pressure ices revealed from single-crystal and powder neutron diffraction

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Abstract

Water ice has remarkable structural diversity, at least 20 crystalline phases are known up to date. Most of those polymorphs exist at relatively low pressures below 2 GPa, and above the pressure, they are limited to ices VII, VIII, X with bcc structures and ice XVIII with a fcc structure, and their structural diversity has seemingly disappeared. However, many unresolved questions about the apparently simple structures of those high-pressure ice phases remain. For example, ice VII shows many anomalous properties at around 10 – 15 GPa, such as electric conductivity enhancing, self-diffusion of protons, X-ray diffraction peak broadening, Raman peak narrowing, and those structural origins are not fully understood (e.g., [1)] and see references therein). Another example is a phase transition from ice VII to ice X which involves hydrogen-bond symmetrisation. It has long been considered that the transition may occur at 60 GPa for H2O and 70 GPa for D2O from spectroscopic studies over 20 years ago[2-4)], but the succeeding studies have suggested multiple changes for hydrogen disordering and proposed different transition pressures ranging from 30 to 110 GPa[5-8)].

Neutron diffraction is a key technique to unravel such unresolved questions of high-pressure ices, because neutrons can interact with hydrogen as well as oxygen and elucidate the detailed crystal structure including hydrogen positions. However, in situ experiments of neutron diffraction under very high pressure, or the detailed structure analyses by single-crystal neutron diffraction have been limited due to the technical difficulty. Our group recently developed new high-pressure cells for single-crystal neutron diffraction up to 5 GPa [9, 10)] and for powder neutron diffraction up to 80 GPa[11)]. The key material for both high-pressure cells is nano-polycrystalline diamond. In this presentation, I will show several neutron diffraction studies for ice VII using the newly developed high-pressure cells, and discuss the detailed crystal structure of ice VII.

References

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