

Unlocking the secrets of ice

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Credit: Pixabay

The complex properties of water and ice are not well understood but a team from UCL and the ISIS Neutron and Muon Source have revealed new information about a phase of ice called ice II.

Given that [water](#) makes up 60% of our bodies and is one of the most abundant molecules in the universe, it's no wonder that water is known as the "matrix of life."

There are many different forms of ice – all of which vary significantly from the ice you'd find in your freezer. Ice takes on many different forms depending on the pressure at which it developed.

As water freezes its molecules rearrange themselves, and high pressure causes the molecules to rearrange in different ways than they normally would. The many distinct phases of ice can be summarised using a phase diagram, which shows the preferred physical states of matter at different temperatures and pressures.

Researchers from UCL and the Science and Technology Facilities Council (STFC) ISIS Neutron and Muon Source have utilised high pressure neutron diffraction to investigate the impact of ammonium fluoride impurities on water's phase diagram.

Their surprising results, published in *Nature Physics*, found the addition of this impurity caused a particular phase of ice, known as ice II, to completely disappear from water's phase diagram whereas the other phases were unaffected.

The many different phases of ice can be grouped into one of two types – hydrogen-ordered phases and hydrogen-disordered phases. In these different phases the orientation of water molecules is either firmly defined or disordered.

Ice II is a hydrogen-ordered phase of ice that forms under conditions of high pressure. Unlike other phases of ice, ice II remains thermodynamically stable and hydrogen-ordered up to very high temperatures and the origin of this anomalous result is not well

understood.

Using neutron diffraction the group revealed the very special properties of ice II. The PEARL high pressure neutron diffractometer at ISIS Neutron and Muon Source is optimised for diffraction studies up to 20 GPa, though here samples were only exposed to 0.3 GPa. Even though this is well below the full capability of the instrument 0.3 GPa is still equivalent to 3 tonnes pressing down on a single fingernail.

For the neutron diffraction measurements ground ice samples were placed inside a titanium-zirconium can, which neutrons easily penetrate. The extreme pressure on PEARL was generated using a gas compressor filled with argon gas. PEARL allows in-situ pressure neutron diffraction measurements to take place, which were essential for this research.

"Without in-situ neutron diffraction we could not have performed this study. It was paramount to demonstrate that ice II has disappeared in the region of the phase diagram where it would normally exist," said Dr. Christoph G. Salzmann (UCL Chemistry).

In addition to collecting high pressure neutron diffraction data, researchers also utilised computational methods to gain very important insights. They found that doping ice II with small amounts of ammonium fluoride caused this particular [phase](#) of ice to disappear altogether, whereas the competing phases of ice were unaffected. This observation allowed researchers to infer important information on the highly unusual properties of ice II.

"Unlike the other phases, ice II is topologically constraint. This means that water molecules in ice II interact with each other over very long distances. In a sense, whatever happens to one water molecule in a crystal of ice II—the effect is "felt" by all other molecules. In our study, ice II experiences a disturbance by the ammonium fluoride which

destabilises all of the ice II and makes it disappear," Dr. Salzmann added.

The knowledge of this effect will be of importance to any study where ice coexists with other materials in nature, for example on icy moons. In addition, the special properties of ice II provide a new explanation as to why the [phase diagram](#) of water displays so many anomalies, including liquid water. These findings may also open up studies into new phases of ice. If dopants have the ability to suppress certain phases of ice this suggests they may also be able to induce the formation of new phases of ice.

Interest in the "matrix of life," and its many phases of ice, certainly shows no sign of wavering. With high pressure [neutron](#) diffraction allowing the study of extreme [pressure](#) environments in a way that no other technique can, we are likely to see the team back at the facility in search of new phases of ice.

More information: Jacob J. Shephard et al. Doping-induced disappearance of ice II from water's phase diagram, *Nature Physics* (2018). [DOI: 10.1038/s41567-018-0094-z](https://doi.org/10.1038/s41567-018-0094-z)

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