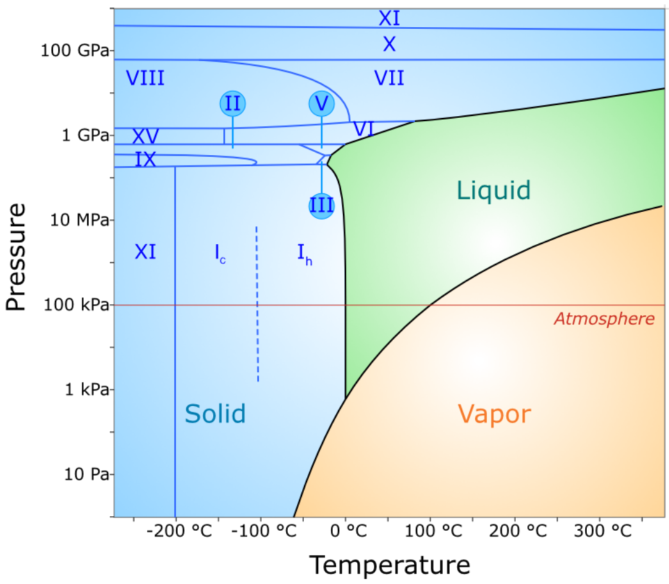
ICE UNDER PRESSURE

Determination of the compressibility of water ice at high pressures

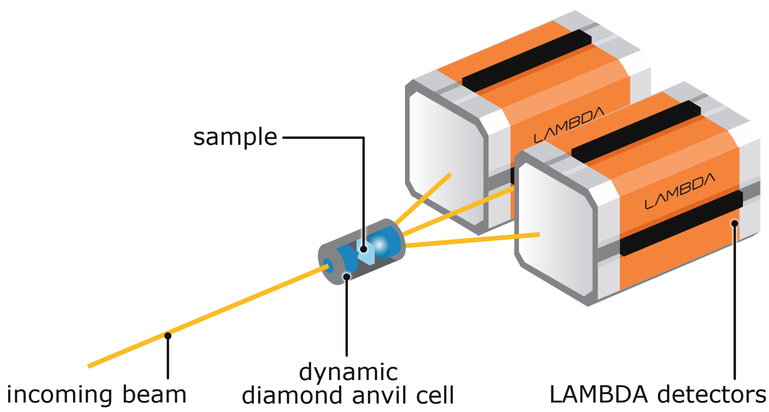
Ice comes in more than one shape: To date, scientists know 19 different types of crystalline solid water (H_2O), or water ice, which can be distinguished by how the H_2O molecules are arranged. This, in turn, determines their physical properties, such as compressibility. In almost the entire ice present on Earth, the H_2O molecules are arranged in hexagonal rings – a type of ice referred to as ice I_h. However, on the inside of other planets – be it in the outer regions of our solar system or in extrasolar planets – ice exists under much higher pressure and thus exhibits different shapes. Above 2 GPa (i.e. 20,000 times atmospheric pressure), ice is present in the cubic crystalline form VII. In this type of ice, the hydrogen (H) atoms are positioned between two oxygen (O) atoms, whereas they are a bit closer to "their" O atom than to the neighboring one. However, if the O atoms are forced even closer together under increasing pressure, the H atoms eventually assume a symmetric position. This form of ice is referred to as ice X. The transition between these two ice forms has now been studied in the lab using X-rays.



Phase diagram of water with different forms of ice.

EXPERIMENTAL SETUP

The international team of researchers from Germany and the United Kingdom performed high-pressure experiments at the Extreme Conditions Beamline P02.2 at PETRA III, DESY. They placed water ice in a dynamic diamond anvil cell (dDAC), a device that allows to subject a sample to a dynamic range of high pressures. While gradually increasing the pressure to up to 180 GPa, they collected X-ray diffraction images of the ice sample using two LAMBDA 2M GaAs cameras. **"We chose the LAMBDA detectors because of their excellent sensitivity and high temporal and angular resolution, features that are crucial in dynamic compression experiments"**, said Alba San José Méndez, lead author of the study. The high sensitivity of the detectors allowed short exposure times, i.e. fast sampling rates, which enabled the researchers to achieve quasi-continuous pressure resolution. On top of that, with a fast dDAC and a fast detector, the total duration of the experiments can be reduced. **"This also facilitates high-pressure experiments at high temperatures, where short experimental times are crucial to avoid thermal damage in diamond anvil cells"**, Méndez explained with reference to previous research that her team conducted with the LAMBDA detectors.

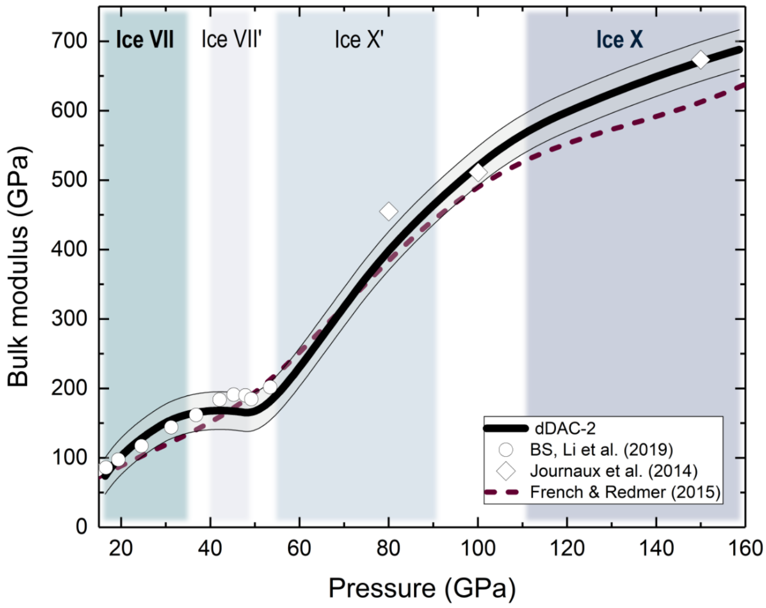


Setup with two LAMBDA 2M cameras recording diffraction images from the sample in a diamond anvil cell.

RESULTS

From the X-ray diffraction images, the researchers determined the unit cell volume as a function of pressure. As a second step, they derived the bulk modulus, which describes a substance's resistivity to compression: the higher its bulk modulus is, the smaller is its compressibility. While the bulk modulus of ice in the experiment generally increased with increasing pressure, the authors found that the transition from ice VII to ice X involves a state of softening at around 35–40 GPa (ice VII'). This, in turn, is followed by a steep increase of the bulk modulus at about 50 GPa. The authors infer that the H atoms assume their symmetric position during this phase (ice X'). At higher pressures, their experimental results agree with computational predictions and confirm the presence of static ice X.

Setup	PETRA III, DESY (Germany), P02.2 beamline
Camera	LAMBDA 2M GaAs detector
Resolution	2,359,296 pixels with 55 µm
Acquisition frequency	0.5–10 Hz
Photon energy	25.7 keV



Bulk modulus as a function of pressure as derived from the experimental run dDAC2. Solid circles represent data from previous studies using a different technique (Brillouin spectroscopy). The dashed line and solid diamonds represent computational results. Background colors indicate approximate pressure ranges for the stability of ice VII, ice VII', ice X' and ice X.

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This information sheet illustrates a real-world application of a LAMBDA 2M camera, developed and manufactured by X-Spectrum. We gratefully acknowledge the voluntary support by the scientists mentioned in this sheet. The optical appearance of the LAMBDA detectors which have been used in the experiment may differ from the depicted detectors.

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