**AN X-RAY VIEW ON THE SHAPE OF HYDROGEN**

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Hydrogen is the most abundant element in the Universe. Our knowledge of celestial bodies such as the Sun, which is made of about 75% hydrogen, relies on our understanding of the properties of hydrogen under extreme conditions of both temperature and pressure. Replicating these extreme conditions in a laboratory is exceptionally challenging, and even the structure of high pressure phases of hydrogen at low temperatures remains an open question. Ji and co-workers have successfully probed the structure of hydrogen at unprecedented pressures, revealing a hexagonal closed-packed structure.

The simplicity of the hydrogen atom, made up of a single proton and a single electron, does not prevent the phase diagram of hydrogen under pressure being rich and complex. Hydrogen is an insulator at ambient conditions, but becomes a metal under extreme compression [1], a state that could for example help generate the magnetic field around Jupiter. Additionally, theoretical proposals suggest that this metallic hydrogen may exhibit a number of exotic phenomena, such as high temperature superconductivity [2] or two-component superfluidity [3].

Over the last few decades multiple solid phases of hydrogen have been identified by increasing the pressure from atmospheric levels to well above those at the centre of the Earth. These experiments have been performed using diamond anvil cells, in which a sample of hydrogen is placed in a gasket, which is in turn screwed between two diamonds to achieve extreme pressures in the centre of the sample. So far, only limited information is known about these phases. The main techniques used are infrared and Raman spectroscopies, which provide insights into the local structure of vibrating hydrogen molecules. These techniques have revealed that upon increasing pressure hydrogen transitions from a solid in which all constituent molecules have similar bond lengths, to a different *mixed* phase in which molecules of different bond lengths coexist [4,5]. These experimental results are consistent with available theoretical models [6].

X-ray diffraction is the predominant technique for the study of long-range order in materials. Bragg’s law tells us that X-rays scattered by the electrons in a crystal interfere with each other, giving rise to a diffraction pattern in which bright spots correspond to waves that are in phase and interfere constructively, and dark spots coming from waves that interfere destructively. X-ray diffraction has been used to make many important scientific discoveries, perhaps the most famous example being that of the determination of the double helical structure of DNA. Unfortunately, the use of X-ray diffraction for the study of high pressure hydrogen has proved extremely difficult up to now.

A major difficulty is that the ability of X-rays to scatter off electrons decreases with the mass of the atoms that make up the material, and therefore hydrogen, as the lightest of all elements, leads to very weak signals. It is very difficult to distinguish the X-rays scattered by hydrogen from those scattered by the surrounding gasket, which is typically made from heavy elements. An additional challenge is that the diamonds that are used to pressurise hydrogen easily break when exposed to X-rays, leading to loss of pressure. Because of these difficulties, X-ray diffraction studies of hydrogen had so far only reached pressures of up to 190 giga-Pascal [7], about half the pressure to which hydrogen can be subjected to in diamond anvil cells, and not high enough to study some of the most exotic phases of hydrogen, such as the mixed phases.

Ji and co-workers have addressed these challenges in a *tour de force*, performing more than one hundred experiments over a period of five years. To increase the signal arising from hydrogen compared to that arising from its surroundings, they have used lighter elements to design the gasket. To avoid the breaking of the diamonds and the associated loss of pressure, they have performed short experiments in order to collect enough data before the inevitable diamond failure.

The results provide the first evidence of the long-range structure of hydrogen across three different high-pressure solid molecular phases, including the mixed phase. In all three phases, hydrogen molecules adopt a hexagonal closed-packed structure, analogous to that of helium atoms, in which the molecules are symmetrically arranged in the shape of a hexagonal prism. Additionally, with increasing pressure the prism becomes *fatter*, with its height becoming increasingly squeezed.

Some questions still remain. Unlike all elements heavier than helium, hydrogen has no electrons tightly bound to its nucleus, and instead all the electrons sit in the molecular bond. This means that the scattering of X-rays by electrons does not directly probe the location of the nuclei in the hydrogen molecule, but instead the location of the bond. As a consequence, the present X-ray results will have to be combined with other experimental techniques, such as the aforementioned infrared and Raman spectroscopies, and possibly also with nuclear magnetic resonance, which has only very recently become available at the extreme pressures under study here [8]. Combining these experimental insights with theoretical models will make the full characterisation of high-pressure hydrogen phases a reality.

In the next few years, experiments will probably focus on even higher pressures. The pressures reached so far in this X-ray study correspond to insulating molecular hydrogen. Studying the higher pressures at which hydrogen becomes atomic and metallic will prove a new challenge for X-ray techniques. In the metallic phase, the electrons will no longer be in the bond of a hydrogen molecule, but instead will be shared by all atoms in the structure, so it is unknown what the corresponding X-ray diffraction pattern would look like. Interesting times lay ahead for the study of the lightest and most abundant element in the Universe.

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