Extreme pressure studies with brucite will lead to advances in areas such as medicine, geoscience, and industrial technology.

Extreme-Pressure Brucite Studies

A collaboration using instruments at both SNS and HFIR has investigated how hydrogen and deuterium differ under pressure, to help both the science community and industry clarify fundamental differences in these isotopes. This research can potentially impact neutron scattering, geosciences research, and industrial applications.

Researchers Juske Horita, Antonio Moreira dos Santos, Bryan Chakoumakos, and Chris Tulk used the WAND instrument at HFIR to study the effects of pressure on the compression properties of hydrogenated and deuterated brucite.

Brucite, or magnesium hydroxide ($Mg(OH)_2$), was chosen because it is one of the simplest hydrogenated materials found in nature. It is made of stacked sheets of magnesium hydroxide octahedra, which are composed of magnesium ions with a +2 charge, bonded to six hydroxides with a -1 charge. Each hydroxide in turn is bonded to three magnesium ions. The result is a neutral sheet, as the charges cancel and the lack of a charge means there is no "glue" to keep the sheets together. The sheets are held together only by weak electrostatic interactions.

"Brucite is what we like to call a model system. It is a system that has so little complexity that phenomena that are observed can be traced directly back to the problem that we want to elucidate," says Moreira dos Santos, a postdoctoral fellow at SNS.

The question was whether a brucite sample made with hydrogen and a second made with deuterium, a heavier isotope of hydrogen, would respond identically to pressure. Researchers favor deuterium for neutron scattering samples because hydrogen scatters incoherently and that generates a lot of what scientists call background in the data. The measurements tend to be lengthier and have poor resolution, Moreira dos Santos explains. "Hydrogen is not a very good isotope to work with."

All conditions being equal, scientists prefer deuterium in their samples for neutron scattering experiments. But all conditions are not equal, as Moreira dos Santos and his colleagues have found. The difference between hydrogen and deuterium in the sample can affect neutron scattering research results, as well as studies of hydrogenation of minerals deep in the earth, some of which store water and hydrogen in other forms, and hydrogen storage applications in industry.

Juske Horita, a researcher in the Chemical Sciences Division, made samples of brucite, one with hydrogen and one with deuterium. Then the researchers went to the SNAP powder diffractometer at SNS and applied pressure to each sample, measuring several diffraction patterns in situ, while increasing the pressure. Says Horita, "By the changes that happen as you increase pressure, you can understand what the pressure is doing to the crystal structure at the atomic level, how much the atoms come closer together. You can quantify that and, because you have both hydrogen and deuterium samples, you can see how the one compares with the other under pressure."

Detectors at different angles collected the diffracted neutron beams. Horita explains, "In this technique, called angle dispersive diffraction, at some angles you measure a peak of intensity. There are a lot of neutrons that scatter in that direction, while at other angles there are very few. Crystals are very ordered systems and the positions of these peaks will provide information regarding the positions of the atoms with respect to each other. The periodicity of the crystal is going to be reflected in a sort of pattern."

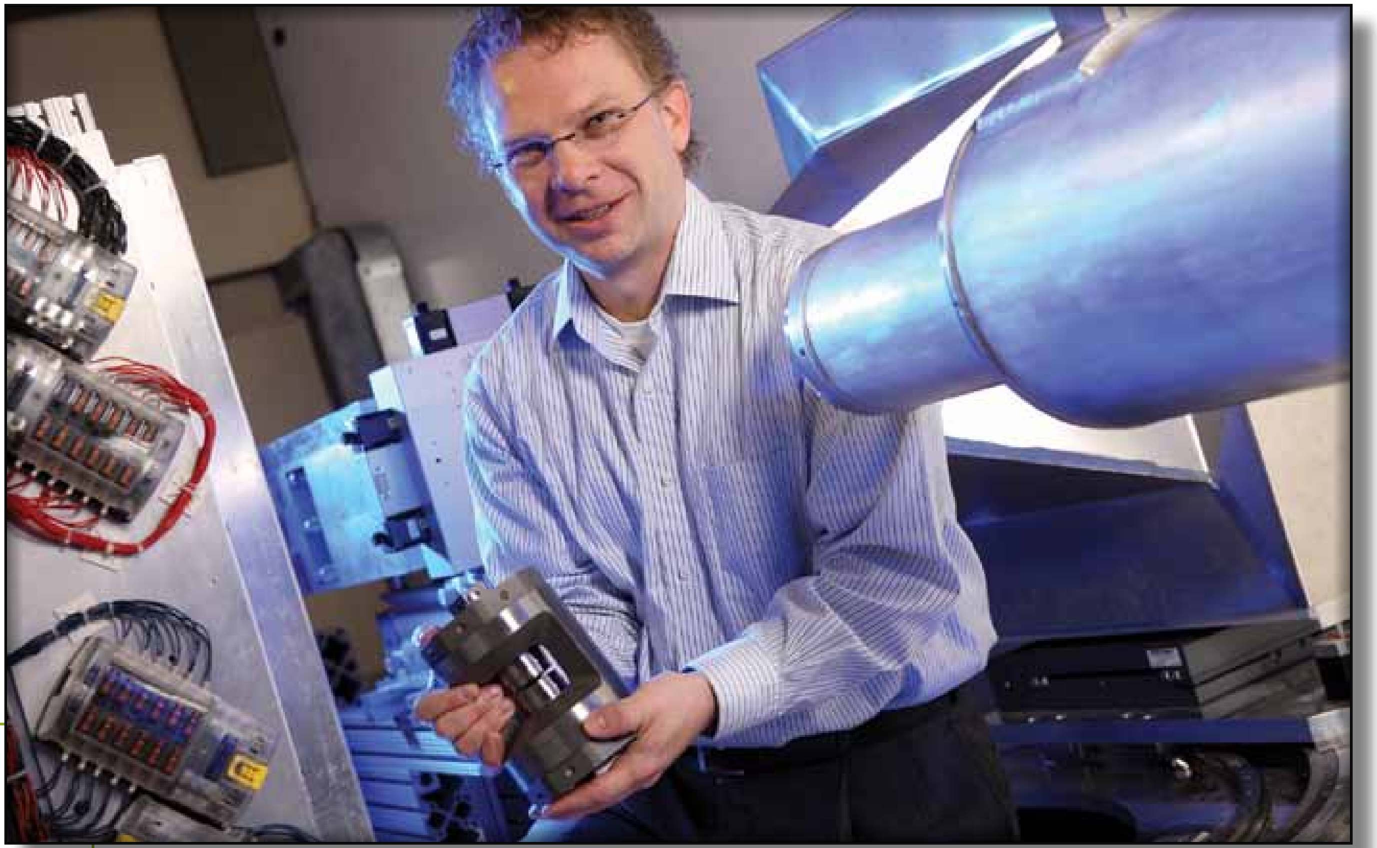
The group was looking for specific changes in unit cell volume (the building block of a crystalline material), which would indicate how close the atoms in the samples became under the pressure applied. What they found was a systematic higher compressibility on deuterium samples of brucite. Moreira dos Santos says this is critically important to him as a researcher. "When I do other sorts of measurements, every time I use deuterium I have to be careful, because things will happen sooner, at lower pressure, than when I use hydrogen. So that will give me clues to establish a standard on what to expect or how to correct the data obtained when doing scientific research on samples containing hydrogen."

The implications may be important across broad fields, from hydrogen storage research to pharmaceutical and even medical research. "When you want to use molecules as a medicine or you want to study mantle minerals underground or you want to study brucite, be careful in replacing hydrogen with deuterium because they are not the same but they actually show a distinctive behavior."

Moreira dos Santos says that a difference in the behavior of hydrogen and deuterium under pressure may be significant at high pressure ranges found in the earth, providing new insight into the abundance of deuterium in nature, and on other planets. "If the deuterium sample is more compressible, deuterium may be more abundant in the earth than previously thought. We mostly measure the things which come to the surface, but of course if hydrogen is less stable under high-pressure conditions, hydrogen will come to the surface first, to escape an adverse environment. If deuterium is actually more compressible, when you compress the rocks it is not such a dramatic change and it may remain in that state. So our estimate for the amount of deuterium and hydrogen in nature can be slightly off."

Finally, the research is important for neutron scattering in hydrogen storage research. "Neutrons are incredibly useful to study hydrogen storage problems, because neutrons can measure hydrogenated samples much better than x-rays. But you still have this background problem with hydrogen. You want to use deuterium, as long as we know what is happening and as long as we have this benchmark.

"If you can just find a good model system it can really open the doors for wonderful research. Horita's work was really important, to find the system in which we were able to isolate the property that we wanted to isolate. Because when you can really clarify something, others can start from that and keep moving forward. This gives us the motivation to move on and do complementary experiments so that we can really probe the bonding of the hydrogen or the deuterium with the oxygen in the structure. This also gives us some ideas to do deeper experiments, to understand the origin of this difference."



Chris Tulk, lead instrument scientist for SNAP, with a Paris-Edinburgh pressure cell.

SCIENCE HIGHLIGHTS