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Feature Story

The J-PARC Neutron BL21 group members gather for a group photo. The total scattering spectrometer, NOVA, is the world's highest resolution neutron spectrometer for the determination of non-crystalline material structure.

NOVA: neutron spectroscopy for a better environment

[Neutron Spectroscopy, Hydrogen Storage, J-PARC]

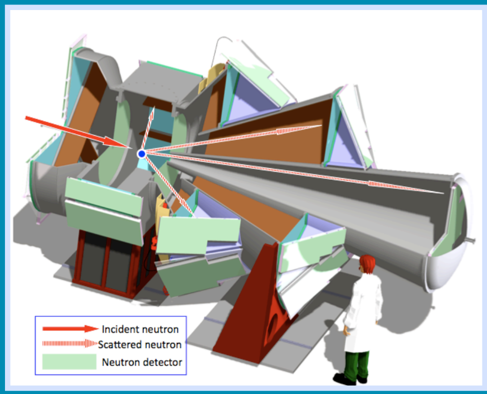
The neutron total scattering spectrometer (NOVA) at the Japan Proton Accelerator Complex is about to begin searching for hydrogen storage materials. Learn here about the unique features of the world's highest intensity wide-angle spectrometer for non-crystalline materials.

If you ask material scientists what the most studied, yet least understood liquid is, often the answer is water. A water molecule is deceptively simple in structure, composed of one oxygen atom and two hydrogen atoms. The difficulty in imaging such a molecule actually comes from the most abundant element in our universe—the hydrogen atom. X-ray diffraction, the most popular type of spectroscopy, determines atomic structure by looking at how X-rays interact with the clouds of electrons surrounding each nucleus. Since a hydrogen atom has just one electron orbiting its nucleus, its electron cloud is thin, has little effect on X-rays, and so is hard to image using X-ray diffraction.

Neutron spectroscopy is the revolutionary tool which changed all this. Neutrons are neutral particles, and do not interact electrically with charged particles. Because of this, neutrons can penetrate deeply into the nuclei of atoms. The strength of the interaction between a nucleus and a neutron, also known as a neutron cross section, does not depend on the atomic number of the target atom, or the size of the atom's electron cloud. This means the neutron cross section of even a small atom like hydrogen is relatively large.

←The installation of NOVA.

↓NOVA measures momentum transfer of neutrons at all scattering angles, allowing for accurate measurements across a wide range of distance scales in non-crystalline, structures, including dynamic structures such as liquids.



In the past, the limiting factor for neutron diffraction had been the low intensity of the neutron beams that could be produced at an accelerator. However, with the start of the world's most intense proton accelerator facility at the Japan Proton Accelerator Complex (J-PARC) in Tokai, neutron spectroscopy is increasingly more accessible and more useful for material scientists, offering a complementary method to the conventional X-ray diffraction.

One of the most important devices at J-PARC for such purpose is the neutron total scattering spectrometer, NOVA. NOVA is a gigantic, five-meter long, three-meter tall, bug-shaped vacuum container with five different detector sections. This device surrounds a sample so as to be able to detect scattered neutrons in all possible directions. NOVA is now almost complete, in good shape to start carrying out experiments late this year.

Materials for hydrogen storage

NOVA's main ambition is to find an efficient form of hydrogen storage. Hydrogen energy is a promising, clean, energy storage technology in which oxygen and hydrogen are combined to produce energy and nonpolluting water. "Hydrogen atoms are abundant, but are also hard to store," explains Prof. Toshiya Otomo of KEK, the leader of NOVA group. "To derive sufficient energy from hydrogen gas, the gas must be often stored at a pressure of 300 to 700 hundred atmospheres. You could not casually carry such a heavy, unsafe container on your car."

One promising solution is an alloy that can store hydrogen in space between atoms of the alloy, called interstitial sites. In order to use hydrogen energy in automobiles, however, the energy discharge must occur instantly when the car accelerator is depressed. Therefore, a hydrogen storage alloy would need to absorb and release hydrogen easily and quickly. More importantly, it should also be light.

"We would not be able to develop a workable material for hydrogen storage by simply mixing and testing. We need to examine what's going on inside the material at the atomic level. We need to understand the mechanism of hydrogen absorption and desorption in order to develop the most efficient materials," says Otomo. He and around 30 other members from 7 research institutions in Japan constructed the spectrometer for just such science.

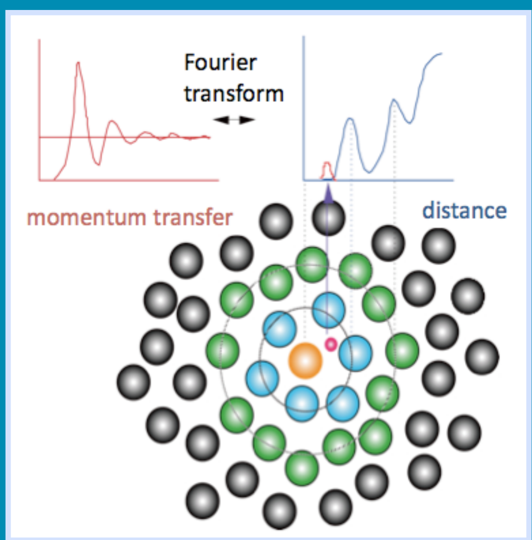
The spectrometer for non-crystalline structure

NOVA will excel in visualizing variety of structures including non-crystalline structures. When hydrogen is absorbed in a crystalline alloy, amorphous—non-crystalline—solid can form, disrupting the regular atomic structure of the crystalline alloy. To obtain high sensitivity to such non-periodic structures, NOVA is designed to detect every neutron diffracted off the sample. Further, in the inelastic scattering of neutrons off each atom, neutrons transfer momentum to the atoms inside sample. NOVA can measure the momentum change, called momentum transfer, of each scattered neutron.

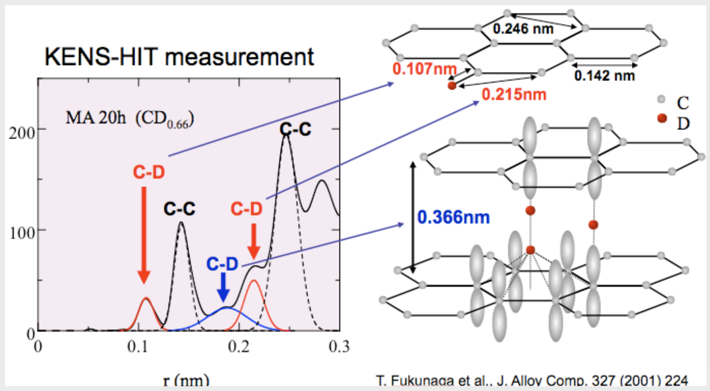
The amount of momentum transfer is related to the scale of atomic distance. In general, for a fixed neutron wavelength, neutrons with small scattering angles have small momentum transfer, while neutrons with large scattering angles transferred large amounts of momentum. Thus, less scattered neutrons infer the large-scale structure of the sample, while more scattered neutrons infer the small-scale atomic arrangements in materials. Data comes in the form of a spectrum showing the number of scattered neutrons at each level of momentum. By applying Fourier transform to this function, scientists can infer the distance between nearby atoms.

Wide momentum transfer range of NOVA

NOVA's precursor at KEK, KENS-HIT, looked at mechanical alloying in graphite hydrogen storage. The alloy was composed of layers of graphite, to which hydrogen atoms had adsorbed. By measuring the distance between hydrogen atoms and nearby carbon atoms, the



Non-crystalline structure is determined by measuring neutron spectrum in momentum transfer, and then applying a Fourier transform.



NOVA's precursor experiment, KENS-HIT, studied hydrogen storage in graphite. The experiment found that half the absorbed hydrogen atoms are stored between the layers of graphite, and the other half are strongly bound to the carbon atoms. The atoms between the graphite layers are easily extractable for use as fuel.

team deduced the positions of the hydrogen atoms. "The KENS-HIT scientists found out that about half of the hydrogen atoms were closely bound to carbon atoms, while the other half were trapped between the graphite layers. The hydrogen atoms that were located further from the graphite were the ones which were easily extracted by bringing up the temperature of the alloy," explains Otomo.

While KENS-HIT provided valuable information, it was only able to observe the small-scale structure of materials. To observe the larger-scale structure of graphite required another spectrometer called KENS-SWAN. "Now, with NOVA, both large- and small-scale structure can be reconstructed from just one shot of neutrons. Further, the resulting images will have more than twice the resolution due to the intense neutron beam," says Otomo.

Utilizing NOVA's ability to detect neutrons scattered at any angle, the team has just demonstrated the ability to determine the position of hydrogen atoms in a sample of vanadium deutrides. Even though neutrons are more sensitive to hydrogen than X-ray, precise determination of the location of hydrogen atoms is still a challenge. Thus, the analysis of NOVA results requires extra care. A hydrogen nucleus has one neutron and one proton. Because the mass of a hydrogen nucleus is comparable to that of a single neutron, the position of a hydrogen atom can easily be disturbed by an inelastic collision with a neutron. Additionally, molecules in liquid water move around. "The correction method for hydrogen has been tested at NOVA," says Otomo. "We were able to confirm the utility of the analytical method."

The bug-shaped vacuum chamber

NOVA's vacuum chamber is probably one of the most bizarre that has ever existed. As Otomo notes, vacuum chambers are not easy to manufacture, and generally have simple shapes, like a cube. Look at the NOVA. The shape you see is exactly the shape of vacuum chamber NOVA has.

There are two points that distinguish the NOVA vacuum chamber from any other vacuum chamber, even from other planned neutron total scattering spectrometers from around the world. First, the chamber has thin aluminum windows on the sides where the detectors are located. Neutrons can pass through these windows and reach the detectors undisturbed. Second, inside the vacuum chamber, neutron shields are installed in radial direction to absorb all unwanted neutrons. For example, neutrons can reflect off the walls of the chamber rather than off the sample, becoming a source of noise. Such neutrons are effectively eliminated by the shields.

"Originally, we were not sure if it would be possible to build a chamber with such a complex shape," says Otomo. "Very few company was willing to accept the original design contract." The team drew the sketches of NOVA vacuum chamber from scratch, and reshaped it a bit to make the design look more reasonable. For example, the original smoothly curving edges became octagonal, because curved vacuum chamber surfaces turned out to be hard to produce.

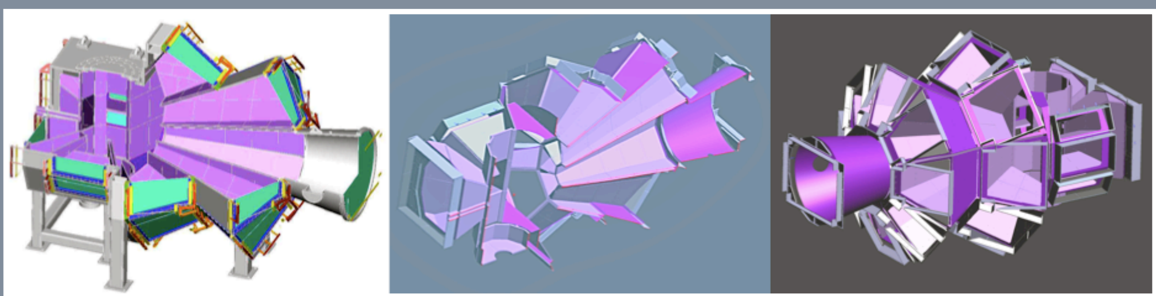
"Luckily, companies were very understanding of our scientific interests. Our project is also well funded by the Department of the New Energy and Industrial Technology Development Organization (NEDO), and so we were able to pursue an optimal design for reliable performance," Otomo says. In March 2009, the vacuum chamber was completed by the Kobe Steel Group, just as designed. The design had been in Otomo's mind since 2001. "It was great to see NOVA materializing, just as we had envisioned."

Interdisciplinary collaboration at KEK

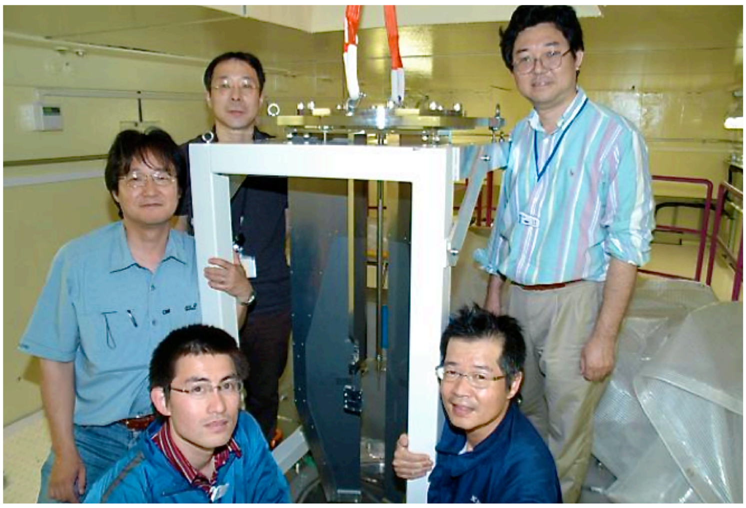
In recent years, a new trend of interdisciplinary collaboration has flowered at KEK. In large part, this trend is due to the efforts of the recently established Detector Technology Project at KEK. "Prior to this, institutes within KEK were rather closed societies. We at KEK's Institute of Materials Structure Science (IMSS) developed everything by ourselves, including detectors," says Otomo. "Now, detector physicists at the KEK's Institute of Particle and Nuclear Studies (IPNS) join our team and help us make the most of advanced detector technology."

An inside view of the NOVA vacuum tank. The complex structure of neutron shields spreads like a web.

In particular, NOVA uses gas electron multipliers (GEM) for the detector to measure



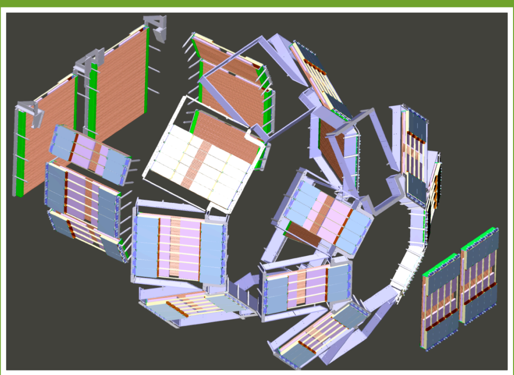
Inside the NOVA vacuum tank, neutron shields (purple) are installed in radial direction to absorb unwanted neutrons.



Top row from left: the leader of NOVA team Prof. Toshiya Otomo of KEK, Dr. Keiji Itoh of Kyoto University, and Dr. Kentaro Suzuya of JAEA. Bottom row from left: Dr. Hidetoshi Oshita of KEK, and Dr. Naokatsu Keneko of KEK.

the incident neutron beam before it hits the sample. GEMs are an advanced gaseous detector technology that allows two-dimensional imaging. The resolution is a 1-millimeter by 1-millimeter, around five times better than the helium wire chamber detectors that NOVA uses for the remainder of the neutron detectors. The detection rate is also two orders of magnitude greater, at one million signals per second.

"J-PARC produces a very intense neutron beam. The beam needs to be well focused to minimize the noise. The high performance GEM allows us to do this with high-quality monitoring," says Otomo. "However, GEM is still a new technology, and has not yet been employed in large scale." Because of the uncertainties surrounding this new technology, the team chose the time-tested and proven helium wire chambers, for detecting the less intense, scattered neutrons.



The 3D arrangement of NOVA helium detectors.

Manyo library

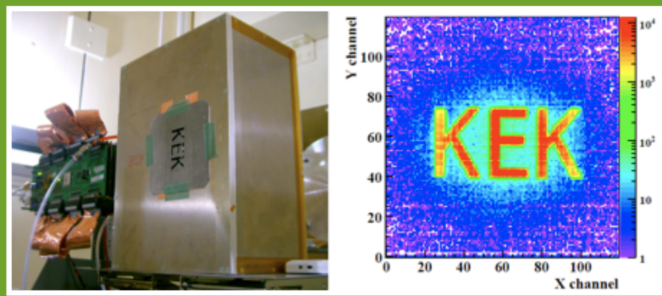
In one way, Otomo's role actually extends to all 23 neutron beamlines at J-PARC. Back in 2003 when NOVA was still seeking approval, Otomo wholeheartedly pursued one ambition: to unify all the software used for neutron analyses at J-PARC. This was not an easy mission because "skilled physicists are inclined to write their own code for their own purposes."

At times, Otomo's quest for unified neutron software was also a lonely pursuit. In terms of unified software, Japan had been lagging behind the international community. Attending international meetings, often the sole attendee from Japan, "contribution from our side was very limited." Now, the neutron software team has grown to include 15 members, including at least one from each beamline. "When completed, we'll be able to share software components among projects." The standard framework, which is the first to be developed and could be an important contribution to the international community, is called the *Manyo*-lib, after the Japanese classic poetry anthology from seventh century B.C., *Manyo-shu*. Just as the poets in *Monyo-shu* were a diverse bunch, ranging from nobles to peasants, the team hopes to make the new software framework accessible to all levels of scientists. Dr. Jiro Suzuki of the computing research center at KEK coded the *Manyo*-lib.

Another important software component, the data acquisition system (DAQ), of the neutron facility has been unified by a separate effort. The DAQ handles everything from the digitization of triggered data, the trigger selection, to storage. DAQ experts from the DTP, in joint effort with Otomo, developed a unified DAQ that can successfully handle the high rate of events at the neutron facility.

NOVA's mission

The NOVA team is currently analyzing the data acquired during last year's trial run. Otomo said that their first priority was to design and develop a stable system using solid technology to realize hard performance. So far it has gone well.



The NOVA beam monitor utilizes gas electron multipliers (GEM) developed by KEK's Detector Technology Project (DTP) group. The GEM is an advanced gaseous detector that allows two-dimensional imaging, with a resolution of 1-millimeter, and a detection rate of 10^9 neutrons every second.

The team will begin examining various hydrogen storage alloys this fall. "Hydrogen energy is an important, environmentally friendly energy source for the future," says Otomo. "NOVA has great potential for examining not just hydrogen storage materials, but more generally non-crystalline structures and liquids. Our biological world is filled with them." Even after the long-awaited discovery of practical hydrogen storage materials, NOVA will continue to provide important advances far into the future.

Related Link:
[KENS Neutron Science Division (Japanese)]

Related Issue:
[Detector technology project connects fields]

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