NBS is Completing New Cold-Neutron Source

For the past 10 years, U.S. scientists could participate in research using high intensity 'cold-neutron" sources only by traveling to the Institut Laue Langevin in Grenoble, France. There, they were able to take advantage of open time available on the joint French-German-British reactor-but only after the research needs of scientists from the sponsoring European nations had been met. In recent years, however, "increased (European) demand for the most frequently used experimental instruments has virtually frozen out the U.S. scientists,' notes Lyle H. Schwartz, director of the National Bureau of Standards' (NBS) Institute for Materials Science and Engineering, in Gaithersburg, MD. But adaptations to the NBS research reactor, which should be completed within a few months, will provide U.S. researchers with a major new domestic source of cold neutrons.

Coupled with a recent doubling of the reactor's power (to 20 megawatts), Schwartz says "the elements are now in place for establishment of a world-class cold-neutron research facility which would bring to U.S. scientists the capabilities for studying advanced materials now primarily reserved to Europeans." That is, in fact, the Reagan administration's plan. A \$10 million request in the FY 1987 budget that the President sent to Congress would go to initiate construction of a new \$27 million facility to make more efficient use of the new NBS cold-neutron source.

Why Cold Neutrons?

To make precise structural measurements with neutrons, one should try to match as closely as possible the wavelength of the radiation to the structure being studied. The atomic-scale wavelengths of neutrons usually emanating from the NBS research reactor make them best for studying atomic structure. Neutrons cooled to temperatures approaching absolute zero, however, have longer wavelengths, making them better suited for studying such things as the molecular structure of polymers, defects in advanced ceramics, protein conformations in biomolecules, the motion of molecules on chemical catalysts, defects causing metallic structures to fail, and sensitive, nondestructive depth profiling of defect concentrations in semiconductor devices. In fact, Schwartz says, such studies "cannot be properly made by any other

The new NBS cold-neutron facility will "chill" neutrons to this longer-wavelength regime. "In many instances," Schwartz says, "the expected results will allow the development of primary reference materials which

will be used for calibration of secondary test methods."

In the 1970s, small-angle neutron scattering (SANS)—a technique best done with very cold neutrons—"stimulated dramatic advances in our understanding of the structure of polymers and biomolecules," according to Schwartz. Although a modest cold-neutron source has existed at Brookhaven National Laboratory since 1980, most of the experimental work with cold neutrons has been conducted in Europe, where there are extensive cold-neutron facilities valued at more than \$140 million.

Schwartz and others voice fear that without at least one major, fully instrumented U.S. facility—one considerably larger than what is now in place at Brookhaven or being completed at NBS—the United States may not only remain inferior to the Europeans, but also may be unable to compete with research expected to come out of the new cold-neutron facilities being constructed in Japan.

The New NBS Source

At NBS, a heavy-water reactor is the source of its probing neutrons. Neutron energy is basically determined by the temperature of the water used to surround the fuel, which at NBS is about 300-350 K. To create a cold source, some of the water surrounding the fuel is being replaced with what is essentially an insulated, frozen block of deuterium oxide, through which cooling helium gas is piped. This will bring the effective temperature in that region down to about 20 K-increasing by more than a factor of 10 its cold-neutron intensity. Explains Michael Rowe, technical leader for the project, "typically, when we talk of cold neutrons, we're talking about those having an energy of about 5 millivolts (one fifth of room temperature) and a wavelength of 4 angstroms."

Rowe says that when the cold source is finally up and running—"hopefully by the end of the year"—it should be "quite comparable" to the existing cold-neutron moderator at Brookhaven. "What really distinguishes our [facility]," he says, "is that we could put a much larger source in"—a factor that could take on added significance if the money eventually comes through to expand the facility to at least four multiplexed beam lines. Two experiments will be tested initially: a small-angle neutron-scattering device and a neutron time-of-flight spectrometer.

The small-angle neutron-scattering (SANS) instrument is an upgrade of one that had been running for three and a half years off ambient-temperature neutrons

from the reactor. It essentially looks at the static properties of materials. The existing, ambient-neutron SANS device is set up to study structures on the scale of the distance between two atoms—about 2 to 3 angstroms. The new cold-neutron version will focus instead on a scale more representative of structures in molecules—from 10 to 10,000 angstroms.

Rowe notes that scaling a SANS up to handle this regime is difficult, because, "as the size of the unit that you're scattering from increases, the scattering is more and more concentrated in the forward direction the same direction the beam came from. In order to resolve scattered neutrons from the incident neutrons, you have to make measurements at very small angles from the main beam." That requires having a very collimated beam. Moreover, the distance between the sample and the point at which one detects the scattered neutrons has to be very large so that in spite of the small angle, there is a large physical separation between the incident and scattered beams.

With the time-of-flight spectrometer, one brings in neutrons moving with a given energy, directs them at a sample, and then looks at not only the scatter angle, but also how the energy of the scattered neutrons has changed—factors that provide data on the motions of atoms within the sample.

Among the first anticipated applications for the new instrument—it will be the first cold-neutron time-of-flight spectrometer in the United States—will be to look at the way molecules move in catalysts used for the production of chemicals. An important aspect of designing a catalyst is not only to make it speed a reaction but also to get the reacting materials in and out of it. And, Rowe says, "that is exactly the sort of thing that we can look at with this spectrometer—the motion of atoms as they move in solids and liquids."

Plans for Immediate Expansion

Space restricts NBS from installing any guide halls or more than two instruments at the new cold source. And that's why NBS is already pushing for construction of a new building around the cold source, with neutron pipes to transport at least four large beams out to 15 experimental stations.

At least four of the 15 stations would be financed by industry and universities which, along with NBS scientists, would form research teams to develop appropriate new techniques as needed. Schwartz notes, "We have received strong expressions of interest in joining such teams from a number of

continued

companies." He reads these as "testimonials to the anticipated impact of this project on the industrial community." Exxon, in fact, has already committed itself to one of the experimental stations—a new small-angle neutron-scattering device (see MRS BULLE-TIN, Vol. XI, No. 2, p.5). For the remaining 11 experiments, NBS is offering to make two thirds of the research time on them available to U.S. scientists "on a competitively reviewed proposal basis."

NBS and the Reagan administration are not the only proponents of this expansion. When the National Academy of Sciences' Major Materials Facilities Committee analyzed the needs of the materials community in a report two years ago, it named as one of its top priorities the immediate expansion of both the NBS and Brookhaven coldneutron sources. (As yet, however, there is no plan for a Brookhaven expansion.)

In particular, the National Academy of Sciences committee recommended the construction of guide halls at those facilities—large experimental areas for situating high resolution spectrometers. Neutrons would be transported to the guide halls via beam guides—pipes whose smooth, interior surfaces will reflect neutrons many meters away from the reactor without significant losses.

The National Academy of Sciences committee observed that although "the United States has no guide halls to improve the versatility and flexibility of cold...neutron instruments," Europe has six fully instrumented ones completed or under construction. Not only do the guide halls offer room for more and larger experimental stations, but they also provide a "cleaner" test environment. When experiments have to be carried out close to the reactor—as they now are at Brookhaven and will be initially at NBS-there will be some stray fast neutrons and gamma rays that could interfere with test results. Guide tubes, which would selectively transmit cold neutrons out to guide halls, would eliminate interference from this other radiation.

However, an immediate expansion of the NBS and Brookhaven cold-source facilities "was only looked at as a stop gap for the next decade," according to Robert J. Birgeneau at the Massachusetts Institute of Technology, who chaired the committee's neutron-scattering panel. "What the [NAS] panel hoped was that by then—1995—we would have a next-generation reactor which was specifically designed around cold sources."

The Next Generation

Work on such a reactor is currently under way at Oak Ridge National Laboratory. Explains Ralph Moon, who's directing the project, the aim is to increase the basic thermal flux of cold neutrons from this new reactor "by a factor of 5 to 10 over anything we have in this country now—even over the best reactor in Europe." He

believes that by planning from the beginning to optimize the reactor's design for the production of cold neutrons, "we could have the best facility in the world not only for cold-neutron scattering, but also thermal-neutron scattering."

Moon says the basic difference between the Oak Ridge and European reactors "would be that we'd develop a much higher flux." The number of cold neutrons is proportional to the number of thermal neutrons, he notes. So where the reactor at Institut Laue Langevin operates at a total power of 57 megawatts, he says Oak Ridge's will aim to produce about 250 megawatts. "Ours would be a more powerful source." And a compact one. "The most critical thing is the power density—megawatts per unit volume in the reactor," Moon says. "And we're going to push that number up as high as we can possibly go."

But for now, Moon believes, the most important thing is to see that the NBS cold source is expanded. Speaking of the United States, he says, "We're woefully inadequate with respect to cold-neutron facilities. The NBS source will allow us to get into the game and learn all the techniques." Which techniques? For starters, he says, "the nature of the NBS cold source is different from any other that has been built." Its cold source will be solid D2O. Liquid deuterium, more commonly used, is probably more effective at cooling the neutrons down, he says, "but the NBS source has the advantage of being inherently safer." Unlike liquid deuterium, its D2O won't explode upon contact with oxygen. And it's Rowe's aim to pioneer a number of other new techniques and instruments at the NBS facility, building from what has been learned in Europe and elsewhere.

Second, U.S. scientists and engineers lack Europe's access to, not to mention experience with, cold neutrons. In Grenoble, Birgeneau points out, "they have something like 20 spectrometers operating [off coldneutron sources]. In the entire United States we only have something like three." Moreover, the NAS committee found, the Institute Laue Langevin instruments currently provide energy resolutions as much as five orders of magnitude better than any available in the United States. Though an expansion of the NBS facility to include 15 experimental stations still won't match the magnitude of research opportunities available at Grenoble, Birgeneau believes, it "probably will help ameliorate the problem."

The inadequacy of cold-neutron facilities in this country "is so drastic that our [NAS committee] hotly debated whether one upgrade [either NBS or Brookhaven] would be enough," Birgeneau recalls. "And the answer was an emphatic no." In fact, the committee labeled U.S. spending on cold neutron research and instrumentation during the past decade "inadequate," noting that it was only one tenth that being

invested by Western Europe.

Though few today question the scientific value of building a large guide hall to make better use of the NBS cold source, there is the issue of finding the money to finance its construction. The administration asked Congress for it last year, without success. And clearly, Rowe says, "this is also a bad year to be going in asking [Congress] for money." Representative Doug Walgren (D-PA) echoed that sentiment during congressional hearings on the NBS research budget earlier this year: Although the coldneutron facility expansion "is certainly a worthy proposal," Walgren said, "whether we can fully fund it right now is an open question."

--JANET RALOFF



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