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A PLAN FOR THE FUTURE OF NEUTRON RESEARCH ON CONDENSED MATTER

An Argonne National Laboratory report
prepared in response to the
"Report of the Review Panel
on Neutron Scattering"

January 27, 1981

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INTRODUCTION

The Argonne management and scientific staff have read and considered carefully the Report of the Review Panel on Neutron Scattering. The Panel has done a creditable job in evaluating the opportunities for neutron research and assessing the present position of this field in the U.S. compared with other parts of the scientific world. The Panel members have tried to maintain the present strengths of the DOE neutron program while paying attention to the long-term (10-20 year) future of the field. They deserve credit for undertaking this difficult assessment.

We strongly support the Panel's recommendation for an expanded budget which will allow the systematic development of the field. The unique abilities of slow neutrons to probe the microscopic structure of condensed matter, together with the need for a fundamental understanding of the effects of fast neutron radiation on materials, argue for a strong neutron research program in the United States. It is clear from the information provided in the Report that a significant investment will be needed to maintain a viable position relative to the new facilities, with innovative instrumentation and large user community involvement, being set up in Western Europe.

We believe that the constrained budget presented by the Panel would have a disastrous effect on the future of neutron research in this country. Since its inception with the advent of nuclear reactors, progress in this field has been bound up with new sources and new types of instrumentation, and there is every reason to believe this will continue to be the case. Pulsed spallation devices represent the most promising line of development for new sources, and the U.S. has in the Intense Pulsed Neutron Source I at Argonne not only the best pulsed spallation source in the world for the next five years but also a program that has been associated from the beginning with novel instrument development. By phasing out IPNS-I as soon as it comes into operation, the constrained budget would cause a damaging and far-reaching set back. In the absence of any major new facility coming on line in the next five years, the U.S. would be relegated to a second-class position for the foreseeable future.

In case it is not possible to provide the systematic development budget, we wish to present an alternative plan which we believe attains the objectives that the Panel was striving for but in a way which will secure a sounder long-term future for the field. It will expand the use of the Brookhaven and Oak Ridge reactors; initiate design work on a very-high-flux facility for the U.S. in the 1990's, which will surely be a spallation (pulsed or quasi-steady-state) neutron source; develop scientific experience at a pulsed spallation source to provide the basis for a decision on the world-class facility within the next five years; develop a user community in the U.S. to exploit the full potential of the field; and accomplish this within a budget scenario which shows a modest and realistic growth.

Our argument proceeds along these lines, discussed in more detail in the following sections:

I. Some omissions from the Report

o First, we wish to point out some important considerations which the Report does not address. Among the more significant of these are the following:

1. The need to view neutron research in a broader context than materials science, considering applications to a wide range of scientific areas in biology, chemistry and fundamental physics as well as contributions to technology.
2. The crucial role in both science and instrument development played by the large user communities at the European centers.
3. The need to maintain continuity in providing facilities for basic neutron radiation effects research.
4. Possible instabilities in the cost-sharing of HFBR, HFIR and WNR by different DOE programs.

II. The essential role of neutrons in condensed matter science

o We strongly endorse the Panel's belief in the essential and unique role that neutrons have fulfilled in materials science, chemistry and biology, and will continue to fulfil if the required sources and instrumentation are available.

III. The importance of pulsed spallation sources

o We believe that the inherent intensity limitations of neutron techniques will continue to drive the need for higher fluxes; that there is very little chance that these fluxes will be provided by reactors; that the hope for the foreseeable future (10-20 years) must lie in spallation sources (pulsed, quasi-steady-state or a combination of the two); and that an intelligent decision will require both the scientific evaluation of the pulsed source and technical development of spallation source concepts.

IV. The need for IPNS-I

o For reasons well documented in the Panel report, IPNS-I provides the only test-bed in the U.S. for the scientific and technical evaluation of pulsed spallation sources at least until 1986; it gives essential input for a decision on a very-high-flux source later in this decade which, as the Panel points out, is essential if such a source is to be available in the early 1990's.

V. The role of WNR-PSR in condensed matter research

o The unsuitable time structure of LAMPF prevents the Weapons Neutron Research Facility at Los Alamos from being a competitive device until 1986 at the earliest, and it would be an uneconomical use of the available resources to duplicate IPNS-I instrumentation and research activities before the Proton Storage Ring becomes available. After 1986, the WNR-PSR facility could provide a pulsed neutron source for condensed matter research that would be more cost-effective than IPNS-I, assuming that the present commitment to availability for this research is met and that funding is provided by the Division of Military Applications at the indicated levels. The transfer of the pulsed source effort (research and instrumentation) could be an option at that time if these assumptions are validated.

VI. A very-high-flux facility for the United States

o Since neither IPNS-I nor WNR-PSR will provide world-class capabilities after 1986, design work aimed at a new dedicated very-high-flux neutron source for the U.S. community should be initiated as soon as possible. Argonne, with its combined expertise in accelerator technology, neutron targetry, time-of-flight instrumentation and radiation effects research, is uniquely qualified to lead this design effort.

VII. The proposed plan

o We present a plan which will allow the DOE neutron program to proceed on a responsible and rational course towards the very-high-flux source while nurturing the scientific capability which will exploit the new facility and the existing high-flux reactors. It is possible, with a near-term real growth averaging about 5% per year in the national (DOE-DMS) budget for neutron research, to realize the basic objectives of this plan.

VIII. Summary

- We recognize that any plan which addresses a subject of this complexity is only as good as the assumptions on which it is based. We strongly suggest that these assumptions continue to be validated as the science and the facilities progress, and that a nationally constituted committee representative of the neutron scientific community be set up to carry out this function.

I. SOME OMISSIONS FROM THE REPORT

We first wish to point out some important considerations which the Report does not adequately address.

1. Neutron research in a broader context

The charge to the Panel, placed in the framework of a restricted DOE Materials Sciences budget, and the ensuing recommendations place neutron research in too narrow a context. Neutron sources are important in many other fields of basic and applied research, and neutron scattering in particular is essential in fundamental physics and biology. The Institut Laue-Langevin in Grenoble, France, has shown how these opportunities can be exploited in a proper institutional context. They can not be addressed in a plan which considers only one type of funding source.

2. Importance of the user community

The Report discusses in some detail the prominent role played by ILL in the European scientific context, the leadership of ILL in innovative instrumentation, and the existence and encouragement of a large user community. There is clearly a relation between these factors--much of the innovation has come about because of bringing in new people and ideas. Yet the Panel's recommendations for the U.S. program do not indicate how or whether the outside user involvement at the major facilities should be strengthened, or how for example the additional funds proposed for HFBR and HFIR might achieve this (apart from a suggested summer visitor program at Oak Ridge). Instead, the recommendations, in the constrained budget scenario, call for the elimination of the only user-oriented U.S. facility. We believe this reflects a serious underestimate of the essential role that a broad user community has played in the development of the European centers and needs to be played in the U.S. if the vitality of the field is to be maintained.

3. Radiation effects facilities

The Report states that neutron radiation damage research is important to the U.S. basic and applied materials science program and is a prime responsibility of DOE. Yet in the constrained budget it recommends elimination of the only facility at which it will be possible to carry out low-temperature basic research with fast neutrons.

4. Funding instabilities

The ability to even consider running four large facilities in a basic research budget of $15-20M per year implies a great measure of sharing costs with other programs. The cost reduction effected by this cost sharing inevitably influenced the Panel's recommendations, since powerful facilities are thereby made available at reduced cost to the basic research community. Yet experience has shown this can lead to an unstable funding situation which in some cases has led to the demise of a reactor (MTR, ALRR, CP-5) We feel that this issue should have been addressed in the report, especially since the charge from DOE raised the prospect of increased reactor charges to the Materials Sciences Program. It may be difficult to assess a risk in an uncertain situation. But there is an obligation to do so when the certainty of shutting down a major facility, to which millions of dollars and tens of scientific and technical careers have been devoted, flows from a principal recommendation.

II. THE ESSENTIAL ROLE OF NEUTRONS IN CONDENSED MATTER SCIENCE

The unique properties of slow neutrons--the ability to penetrate bulk matter, their low energy and short wavelength being well matched to the ranges of interest in condensed matter, their coupling to magnetic systems through their magnetic moment, their relatively strong and isotope-dependent interaction with light atoms like hydrogen and carbon--make them an excellent probe of the microscopic nature of a broad range of physical, chemical, and biological phenomena. The importance of neutrons to the study of condensed matter was emphasized succinctly in the 1977 National Academy of Sciences report on Neutron Research on Condensed Matter. To quote this report:

> "Neutrons . . . provide basic information about the structural and magnetic properties of condensed matter that is not accessible via any other experimental technique. Such information is essential for the understanding of all properties of materials"

and:

> "In many cases, completely new areas of research investigation have been opened up by the exploration of the unique properties of neutrons".

Three years after the publication of this report, the above statements assume greater urgency in the light of the grave situation which faces the field of neutron scattering in this country. This urgency is prompted by the need to plan now for effective new neutron sources to continue this vital area of condensed matter and materials research into the 1990's and beyond, in spite of the serious budgetary restraints facing basic research in the U.S. at the present time. As the present report of the Review Panel on Neutron Scattering points out, in one of its most startling and important findings, the three major nations of Western Europe, namely the United Kingdom, France and West Germany, have not only appreciated and assimilated the facts about the importance of neutron scattering but have effectively laid the basis for both present and future excellence in the field via existing facilities such as the ILL in France, and future facilities such as the SNS at the Rutherford Laboratory in England and the SNQ spallation source being planned in West Germany. By spending five times as much on this field as the U.S., by involving a very large user community and by developing novel technology and instrumentation, they have already surpassed the U.S. in this field and will clearly inherit it almost completely if the U.S. finds itself, by the early 1990's, with no effective new neutron source. We believe this would constitute a major setback for condensed matter and biological research in this country with a chain of serious consequences to the health and vitality of the scientific community.

We will briefly examine the impact made by different neutron techniques on condensed matter and biological sciences. First, inelastic neutron scattering studies processes where the neutron exchanges both energy and momentum with the system under study and can thus be used to probe the spectrum of "excitations" (i.e. the dynamics) of the system at a truly microscopic level. Past accomplishments of inelastic neutron scattering have greatly transformed whole areas of condensed matter science. Unlike optical and Raman spectroscopy, which probe long-wavelength phonons in crystals, neutrons can probe the spectrum of waves in crystals with wavelengths ranging from long to short compared with the interatomic spacings of the solid or fluid under study, thus providing a wealth of much more detailed information on the interactions (chemical bonding or magnetic) between the constituents. For example, the intricate knowledge of the existence and spectrum of phonons have enabled us to construct theories of bonding and cohesion of metals, semiconductors and insulators far more sophisticated and detailed than anything which would have been possible without such information. In addition, inelastic neutron scattering has enabled the construction of test models of the electron-phonon interaction which are vital to understanding the transport and superconducting properties of metals and of highly sophisticated models of non linear phenomena in anharmonic crystals and quantum solids. The knowledge of the existence and the dispersion of spin excitations in solids has done the same thing for the understanding of the fundamental nature of magnetism in metals and insulators, of crystal field levels in systems containing magnetic ions, and of the physics of mixed valence (interconfigurational fluctuation) materials. The study of soft mode phenomena and critical scattering has been essential to the understanding of the important field of phase transitions, both structural and magnetic. Inelastic neutron scattering studies are currently contributing to the understanding of amorphous solids, fluids and spin glasses, all frontier fields at the present time.

Neutron diffraction is concerned with the structural arrangement of the atomic particles (and sometimes magnetic moments) in a material and the relation of this arrangement to its physical and chemical properties. In the past 25 years crystallography has revolutionized the biological sciences, has become the major cornerstone of transition metal coordination chemistry, and has played a crucial role in the fields of organic chemistry, the earth sciences and materials research. To understand the fundamental, physical, chemical or biological properties of a material or compound it is usually essential to know its structure. The scattering of radiation (electrons, x rays, neutrons, etc.) offers the most effective experimental means of acquiring such information. Electrons can only be used to study surfaces or thin films because they have low penetrability. X rays, being a highly energetic form of radiation, are capable of inducing damage in certain systems, particularly those containing biological molecules. On the other hand, neutron radiation of the type used to investigate molecular structure does not induce damage and has the following unique features:

(a) the ability to detect hydrogen and other light atoms easily;

(b) low absorption in all but a few cases;

(c) the ability to obtain true nuclear (as opposed to electronic) position and motion;

(d) interaction with unpaired electron spins in magnetic materials; and

(e) the irregular variation of the scattering cross section with atomic weight.

For these reasons, neutron diffraction has had a major impact on studies of broad classes of materials: homogeneous catalysts, metal hydrides, hydrogen-bonded materials, solid electrolytes, one-dimensional electrical conductors, ferroelectrics and antiferroelectrics, organic compounds, ferro-, antiferro- and ferri-magnetic materials, and polymers. Neutron diffraction is also beginning to play a major role in the study of biological systems like viruses, proteins and enzymes. The ability to selectively substitute deuterium for hydrogen is especially advantageous. This application is being heavily exploited in Europe where facilities for sample preparation and wet chemistry are being set up at the neutron sources, for example, the new European Molecular Biology Organization's laboratory adjacent to the ILL reactor.

Neutron radiation effects studies are of primary importance to the use and safety of fission nuclear energy and to the development and use of fusion energy. In addition, neutron radiation damage is an effective tool in the study of the defect solid state, particularly in the area of defect interactions. Let us consider what happens when a solid is bombarded by fission neutrons. The energetic neutron collides elastically with a host lattice atom imparting to it some tens of keV of kinetic energy. The net result is a localized area called a displacement cascade containing a high concentration (10^{-3}) of vacant lattice sites and self-interstitial atoms. At this concentration, these defects interact with each other, producing a very complex defect array whose properties greatly differ from the simple situation of a single vacancy/interstitial pair that is produced by low-energy electron irradiation. It is this complexity which is responsible for the changes in the mechanical properties that are so important to material problems arising in nuclear reactors and magnetic fusion devices, and which therefore needs to be understood on a fundamental level.

As well as these primary applications, neutrons have relevance in other areas of science and technology. In fundamental physics, the measurement of the very small electric dipole moment of the neutron, an experiment which is very demanding on the intensity of the source of neutrons, provides a crucial test of theories of the weak interaction. In addition, there are large numbers of technological applications of neutrons, including activation analysis, tomography, radiography and so on, which need to be further developed at neutron sources under research conditions to fully exploit their usefulness to technology.

In conclusion, the availability of state-of-the-art neutron sources continues to be vital for the development of knowledge about the structural arrangements and fundamental processes occurring in condensed matter and the relation of these to problems of national technological importance. We strongly support the Panel in their recommendation for an expanded budget which will enable the U.S. to proceed with a systematic development of these facilities.

III. THE IMPORTANCE OF PULSED SPALLATION SOURCES

The way to higher fluxes

The most pressing argument for the rapid development of pulsed spallation sources in the U.S. is that they provide the only practical way to achieve new high-flux neutron sources in the U.S. and thus assure the continued vitality of the field. As the Panel indicates in its report, neutron scattering is intensity limited, and history has shown that increases in intensity have provided new and often unexpected breakthroughs. The Panel also points out that the present high-flux reactors, which have fluxes around 10^{15} n/cm^{2}sec, will be 25 years old by 1990 and their age makes it prudent to plan for a new source by the 1990's. For technological, as well as political and economic, reasons it is unlikely they will be replaced by a "super high-flux" reactor in the U.S. at that time. The pulsed source can, however, offset many of the apparent advantages of a reactor if the peak flux and repetition rates are high enough. It can be shown that, for neutron scattering experiments with "conventional" (thermal) neutron energies, a pulsed source *with a peak flux of* 10^{16} *n/cm*^{2}*sec and 60 Hz* repetition rate is more powerful than the present high-flux reactors by a factor ranging from about 1 to 100, depending on the experiment to be done.

New experiments

There lies an important class of inelastic neutron scattering experiments which have heretofore not been explored because of severe limitations on the flux of epithermal neutrons and crystal reflectivities for high-energy neutrons at reactors. These correspond to experiments in the 60 meV - 500 meV energy transfer range. The abundant epithermal flux of a pulsed spallation source ($\sim$ 100 times larger than that available at the ILL "hot source" at 1 eV for a 10^{16} pulsed spallation source), the short ($\sim$ 1 μsec) burst width and chopper technique make these the only feasible neutron sources for performing such experiments. These include studies of:

(a) electronic densities of states (in the range 0.1-0.5 eV around the Fermi level) of *transition, mixed-valence and actinide metals;*

(b) high-lying magnetic excitations in transition and rare-earth metals, for example, of the spin density wave in metallic chromium;

(c) the dynamics of light, tightly bound interstitials in metal hydrides and superionic conductors (leading to a detailed understanding of the potentials for these interstitials),

(d) magnetic and collective excitations in amorphous solids (where the severe kinematic restrictions on requiring large energy transfers at small neutron momentum transfers force one to use high-energy incident neutrons);

(e) high-energy molecular vibrational spectra--particularly those of intermediate products formed in catalytic reactions at surfaces;

(f) crystal-field levels in actinide metals and compounds; and

(g) studies of the atomic momentum distributions of quantum fluids and solids, such as helium-3 and -4.

It is our belief that neutrons will be the best probe for excitations at such energy transfers from the point of view of energy resolution, signal to background ratios and ease of sample preparation (e.g., bulk samples will do), that they will open up a whole new area of condensed matter science, and that the nature of pulsed spallation sources is uniquely suited to such investigations.

Pulsed neutron sources will play a dominant role in powder diffraction because they offer a particularly simple and effective way to obtain the high resolution needed for refinement of small complex structures. The time-of-flight technique allows data to be taken at a single scattering angle. Thus, back-scattering detectors can be used to achieve high resolution and time-focusing techniques can be employed to dramatically increase the detector area with no loss of resolution. Because no chopper is required, a large source area can be viewed; thus long incident flight paths can be used to achieve high resolution. Since typical pulsed source moderators produce pulses whose widths are roughly proportional to wavelength, the time and geometrical resolution contributions remain matched over a wide range of Q. Thus, the resolution function is nominally constant over a wide Q range and can therefore be made superior to that available on a conventional diffractometer over part or all of the Q-range of interest. The high-resolution powder diffractometer (HRPD) operated at the prototype pulsed source ZING-P' has demonstrated these principles. It achieved resolution of $\Delta d/d$ = 0.003 with counting times of one to two days for typical samples. Presently operating conventional diffractometers match this resolution only in the limited Q-range for which they are optimized. The HRPD also exhibited a better peak-to-background ratio for a standard Al_2O_3

sample than that reported for any reactor diffractometer, probably resulting from the source being off between pulses. Rietveld refinements gave results as good as or superior to those obtained on the best conventional diffractometers, despite the low peak flux of the ZING-P' source relative to the high-flux reactors.

Thus, powder diffraction at a high-flux source will provide extremely powerful capabilities which can be used for measuring very small samples (e.g., transuranics) or making rapid sequential measurements, for example, in an electrochemical cell in the process of charging and discharging. The single-angle diffraction is especially powerful for high-pressure studies and with multiple-anvil presses neutron diffraction at pressures of 100 kbar with a high-flux source can be expected.

In single crystal diffraction, crystals with more than 100 atoms in the asymmetric unit can now be solved routinely by conventional neutron techniques. There are, however, two problems with these techniques:

(a) Even at a high-flux reactor with a suitable crystal, data collection can be long and tedious; and

(b) Compounds with large molecular weights are often the most difficult to obtain in the form of suitably large crystals

The use of time-of-flight techniques with large position-sensitive area detectors at a high-flux pulsed source will lead to higher data collection rates, perhaps by two orders of magnitude, than are obtained at single-detector instruments at reactors. This will permit the study of more complex structures, including those of biological molecules, and smaller crystals than are now feasible to measure . These advances should be particularly effective in the study of transition metal coordination and cluster complexes which are homogeneous catalysts or model the surface chemistry of heterogeneous catalysts. In addition, the single crystal diffractometer will provide a totally unique three-dimensional sampling of reciprocal space, which is especially powerful for studying phase transitions, superlattices, and diffuse scattering. Since it is possible to obtain these 3-D views of reciprocal space with the sample in a fixed position, special pressure and temperature equipment is easily accommodated.

Pulsed sources can utilize all of the characteristics of neutrons which render them so important for biological structural studies and, in addition, offer several unique advantages. An important application lies in the utilization of anomalous scattering at nuclear resonances. At certain wavelengths, characteristic isotopes exhibit an anomalously larger cross section for elastic scattering than they exhibit at other wavelengths removed from the resonance. Thus at the resonant wavelength these anomalous scatterers have a significantly larger scattering density than normal. If several such isotopes are sequestered in localized areas of the molecule, the molecule will be labeled at resonant wavelengths. In addition, many enzymatic cofactors can be replaced with resonant lanthanides to provide labels on functional regions of molecules. Calcium, for instance, can be replaced by gadolinium within many Ca^{++} binding proteins and the distances between active sites can be obtained.

Basic research in neutron irradiation effects is aimed at an understanding of the displacement cascades and the changes which occur in them as a function of temperature. The damage mechanisms and defect state can best be understood by "freezing in" the defects as they are produced, which generally means irradiation below 10°K. The motion and agglomeration of the defects are studied by subsequent systematic warming. Of primary importance in these studies is the ability to control and characterize the neutron energy spectrum as well as the bombardment temperature. The flux does not need to be very high provided it is high enough to produce a sufficient density of cascades in a reasonable time so that the property changes induced by the cascades can be measured. Pulsed spallation sources have adequate time-average fast neutron fluxes (10^{12} - 10^{13}n/cm^{2}sec) and the low gamma heating means that temperature control down to 4°K can be easily maintained.

World-wide activity

Thus, not only do pulsed sources offer the most promising approach to obtaining higher effective intensities, they also have some unique features compared with reactors which will enable qualitatively new types of scientific investigation to be carried out. A workshop on "Applications of a Pulsed Spallation Neutron Source" held at Argonne in 1973 identified many exciting research opportunities with these devices, and consequently activities were begun in several countries, including Japan, where a new source of this kind came on line in the fall of 1980, and Great Britain, where the SNS, providing peak fluxes of 5×10^{15} at 50 Hz (a higher intensity than any pulsed source now planned in the U.S.) will come up to full power in 1986. In Germany, a large-scale ($\sim$ \$10M) study is underway for a somewhat different kind of spallation source, a quasi-steady-state source (5% duty cycle) which could provide competitive intensities for steady-state techniques as well as enhanced performance for time-of-flight experiments, further enhancement being possible with the further addition of a compressor ring to provide short ($\sim 1\ \mu$sec) proton pulses. The relative scientific merits of this type of source, more versatile but correspondingly more costly in terms of both construction and operation compared with a pulsed source of the same peak flux, should be considered in the process of making a decision on the very-high-flux U.S. facility.

IV. THE NEED FOR IPNS-I

Future goals

If the scientific community in the U.S. is to have a very-high-flux neutron source in the early 1990's, it is clear that a decision to construct such a source must be made within the next five years or so. A decision by the community to go ahead by 1986, for example, followed by the appropriation of funds and the design and construction of a project of this magnitude, would likely provide a facility available for research by 1993. Two kinds of activity must therefore proceed immediately:

(a) The scientific evaluation of the type (steady-state, quasi-steady-state or pulsed) and performance (peak flux, repetition rate, neutron energy range) required; and

(b) The technical evaluation of the cost and feasibility of the different options.

As discussed in the previous section, we believe that the next source must be a spallation source. We also believe that a pulsed source can exceed the capabilities of the present reactors even in those areas which have traditionally been the province of the steady-state techniques, as long as the intensity is sufficient, in addition to providing radically new capabilities in other areas. The option of a quasi-steady-state spallation source should also be considered, although we believe it will turn out to be much more costly. In any case, an evaluation of the pulsed sources over the entire range of scientific demand must be explored before a responsible scientific decision can be made. In addition, there is a need to maintain continuity in the technical development of spallation sources which involves new technology in either case. (In fact, the problems are largely common to the pulsed and steady-state sources, as the recent expansion of the International Collaboration on Advanced Neutron Sources, to include the steady-state sources, implies.)

The systematic development of pulsed sources at Argonne

The IPNS-I facility now being built at Argonne and scheduled for completion in the Spring of 1981 provides the only way of making a thorough scientific evaluation, and a highly effective way of continuing the technical development, of the pulsed spallation source within the required time scale. It is part of a deliberate and systematic plan which Argonne set up to develop advanced spallation sources, starting with the world's first prototype pulsed spallation source (ZING-P, 1974-5), leading through an advanced prototype (ZING-P', 1977-80) to IPNS-I, an intermediate-level facility designed to demonstrate the scientific promise of this kind of source prior to the major investment required for a high-flux source. As part of this plan, Argonne also developed a complete concept for such a high-flux source (IPNS-II) which provides a point of reference for the decision on the future world-class facility.

To execute this plan, Argonne assembled a team of scientists with expertise in neutron scattering techniques, radiation effects research, instrument development, target and moderator optimization and accelerator development. The scientific disciplines involved include the various subfields of materials science--solid state physics, metallurgy, ceramics and materials chemistry--and extend into biology and elementary particle physics. To support this expanding effort within an essentially constant materials research budget, Argonne reprogrammed, with DOE approval, about $3.2M (1981 dollars) of existing materials research funds into the pulsed neutron source activity.

The role of outside users

Realizing the crucial role which outside user communities have played at ILL and other European centers, Argonne from the beginning has made a major commitment to involve university and other outside users, taking advantage of the Laboratory's central location. Two major workshops on scientific applications have been held at Argonne. An International Symposium on Neutron Scattering will take place at Argonne this August, with emphasis on pulsed neutrons, and an International Conference on Neutron Irradiation Effects is scheduled for this November. A special advisory committee composed of distinguished university and industrial scientists was appointed under the auspices of the Argonne Universities Association. An IPNS Program Committee was formed with outside users holding prominent positions. Already at the IPNS-I level over 100 scientists have demonstrated an interest in using the facilities.

Achievements of the prototype sources

At the present time, Argonne has successfully completed the second stage of the ZING-P/ZING-P'/IPNS-I/IPNS-II program. Over the period 1977-80, the ZING-P' target was used to bring the accelerator up to stable production operation at the current levels needed for the start of IPNS-I operation, to develop uranium targets for spallation sources, to develop moderator techniques to maximize neutron fluxes, to develop instruments to be used on the IPNS-I target, and to perform scientific experiments by ANL, university, other outside user scientists. Many crucial innovations came out of ZING-P':

(a) the first time-of-flight single-crystal diffractometer with a position-sensitive area detector;

(b) the highest resolution powder diffractometer ($\Delta Q/Q$ = 0.3%) in the world;

(c) a new type of two-dimensional scintillation detector based on the Anger principle;

(d) ultracold neutrons produced by a pulsed Doppler-shifting technique;

(e) demonstration of resonance radiography with epithermal neutrons from a pulsed source;

(f) the first uranium target in a pulsed spallation source for neutron scattering;

(g) the first liquid hydrogen moderator in a pulsed neutron source (until now the only working cryogenic moderator in the U.S.); and

(h) crystal-oscillator stabilized operation of proton accelerator-neutron chopper phasing.

Two of the prototype instruments, the high-resolution powder diffractometer and the crystal analyzer spectrometer, became scientifically productive devices. The high resolution powder diffractometer completed 17 experiments performed by outside users from ten universities, one national laboratory, and two industrial research laboratories, and 21 experiments by ANL scientists. The crystal analyzer spectrometer completed 10 experiments by outside users from four universities and two national laboratories and six experiments by ANL scientists.

The capabilities of IPNS-I

The first phase of the Intense Pulsed Neutron Source project, IPNS-I, is now in the final stages of construction. Startup for research use is scheduled for May 1981. By using equipment and buildings set up previously at Argonne under the national high-energy physics program, estimated to have a replacement cost of $35M, a well-designed source with a broad complement of research instruments (seven diffractometers and spectrometers for neutron scattering, three radiation effects facilities, and six additional beam tubes for other types of experiment) has been constructed for a construction outlay of nearly $9M. IPNS-I is designed as a intermediate level facility ($\phi_{th} = 5 \times 10^{14}$ n/cm^{2}sec at 45 Hz) in which the scientific promise of this kind of source can be fully demonstrated prior to the major investment on a high-flux source.

The IPNS-I source is dedicated to condensed matter research: the materials science and biology communities will have control, within the budgetary constraints, of scheduling and configuring the facilities to optimize the scientific output in their field. It provides new capabilities in several areas of scientific research. Above 150 meV, the flux is higher than that of the high-flux reactors. In inelastic scattering, this provides the capability for experiments analogous to x-ray Compton scattering where the momentum distributions of the atoms in a quantum system like liquid or solid helium-3 or -4 can be measured. Inelastic scattering will also be possible at high energy transfer (> 100 meV) so that the collective and single-particle excitations can be studied in ordered magnetic materials.

For diffraction studies, the IPNS-I pulsed neutron source offers some distinct advantages for the continued development of high-resolution powder diffraction techniques. High resolution diffractometers demand a properly optimized pulse length and repetition rate to achieve the unique advantages that the time-of-flight method can offer over conventional diffractometers. The HRPD at ZING-P' utilized an 18.4 m flight path and required a repetition rate of 50 Hz or less to avoid frame overlap. The development of instruments which achieve even higher resolutions will only be possible at a source like IPNS-I which provides adequate intensities at low repetition rate (< 50 Hz). The short wavelength of the epithermal neutrons, which can be exploited because of the short (100 nsec) pulse length of the accelerator, lends itself to high-resolution studies of the spatial structure of amorphous solids like ternary metallic glasses. Also, IPNS-I will be the only U.S. source where biological materials can be studied with the small-angle resonance scattering discussed in the last section.

Important developments of neutron scattering techniques will be explored on IPNS-I as part of the relative demonstration of the value of high-flux (> 10^{16} at 60 Hz) pulsed sources including: an area-detector pulsed Laue technique for single-crystal diffraction studies of complex molecular and biological systems; studies of dynamical effects in solids to evaluate the power and versatility of the pulsed-source, time-of-flight method for "conventional" (thermal) neutron energies; and the use of correlation and spin-echo methods in a pulsed-source context.

For radiation effects research, IPNS-I will be the only facility in the U.S. meeting the two criteria for basic radiation effects studies: low nuclear heating and moderate neutron intensity with a well-characterized spectrum. In addition, there are two special features which promise to open up new research areas:

(a) the production of neutrons by proton bombardment (evaporation and spallation) that does not in itself produce γ rays; and

(b) the fact that the neutrons are produced in pulses $\sim$ 100 nanoseconds in width with $\sim$1/30 sec between pulses.

The IPNS-I Radiation Effects Facility is the only facility available in the U.S. where the effects of fast neutron irradiation on fusion magnet materials can be studied. Mechanical property studies of the organic insulating materials must be made in a neutron flux at 4°K to a fluence of 10^{18} n/cm^2 to simulate the magnet operating conditions. The large volume available in the IPNS-I cryostats permits the irradiation of a large number of samples so that a data base can be obtained, and a transfer cryostat allows transfer without warmup for testing purposes. Samples can also be irradiated under tensile or compressive stresses. In like fashion, the stabilizing material (copper or aluminum) is limited by the irradiation induced resistivity. Proper magnet designs require measurements of the resistivity changes in a high magnetic flux (12 T) and repetitive thermal cycling at room temperature. IPNS-1 is the only facility in the U.S. capable of performing this experiment.

Argonne has pioneered the development of pulsed source neutron sources and has embarked, in concert with the national scientific community, on a logical and coherent plan to develop the scientific and technical basis for a decision on a world-class facility by the middle of this decade. At present, the Laboratory is poised ready to complete and promote the use of the only source in the world with an intensity and pulse length sufficient to adequately test the pulsed concept consistent with a decision on this time scale. An integrated in-house team with demonstrated capability and ingenuity in this area of science has been assembled to lead this effort, and user policies have been established from the beginning so that the best ideas from the national scientific community are exploited.

V. THE ROLE OF WNR-PSR IN CONDENSED MATTER RESEARCH

The Weapons Neutron Research (WNR) facility at Los Alamos is available for neutron scattering experiments utilizing pulsed neutrons. As the Panel points out, because of the restrictions of the source (long pulses , high repetition rate, difficulty in synchonizing choppers, small experimental area) only limited neutron scattering research can be accomplished at the present time. Also, there are no provisions for radiation effects research. For these reasons, the development of the science and technology of spallation sources should be based on IPNS-I at least until the WNR facility becomes attractive with the advent of the Proton Storage Ring (PSR). Until this time DOE should not, in a constrained budget situation, try to duplicate the IPNS-I research and instrumentation effort at Los Alamos.

In 1986, LASL plans to have the Proton Storage Ring in operation at WNR, which will then be a competitive facility for condensed matter research, overcoming most of the current limitations of the WNR facility. The neutron pulses can be shortened, allowing epithermal neutron measurements, while the repetition rate will be reduced, allowing high-resolution time-of-flight diffraction without frame overlap, and the chopper synchronization problem is simplified. The intensity goal of 10^{16} at 12 Hz is overall four times and availability about half that of IPNS-I (see Table 1 of the Panel report). The experimental area is still limited but the inadequacies will be partially alleviated by a new laboratory building being built adjacent to the WNR site. A radiation effects facility would have to be installed if this field is to be continued. Los Alamos management has made a commitment to make the WNR-PSR facility available 80% of the time for condensed matter research, providing about 110 days per year at a cost of $2M, assuming the condensed matter community supports 40% of the WNR-PSR costs as suggested in the Neal report. Provided the performance goal is met and funding is provided by DMA at the proposed levels, this could be cost-effective compared with IPNS-I, thereby freeing up funds to develop and conceptually design the very-high-flux facility. The transfer of the pulsed spallation effort to WNR-PSR during this period could therefore be a possible option. If it were taken, Argonne scientists would participate in the transfer of the IPNS-I instrumentation to WNR-PSR and would continue the collaboration on neutron scattering instrument development which has already been actively pursued in helping to get instruments in operation at WNR, as well as help to set up a radiation effects facility at WNR-PSR.

VI. A VERY-HIGH-FLUX FACILITY FOR THE UNITED STATES

Neutron research in the U.S. will be in great jeopardy in the 1990's unless there is a new, very-high-flux facility which will provide capabilities comparable with the SNS pulsed spallation source (5 x 10^{15} at 50 Hz) in Britain, the heavily re-equipped and re-instrumented reactor at the Institut Laue Langevin, and the high-flux quasi-steady-state spallation source (1-5 x 10^{16} at 100 Hz) likely to be built in Germany. Clearly, the U.S. needs at least one facility which will be competitive at this level, whereas it appears that our high-flux reactors will not, at least without a major reinvestment on both the reactors and the instrumentation, compete with ILL; WNR-PSR will be less than half as intense and much more limited in experimental capability than the high-flux, dedicated British source. The German project, if completed in any of the presently proposed forms, will be superior to all the proposed U.S. facilities.

Argonne strongly endorses the Panel's recommendations to start the planning and designing for a new facility as soon as possible. It will be necessary to consider, at least briefly, the possibility of a very-high flux reactor and the various options for a spallation source which can, in principle, be either a stand-alone facility or one based in part on existing accelerator hardware (ANL, BNL, FNAL or LASL). Argonne should play a lead role in this activity, in view of the Laboratory's expertise in reactor and accelerator technology, spallation neutron targetry, steady-state and time-of-flight neutron scattering instrumentation and neutron radiation effects research. This body of expertise has been built up at Argonne from 1972 onwards to carry out the systematic plan for the development of advanced spallation sources, as discussed in Section III. It would be most cost-effective for the nation to utilize this assembly of competence, ingenuity and dedication for the design of the very-high-flux facility. Further, Argonne is well coupled to the materials research and biology communities and therefore in a good position to react to the desires and needs of these communities for new capabilities in neutron research. We would view the IPNS-II concept developed three years ago as a reference against which to judge the various alternatives.

The size of the effort for designing and planning for this source recommended by the Panel ($1M/year by 1984) is adequate up to that point but will need expansion as the concept becomes more firm and conceptual design studies leading up to a funding appropriation are required. Economies can clearly be effected by the joint use of expertise funded under IPNS-I operations.

VII. THE PROPOSED PLAN

We have discussed in the previous sections our belief in the essential role of neutrons in condensed matter science, the importance of pulsed spallation sources in the drive for higher neutron intensities, and the need to plan now for a very-high-flux facility for the United States. We now present a plan which will allow the DOE neutron program to proceed on a reponsible and rational course towards the very-high-flux source while nurturing the scientific capability which will exploit the new facility and the existing high-flux reactors. This plan has four principal components:

1. Continued support of the mainstay of the present research programs at the high-flux reactors with additional funding to enable the user community to carry out research at these facilities.
2. The timely scientific demonstration and technical development of pulsed spallation sources at IPNS-I up to 1986 (Section IV).
3. Continued development of the Proton Storage Ring and preservation of a future option to transfer the pulsed spallation program to WNR-PSR in 1987 (Section V).
4. Design and planning leading to a new very-high-flux facility, aiming for a 1986 decision and availability in the early 1990's (Section VI).

Tables 1 and 2 present the estimated costs of this plan based on the input from the Laboratories presented to the Neutron Scattering Review Panel. For simplicity, we follow the Panel Report in showing only costs for Fiscal Year 1984, expressed in FY81 dollars. Table 1 shows the total operating costs for running the DOE neutron facilities and associated neutron research programs. Table 2 shows the components of the costs expected to accrue to the Division of Materials Sciences (DMS)

The cost figures are derived on the following bases:

1. For the reactor programs at BNL, ORNL and Ames, we use data supplied to the Review Panel on Neutron Scattering (these do not include the costs associated with the new fuel supplier which will likely increase these totals). An additional funding of \$1.5M is provided to expand the outside user program at the two reactors.

2. For IPNS-I, the budget is $1.1M below the lower (B) budget presented to the Review Panel. With this reduced budget it will be necessary to cut back on some of the goals of IPNS-I as presented to the Panel. Nevertheless, we believe that the basic objectives of the program as discussed in Section IV can still be met.
3. For WNR-PSR, we use data given in the Neal Report (these assume that construction of the PSR and the upgrading of WNR target cell and shielding are covered by separate funds). We assume that the Materials Sciences research program is delayed to an FY86 start, for reasons discussed in Section V.
4. The cost-sharing arrangements between DMS and other parts of DOE will continue at the present levels.

Since IPNS-I is a facility dedicated to condensed matter research, the costs to the DMS program are of course higher than for the other facilities. We should point out, however, that the Argonne program is also distinguished from the other four in its support of a neutron radiation effects program, accounting for about one-fourth of the total effort. As discussed in Section IV, about $3.2M of the IPNS-I budget represents funds reprogrammed from other materials research programs.

Based on the FY80 DOE-DMS budget of $12.6M (Table 2 of the Panel report), the budget schedule shows an increase of 22% over the period FY80-84, an average of 5% per year in constant dollars. We feel that these are realistic increases amply justified in view of the importance of neutron research to the nation's scientific effort and the presently eroding position with respect to international competition.

COST OF NEUTRON FACILITY OPERATIONS AND RESEARCH

FY 1984 (in millions of FY 1981 dollars)

Table 1. Total Costs

Facility	Costs
Reactors	$ 22.0
IPNS-I	7.3
WNR-PSR	5.8
New Source	1.0
TOTAL	$ 36.1

Table 2. Costs to DOE Division of Materials Research

Facility	Costs
Reactors	$ 8.4
IPNS-I	7.0
WNR-PSR	0.4
New Source	1.0
TOTAL	$ 16.8

VIII. SUMMARY

We strongly support the Panel's recommendation for an expanded budget which will allow the systematic development of the field. In case it is not possible to provide this budget, however, we have presented an alternative plan for the future of neutron research on condensed matter. This plan leads, in a rational and logical way, to a world-class neutron source which will ensure the vitality of the field and exploit the many benefits which state-of-the-art neutron facilities can bring to the nation's materials and biological sciences programs.

The plan has four essential stages in arriving at the world-class facility:

1. The scientific demonstration and technical development of the pulsed spallation concept at IPNS-I through 1986.
2. Feasibility and design studies leading to a construction decision on a world-class facility in 1986, to be available for research in the early 1990's.
3. Continuation of the DOE neutron research programs at the High-Flux Beam Reactor and the High-Flux Isotope Reactor and preservation of the option to transfer the pulsed spallation program to the Weapons Neutron Research-Proton Storage Ring Facility after 1986.
4. Development of an expanded user community.

We must emphasize that this plan is based on certain assumptions which must be continuously validated as the development and construction of the facilities involved progresses. These include the assumption that the Proton Storage Ring at Los Alamos will be built as planned and available over 100 days per year for condensed matter research from 1987 onwards.

We propose that about two years from now a national committee in the fields related to neutron research be organized to review the development of the science and the facilities and to represent the community in recommendations on priorities to the funding agencies. Such committees have been set up in other fields and appear to have had beneficial effects. Some specific functions we foresee this committee addressing are the following:

1. Validation of assumptions of facility availability, performance anl cost figures used in previous planning.
2. Assessment of costs and benefits of plans for the very-high-flux source as developed by that time.
3. Assessment of costs and benefits of operating existing facilities.
4. Optimization of the involvement of the general scientific community with the neutron facilities.

We believe that the plan we have presented will enable the exploitation of the full potential of neutron techniques to a broad range of scientific arcas.

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